On gauge freedom and subsystems in quantum electrodynamics

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I confirm that the work submitted in this thesis is my own, except where work which has formed part of jointly authored publications has been included. The contribution of myself and the other authors to this work has been explicitly indicated below. I confirm that appropriate credit has been given within the thesis where reference has been made to the work of others.

Publications

1. STOKES, A., KURCZ, A., SPILLER, T.P., BEIGE, A. (2012). Extending the validity range of quantum optical master equations. *Physical Review A*, **85**, 053805. (Stokes *et al.* (2012)).

Chapter 8 is based on results from this paper. The main new result obtained is the general master equation 8.29. The method of derivation of this master equation is also original. This method, which is presented in sections 8.1 and 8.2, was developed in discussions with all of the above authors. All analytic calculations were made by myself. All of the above authors contributed to the physical interpretation of the master equation constants presented in 8.3.

2. STOKES, A. (2012). Noncovariant gauge fixing in the quantum Dirac field theory of atoms and molecules. *Physical Review A*, **86**, 012511. (Stokes (2012)).

Section 3.3 in chapter 3 is based on results from this paper. The main new result presented is the arbitrary noncovariant gauge Hamiltonian 3.96. Section 9.3 in chapter 9 also contains results from this paper. Specifically the material from page 189 onwards. All work presented in section 3.3 is directly attributable to myself.

3. STOKES, A. (2013). On the gauge of the natural lineshape. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **46**, 145505. (Stokes (2013)).

Sections 7.2-7.4 in chapter 7 are based on results from this paper. This includes the entire analysis of the spectral lineshape of light emitted by an excited bare atom undertaken in these sections. All work presented in sections 7.2-7.4 is directly attributable to myself.

For Helen.

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Abstract

I analyse different decompositions of composite light-matter systems into constituent subsystems. I show that given a single description of a composite atom-field system, many different decompositions into "atom" and "field" subsystems can be made. I show that these decompositions are generally physically inequivalent, and that they can be understood as corresponding to different choices of gauge. I discuss some of the implications this has for the ontology of QED, and find experimental signatures that could be used to distinguish between different theoretical subsystem decompositions.

Abbreviations

QSR	Quantum subsystem relativity
QED	Quantum electrodynamics
EDA	Electric dipole approximation
PZW	Power-Zienau-Woolley
WW	Weisskopf-Wigner
2LA	Two-level approximation
RWA	Rotating wave approximation
MA	Markovian approximation
EMED	Electromagnetic energy density
AQFT	Axiomatic/algebraic quantum field theory

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Introduction

Altogether this thesis is unusually long, which is the result of my desire to produce an essentially self-contained work. I begin by identifying a problem regarding the notion of subsystem in quantum theory. Subsystems of a composite quantum system can only be uniquely defined *relative* to a particular choice of basis for the composite system's Hilbert space $\mathcal{H}$. Different representations of $\mathcal{H}$ incur different tensor product decompositions of $\mathcal{H}$, and these decompositions generally constitute physically *inequivalent* means by which to identify physical subsystems. I call this phenomenon *quantum subsystem relativity* (QSR). My aim in the remainder of the thesis is to present a clear view of the implications of QSR in quantum optics and quantum electrodynamics (QED). The thesis is divided into three parts with three chapters in each part. Below I summarise the structure and main objectives of each part.

PART I

Quantum mechanics and classical mechanics are radically different theories, yet they retain formal similarities. In both theories one specifies physical states and observables. Both theories use a Hamiltonian together with a Lie algebraic bracket structure to generate dynamics, and both theories utilise canonical variables satisfying canonical bracket relations. It is these formal similarities that lead to the idea of canonical quantisation.

The decomposition of a classical mechanical system into component subsystems seems to be relatively uncontentious and natural. It is assumed that a *system* is a collection of particles each objectively possessing a definite position and velocity at each moment in time.[1] The physical observables of interest such as energy, momentum, force, work etc., are defined in terms of particle motions. These motions are in turn described by the (empirically verified) *equations of motion*. Viewed as a physical subsystem, an individual particle's state is unambiguously specified through its position and velocity variables. These variables do not generally coincide with any given set of canonical variables.

In contrast to this the underlying mathematical structure of quantum mechanics generally forces one to use the canonical variables to specify physical subsystems. This makes the notion of quantum subsystem fundamentally different to the corresponding classical notion. In particular, the non-uniqueness of canonical variables implies a certain relativity in the

[1] In the relativistic setting these positions, velocities and moments in time are specified with respect to some *inertial frame of reference*. The specification will generally be different in different inertial frames.

decomposition of a composite quantum system. In the case of massive particles interacting with electromagnetic fields this non-uniqueness is directly related to gauge freedom.

Part I of this thesis is entitled "gauge-freedom and physical systems" and consists of three chapters. The material I present in chapter 1 is elementary, and can be found in numerous textbooks. My presentation is specifically aimed at elucidating the assumptions that are conventionally made regarding classical and quantum subsystems. I begin in 1.1 by reviewing the classical notion of physical subsystem. In 1.2 this classical idea is compared and contrasted with the corresponding quantum notion of subsystem. In section 1.3 I illustrate the differences between the classical and quantum viewpoints by using a particularly simple composite system example.

In chapter 2 I look at how QSR manifests itself in the context of nonrelativistic QED. I start off by reviewing free electrodynamics and discussing the gauge freedom present (2.1-2.2). Moving on to the case of electrodynamics with sources, in 2.3 I obtain an arbitrary gauge formulation of interacting nonrelativistic QED by following the approach of Woolley (1999). Again the ideas of this chapter are not new or original, but the presentation is intended to emphasize the interplay between gauge freedom and subsystem relativity. The arbitrary gauge quantum Hamiltonian obtained in 2.3.3 (equation 2.71) shows precisely how the canonically defined material and electromagnetic subsystems depend on the choice of gauge.

In chapter 3 I extend the ideas of chapter 2 to describe relativistic QED in noncovariant gauges. I begin in 3.1 by reviewing the free Dirac field. In 3.2 I review a method of *quantum mechanical gauge fixing* due to Lenz *et al.* (1994) and use this method to extend the results of chapter 2 to the relativistic setting. This section summarises (and in places elaborates upon) the results presented in the paper Stokes (2012). The main new result presented in this section is the arbitrary noncovariant gauge Hamiltonian 3.96. Like the corresponding Hamiltonian 2.71 obtained in chapter 2, this Hamiltonian shows how the canonically defined material and electromagnetic subsystems depend on the choice of gauge.

PART II

Part II is entitled " the classical and quantum theories of radiation". The aim in this part is to consider what physical interpretations of light-matter interactions QSR necessitates. I consider whether or not it's possible to establish a clear ontology within QED? There are no new results presented in this part; the aim is simply to review conventional interpretations of QED, and to compare the theory with the corresponding classical theory. This part can be used as and when it is needed as a reference section that provides the appropriate context for the new material presented in part III.

I begin part II by reviewing the classical theory of electromagnetism (chapter 4). The most severe problems in classical electromagnetism are encountered when one considers the effects of the electromagnetic fields produced by a charge acting back on the charge itself.

My aim in chapter 4 is to summarise these and other aspects of classical electromagnetism in a way that facilitates a clear comparison with the quantum theory in the subsequent chapters.

In chapter 5 I review QED from the quantum field-theoretic perspective, QED being the prototypical quantum field theory. I introduce the terminology *bare* subsystems to refer to canonically defined material and electromagnetic subsystems. I then review the central tool used in quantum field theory—the gauge-invariant S-matrix formalism, which describes interactions between bare subsystems over infinite durations. This ultimately leads to the notion of virtual particles, which *dress* bare particles giving rise to *dressed* particles.

Having introduced the notions of bare and dressed systems in chapter 5, in chapter 6 I begin to address the question as to their respective physical realities. This is carried out within the nonrelativistic arbitrary gauge QED formalism laid out in chapter 2, and I use nothing but conventional quantum optical techniques and approximations. My analysis concentrates on two well-known quantum-optical effects; atomic level shifts and spontaneous emission. I also review an analysis of the virtual cloud of photons that is hypothesised to surround a bare atom.

PART III

In part III I look at specific signatures associated with different decompositions of light-matter systems into subsystems. These signatures come in the form of concrete physical predictions.

In chapter 7 I consider the spectral lineshape of spontaneous emission of photons by an excited atomic source using the formal theory of radiation damping. I begin in 7.1 by obtaining some standard results concerning bare atomic states (including their decay) and how they relate to excited dressed states of the total atom-field Hamiltonian. In sections 7.2-7.4 I move on to tackle the problem of the spectral lineshape of light emitted by an excited bare atom. This analysis constitutes all of the new work presented in this chapter. The procedure by which the atom is initially excited is described in two ways; through the absorption of incident radiation with a sharp line, and through irradiation with laser light treated semi-classically. The results of sections 7.2-7.4 are presented in the paper Stokes (2013).

In chapter 8 I adopt an open quantum systems approach to study the dynamics of a single bare atom in an electromagnetic reservoir. This involves deriving a master equation that describes the dynamics of the reduced density matrix associated with the bare atomic source. The aim in this section is to discern the dependence of the (Markovian) quantum optical master equation and its associated photon emission rates on the decomposition of the atom-field system into subsystems. In order to do this various standard approximations must be avoided. The results of this chapter are summarised in the paper Stokes *et al.* (2012). The main new result obtained is the general master equation 8.29. The method of derivation

of this master equation is also original. It works by combining the quantum jump approach (cf. Hegerfeldt & Wilser (1992), Gardiner *et al.* (1992), Mølmer *et al.* (1993), Carmichael (1993)) with the ideas of Zurek (2003) on einselection. This method which is presented in sections 8.1 and 8.2, was developed by myself along with the coauthors A. Kurcz, A. Beige and T. P. Spiller of the paper Stokes *et al.* (2012). A. Kurcz, A. Beige and T. P. Spiller also contributed to the physical interpretation of the master equation constants presented in 8.3.

In the final chapter 9, I discuss the famous *Fermi (1932) two-atom problem*. An apparent violation of Einstein causality within this problem has been the subject of intense debate in the past. I point out that this issue is intimately related to questions regarding the precise nature of bare and dressed subsystems, and to their localisation properties. I begin in 9.1 and 9.2 by briefly discussing Einstein causality in the contexts of quantum mechanics and (algebraic) quantum field theory. Section 9.3 on the Fermi problem includes some material from the paper Stokes (2012).

Summary of the thesis' structure

In part I I review what I have called *the problem of quantum subsystem relativity*, and relate this to gauge freedom in quantum electrodynamics. The new results in this part are to be found in chapter 3 section 3.2. Part II contains no new results and is simply included to provide a broader context within which any new work can be placed. In it I review the conventional interpretations of the classical and quantum theories of radiation. In part III I look at experimental signatures that could be used to distinguish between different theoretical subsystem decompositions of an atom-field composite system. The new results presented in this part are to be found in chapter 7 sections 7.2-7.4, and in chapter 8.

Appendices

I have provided extensive appendices to be used as a reference for information on the mathematical details of the theories reviewed and developed in part I.

Units

Throughout the thesis I use natural Lorentz-Heaviside units $\hbar = c = \varepsilon_0 = 1$, $e = \sqrt{4\pi\alpha}$.

PART I

Gauge-freedom and physical subsystems

CHAPTER 1

Physical systems

In this opening chapter my aim is to review the conventional definition of a subsystem in quantum mechanics, and to compare this with the definition of a subsystem as it most naturally occurs in classical mechanics. To this end I review both theories and attempt to determine precisely what physical assumptions are encoded into their mathematical structures. The first section is dedicated to classical mechanics; its basic postulates and mathematical setting.

In the second section I carry out a parallel analysis of quantum mechanics, again starting with the basic postulates. Then I review the conventional approach to defining subsystems of a composite quantum system. In the final section I compare the way in which subsystems are defined in the classical and quantum settings by using the simple example of two interacting oscillators. My conclusion is that there are some very important differences, which could present a formidable problem of subsystem ambiguity within interacting quantum theories. This is what I have called the phenomenon of QSR.

1.1 Classical mechanics

In 1687 Newton published his *laws of motion*. What Newton noticed was that the motion of an object doesn't change unless something changes it. This was his first law. His second law $F = ma$ can be viewed as a quantitative version of his first. A *force* is defined as that which gives rise to changing motion i.e., acceleration. Implicit within Newton's laws is the assumption that what we are physically interested in is *motion*, and how motions change in space and time. In other words we are primarily interested in the quantities position, velocity and acceleration. Force, energy, momentum and other interesting observable quantities, are each defined in terms of these three. Space and time are themselves primitive concepts for which it seems that any attempt at a definition would end up being circular.

We now know that Newtonian mechanics is incapable of explaining a number of phys-

ical phenomena, and we have upgraded the theory accordingly. For example, in special relativity we realise that time is not absolute, but rather an observer dependent coordinate, that changes between different *frames of reference*. Nevertheless, it seems that we are still interested in *motion* of objects with respect to some frame of reference, so motion still plays a key role. In quantum mechanics we realise that we cannot prescribe a system with a definite value of a physical observable, unless it is in an eigenstate of the observable when it is measured. Despite this, it remains meaningful to talk about *observables*, and moreover, it appears that the observables in which we are interested are still those like energy and momentum defined in terms of motion.

The canonical (Hamiltonian) formalism was originally developed to describe classical systems. It seems to me that in adapting this formalism so as to describe quantum reality, we may be forced to abandon the idea that it is the motional degrees of freedom that are physically relevant. If this is the case we must decide what the physically relevant degrees of freedom are? To properly understand what I mean by this it is necessary to understand the precise nature of the classical canonical formalism. It's for this reason that I begin with classical mechanics. My treatment closely follows the treatment of Fecko (2011) chapter 18. The definitions and basic results required to make full sense of this section are presented in B.1.

1.1.1 Lagrangian systems

The natural setting for Lagrangian mechanics is the tangent bundle TM of an m-dimensional base manifold M called configuration space. For example, M could be Euclidean space E^3 or Minkowski space-time $E^{1,3}$. A curve $\gamma : \mathbb{R} \to M$ could represent the motion of a particle in configuration space and the tangents v_x to γ at $x \in M$ would then represent possible instantaneous velocities of the particle at x. A point $(x, v_x) \in TM$ would thus constitute a physical state of the particle system. Any tangent $v_x \in T_xM$ can be written $v^i(x)\partial_{i,x}$, $i = 1, ..., m$ in terms of some set of local coordinates $\{x^i\}$ on M (cf. B.1.3). Thus the (x^i, v^i) constitute coordinates on the $2m$-dimensional manifold TM (cf. B.4.1).[2]

In Lagrangian mechanics one starts off with some equations of motion, that the system has been empirically verified to obey. A Lagrangian is a function on the tangent bundle i.e., a map $L : TM \to \mathbb{R}$, which is chosen to yield the equations of motion when it is plugged into the *Euler-Lagrange equations*;

$$\frac{d}{dt}\frac{\partial L}{\partial v^i}\bigg|_{\gamma(t)} = \frac{\partial L}{\partial x^i}\bigg|_{\gamma(t)}. \tag{1.1}$$

Here $\gamma(t)$ is a curve of motion of the system with values in M. A fact that will be important

[2] I am using the same symbol x to denote a point in M and the coordinates $\{x^i\}$ on $U \subset M$. The restriction of quantities to a point $x \in M$ will be denoted with a subscript $_x$, otherwise the coordinate expression of a quantity is valid at any $x \in U \subset M$.

to us is that

> any two Lagrangians L and L' such that
>
> $$L' = L + \left.\frac{df}{dt}\right|_{\gamma(t)} \tag{1.2}$$
>
> for some function $f : TM \to \mathbb{R}$, yield the same equations of motion. One therefore has considerable (*gauge*) freedom in choosing the Lagrangian for a system.

The Euler-Lagrange equations can be derived from a *least action principle*, in which the *action* is obtained by integrating L over a temporal interval with fixed endpoints. The freedom 1.2 arises because the action will not be changed by the presence of f whenever f vanishes at the endpoints. The determination of the physical significance of the principle of least action seems to constitute a rich branch of philosophy, but one that I would rather not get into. Regardless of any such considerations what is known is that most all of the fundamental equations of physics take the form of Euler-Lagrange equations for some Lagrangian.[3] This means a Lagrangian often constitutes the starting point for a fundamental theory like QED.

A complimentary approach to mechanics is the Hamiltonian approach, which is the one most commonly adapted to describe the quantum universe. In order to investigate the link between the Lagrangian and Hamiltonian formulations I will develop some technical ideas. Namely, these are the *vertical endomorphism* and the *Liouville field*.

The vertical endomorphism is defined using the vertical lift operation. In B.4.1 I define vertical tangent vectors over a point in a base manifold M. The vertical lift of a vector $u_x \in T_xM$ to $v_x \in T_xM$ is a vector $u_{(x,v_x)} \in T_(x,v_x)TM$;

$$u^{\uparrow}_{(x,v_x)}(f) := \left.\frac{d}{dt} f(x, v_x + t u_x)\right|_{t=0} = u^i(x)\frac{\partial f}{\partial v^i_x} \tag{1.3}$$

where the last equality gives the coordinate expression. The lifted vector field is given by the "de-restriction" of this expression to all of some neighborhood $U \subset TM$, on which the coordinates (x^i, v^i) are defined, explicitly $u^{\uparrow} = u^i \partial/\partial v^i$. Similarly one can define the vertical lift of a type $\binom{1}{1}$-tensor field A on M, which in coordinates reads $A^{\uparrow} = A^i_j dx^j \otimes \partial/\partial v^i$. In particular the *vertical endomorphism* is defined by

$$S := I^{\uparrow} = dx^i \otimes \frac{\partial}{\partial v^i}, \tag{1.4}$$

where I denotes the identity.

[3] Newton's laws, Maxwell's equations, Einstein's field equations, the Dirac equation and the Schrödinger equation in wave mechanics are a few examples of Euler-Lagrange equations.

Now for the Liouville field. Consider a curve $\phi : \mathbb{R} \to TM$ such that $(x(\phi(t)), v_x(\phi(t))) = (x^i, e^t v_x^i)$. This can be viewed as a right action R on TM defined by $R((x, v_x), e^t) := (x, e^t v_x)$ (cf. A.3.5). The corresponding infinitesimal generator is a vertical vector field denoted $\Delta \in \chi TM$, called the Liouville field (cf. B.3.6). In coordinates

$$\Delta = v^i \frac{\partial}{\partial v^i}. \tag{1.5}$$

Given a Lagrangian $L : TM \to \mathbb{R}$ one can define the following so-called *Cartan forms*

$$\begin{aligned} \theta_L &:= S(dL) = \frac{\partial L}{\partial v^i} dx^i, \\ \omega_L &:= -d\theta_L = dx^i \wedge d\left(\frac{\partial L}{\partial v^i}\right) = -\frac{\partial^2 L}{\partial x^i \partial v^j} dx^i \wedge dx^j + \frac{\partial^2 L}{\partial v^i \partial v^j} dx^i \wedge dv^j \end{aligned} \tag{1.6}$$

where again the second equalities give the coordinate expressions. The two-form ω_L is symplectic (non-degenerate) in the sense of B.2.1, if and only if

$$\det\left(\frac{\partial^2 L}{\partial v^i \partial v^j}\right) \neq 0 \tag{1.7}$$

in which case the Lagrangian is said to be *non-degenerate* or *non-singular*. The *energy* associated with a Lagrangian L is defined as

$$E_L := \Delta L - L = \frac{\partial L}{\partial v^i} v^i - L(x^j, v^j). \tag{1.8}$$

Thus, one obtains a Hamiltonian system (TM, ω_L, E_L) provided the Lagrangian is non-singular. The dynamics generated by the Hamiltonian E_L are strictly equivalent to the dynamics governed by the Euler-Lagrange equations. Something particularly important to note about the Hamiltonian system obtained is that

> the canonical momentum
>
> $$p_i := \frac{\partial L}{\partial v^i} \tag{1.9}$$
>
> clearly depends on the Lagrangian chosen. Since there is a freedom in the choice of the Lagrangian we should expect that canonical momenta are non-unique. Furthermore, for a point particle of mass m with path $\gamma(t) \in M$, there exists no explicit requirement that the canonical momenta must coincide with the *mechanical momenta* $p^i_{\text{mech}}(t) := m v^i(\gamma(t))$.

1.1.2 The Legendre map

I have described how a Hamiltonian system can be constructed on TM from a non-degenerate Lagrangian. However, the natural setting for Hamiltonian mechanics is not TM, but rather the cotangent bundle T^*M dual to TM. The map associating a Hamiltonian system on TM with one on T^*M is called the *Legendre map*. The Legendre map $\mathbb{L}_x : T_xM \to T_x^*M$ is defined by

$$(\mathbb{L}_x v_x)(u_x) := u^{\uparrow}_{(x,v_x)}(L|_{(x,v_x)}) \tag{1.10}$$

where $u_x, v_x \in T_xM$ and $L : TM \to \mathbb{R}$ is a Lagrangian. In coordinates this definition yields

$$[\mathbb{L}_x(v_x)]_i(x)\, dx^i_x = \frac{\partial L}{\partial v^i}(x)\, dx^i_x, \tag{1.11}$$

which without the restriction to the point $x \in M$, can be written

$$[\mathbb{L}(v)]_i = \frac{\partial L}{\partial v^i} =: p_i. \tag{1.12}$$

I give the definition of the pullback map in B.1.9. Assuming the Lagrangian L is non-singular, the pullback of the Legendre map $\mathbb{L}^*$ is used to obtain the Hamiltonian H, canonical form θ and symplectic form ω on T^*M, from the energy E_L, and Cartan forms θ_L and ω_L respectively. More precisely

$$E_L = \mathbb{L}^*H, \qquad \theta_L = \mathbb{L}^*\theta, \qquad \omega_L = \mathbb{L}^*\omega. \tag{1.13}$$

In coordinates this yields

$$H = p_i v^i(\{x^j\},\{p_j\}) - L(x^i, v^i(\{x^j\},\{p_j\})), \quad \theta = p_i dx^i, \quad \omega = -d\theta = dx^i \wedge dp_i \tag{1.14}$$

where the components of velocity v^i are expressed in terms of the coordinates (x^i, p_i) on T^*M.

It is worth noting that in either formulation it is easy to identify symmetries of the system. If x^i is a cyclic coordinate i.e. the Lagrangian does not explicitly depend on x^i, then

$$\begin{aligned} p_i = \frac{\partial L}{\partial v^i} &\text{ is conserved in Lagrangian mechanics, and...} \\ p_i &\text{ is conserved in Hamiltonian mechanics.} \end{aligned}$$

This is the most basic form of *Noether's theorem* as applied to classical mechanics (Butterfield (2005)). It is not too difficult to formulate classical mechanics in such a way that time t is a coordinate (Howland (2005), Fecko (2011)). One then sees that for an explicitly time-independent Hamiltonian, energy i.e. the Hamiltonian itself, is the conserved quantity.

In summary, given some equations of motion and a non-singular Lagrangian, we can construct two Hamiltonian systems, one on TM and one on T^*M. M is often some real m-dimensional vector space, which supports global coordinates. The tangent and cotangent bundles are then both isomorphic to $\mathbb{R}^{2m}$. For example $M = E^3$ for a single Euclidean point particle, so $TM \cong T^*M \cong \mathbb{R}^6$. The dynamics are generated by the Hamiltonian H, which can be written in terms of the $p_i = \partial L/\partial v^i$, or the v^i. In the latter case the Hamiltonian is referred to as the energy and is denoted E_L instead. The component functions v^i of tangents in $TM \cong \mathbb{R}^{2m}$ have the unambiguous interpretation *as velocity components*, whereas the canonical momenta are coordinates on $T^*M \cong \mathbb{R}^{2m}$, that depend on the choice of Lagrangian. They have the advantage of enabling one to find the dynamics $\gamma(t) \in M$ by solving Hamilton's first order dynamical equations without having to solve the second order Euler-Lagrange equations.

1.1.3 Observables, states and dynamics in classical mechanics

I'm now set up nicely to expound the physical assumptions underpinning classical mechanics, so I will jump straight in. The definition of a Hamiltonian system (M, ω, H) is given in B.2.2. Given such a system, states of the physical system it describes are points in M. The manifold M is usually a tangent or cotangent bundle of some underlying base manifold representing space or space-time. The images of the integral curves $\gamma : \mathbb{R} \to M$ of the Hamiltonian vector field X_H are the paths of evolution of states in M;

$$(\dot{x}^i(t), \dot{p}_i(t)) = X_H(\gamma(t)) = \left(\frac{\partial H}{\partial p_i(t)}, -\frac{\partial H}{\partial x^i(t)} \right). \tag{1.15}$$

Curves with different starting points correspond to different initial states. The associated flow $\{F_t : M \to M\}$ where $F_t(\gamma(0)) = \gamma(t)$, is the set of dynamical maps that govern the evolution of the system by deterministically mapping a state at some initial time to state at a later time. This perspective on dynamics constitutes the *Schrödinger picture* of classical mechanics whereby states evolve and observables stay fixed.

Observables are represented by functions on M i.e., smooth maps $f : M \to \mathbb{R}$. The value the physical system in state $P \in M$ possesses for an observable $f \in F^\infty M$ is $f(P) \in \mathbb{R}$. This idea clearly reflects the classical intuition that a system possesses a definite value for f irrespective of whether or not it has been measured. In the *Heisenberg picture* the observables evolve while the states remain fixed. If states in the Schrödinger picture evolve according to a map $F_t : M \to M$, then the evolution of observables in the Heisenberg picture is governed by the pull-back $F_t^* : F^\infty M \to F^\infty M$, which is defined by $F_t^* f := f \circ F_t$. Clearly both pictures yield the same results as far as physical predictions are concerned;

$$f(F_t(P)) =: (f \circ F_t)(P) =: (F_t^* f)(P) \tag{1.16}$$

$\forall P \in M$. It is easy to determine a differential equation for the evolution of an observable f;

$$\dot{f}(0) := -\frac{d}{dt} F_t^* f \Big|_{t=0} =: -L_{X_H} f = -X_H(f) = \{f(0), H\}, \tag{1.17}$$

which for arbitrary t generalises to

$$\dot{f}(t) = \{f(t), H\}. \tag{1.18}$$

Thus, one defines the classical *algebra of observables* $\mathcal{A}(M) := (F^\infty M, \{\cdot,\cdot\}, \cdot)$, which is a Lie algebra with respect to the Poisson bracket $\{\cdot,\cdot\}$, and an associative commutative (Abelian) algebra with respect to the pointwise product $\cdot$ defined by $(f \cdot g)(P) := f(P)g(P)$.

I'll now briefly go over the example of a single particle with mass m, in Euclidean space to demonstrate the above formalism in action. For this simple system the base manifold M is E^3, so the tangent and cotangent bundles are isomorphic to $\mathbb{R}^6$. If the particle moves in a potential V then

$$\begin{gathered} L = \frac{1}{2} m \sum_i v^{i2} - V\{x^j\}, \quad E_L = \frac{1}{2} m \sum_i v^{i2} + V\{x^j\}, \\ \theta_L = \sum_i m v^i dx^i, \qquad \omega_L = \sum_i dx^i \wedge dm v^i. \end{gathered} \tag{1.19}$$

As is common the Lagrangian is the difference in kinetic and potential energies, while the total energy E_L is their sum. The equations of motion read

$$(\dot{x}^i(t), \dot{v}^i(t)) = \left(v^i(t), -\frac{1}{m} \frac{\partial V}{\partial x^i} \right) \tag{1.20}$$

which expresses the fact that the $v^i(t)$ are components of the particle's velocity, and that the force exerted on the particle is the negative of the gradient of the potential; $\mathbf{F} = m\mathbf{a} = -\nabla V$. In the Hamiltonian formalism one has

$$p_i = \frac{\partial L}{\partial v^i} = m v^i, \quad H = \frac{1}{2m} \sum_i {p_i}^2 + V\{x^j\}, \quad \theta = p_i dx^i, \quad \omega = dx^i \wedge dp_i, \tag{1.21}$$

which shows that in this example the canonical momentum $\mathbf{p}$ coincides with the mechanical momentum $m\mathbf{v}$. This is predominantly the case when dealing with non-interacting systems.

As a technical extension to conclude this section I remark that the points in the state space M actually correspond to the so-called *pure states* of the system. More generally one can define a *mixed state* as a probability measure ρ over M. The integral of a function f with respect to ρ yields the average result of a measurement of the associated observable in the state ρ. The probabilistic nature of classical mechanics is purely epistemic meaning that the measure ρ merely represents the observer's ignorance of the state of the system,

which objectively possesses a definite value for every observable. The pure states are just those mixed states for which ρ is concentrated at a single point in M. For example if $M = \mathbb{R}^6$ for a Euclidean point particle, a pure state $(\mathbf{x}, \mathbf{p})$ would be associated with a measure $\delta(\mathbf{x} - \mathbf{x}')\delta(\mathbf{p} - \mathbf{p}')$. The average result of measuring an observable f in this state, would be

$$\int d^3x' \int d^3p' \, f(\mathbf{x}', \mathbf{p}')\delta(\mathbf{x} - \mathbf{x}')\delta(\mathbf{p} - \mathbf{p}') = f(\mathbf{x}, \mathbf{p}). \tag{1.22}$$

1.2 Quantum mechanics

Having done classical mechanics it's now time to move on to quantum mechanics. The ultimate goal of this chapter is to compare how the two theories differ with regards to how subsystems are defined. The definitions and basic results required to make full sense of this section are presented in A.3.

1.2.1 Postulates

I start by presenting the rules of quantum mechanics:

1. States of a physical system are represented by normalised vectors in a complex Hilbert space $\mathcal{H}$.[4]

2. Observables associated with a physical system are represented by self-adjoint operators in $\mathcal{L}(\mathcal{H})$.

3. The average result of repeated measurements of an observable A with non-degenerate eigenvalues, associated with a system in state $|\psi\rangle$, is

$$\langle\psi|A|\psi\rangle. \tag{1.23}$$

   This is equivalent to the requirement that the individual measurement outcomes are eigenvalues a_m of A, and that the probability of a measurement yielding the value a_m is given by

$$\langle\psi|(|a_m\rangle\langle a_m|)|\psi\rangle \equiv |\langle\psi|a_m\rangle|^2 \tag{1.24}$$

   where $|a_m\rangle$ denotes the eigenvector corresponding to a_m. This rule is easily extended to the case of operators with degenerate eigenvectors.

4. The state $|\psi\rangle$ of a closed system evolves in time according to the *Schrödinger equa-*

[4] States are actually subspaces called *rays* in the Hilbert space. The elements in a ray are allowed to differ by a complex phase with magnitude 1. I'm going to ignore this point for now, but will revisit it at the end of section 1.2.2

tion

$$i\frac{d}{dt}|\psi\rangle = H|\psi\rangle \quad \Rightarrow \quad |\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle \tag{1.25}$$

where H is a distinguished observable called the *Hamiltonian*. This perspective on dynamics constitutes the *Schrödinger picture* of quantum mechanics in which states evolve and observables are held fixed. In the *Heisenberg picture* observables evolve and states are held fixed. If at time $t = 0$, A denotes an observable in the Schrödinger picture, then in the Heisenberg picture at time $t > 0$ this observable is represented by $A(t) := e^{-iHt}Ae^{iHt}$. Differentiating this expression with respect to t yields the *Heisenberg equation*

$$i\dot{A}(t) := i\frac{d}{dt}A(t) = [A(t), H] \tag{1.26}$$

where $H(t) \equiv H(0) =: H$. Clearly both pictures yield the same results as far as physical predictions are concerned;

$$\langle\psi(t)|A|\psi(t)\rangle = \langle\psi|e^{iHt}Ae^{-iHt}|\psi\rangle = \langle\psi|A(t)|\psi\rangle \tag{1.27}$$

where $|\psi\rangle := |\psi(0)\rangle$.

The vectors $|\psi\rangle \in \mathcal{H}$ actually represent the so-called *pure states* of the system. As in the classical case one can generalise the rules, so as to be able to describe *mixed states*. A mixed state is represented by a *density operator*, which is a Hermitian operator ρ such that

$$\mathrm{tr}\rho := \sum_i \langle i|\rho|i\rangle = 1, \qquad \langle\psi|\rho|\psi\rangle \geq 0 \ \ \forall|\psi\rangle \in \mathcal{H}. \tag{1.28}$$

Any density operator can be written as a sum of projection operators onto pure basis states;

$$\rho := \sum_i p_i|i\rangle\langle i| \tag{1.29}$$

where p_i represents the "classical" probability that the system is in state $|i\rangle$. The probability that the eigenvalue a_m is found when a measurement of the observable A is carried out on a system with state ρ, is $\mathrm{tr}(|a_m\rangle\langle a_m|\rho)$ where as usual $|a_m\rangle$ denotes the eigenstate corresponding to a_m. The expectation value of A in the state ρ is simply $\mathrm{tr}(A\rho)$. This reduces to the usual probabilistic rule 3 above, whenever $\rho = |\psi\rangle\langle\psi|$ for some pure state $|\psi\rangle \in \mathcal{H}$. In the Schrödinger picture the density operator evolves according to the equation

$$i\dot{\rho}(t) = [H, \rho(t)]. \tag{1.30}$$

In the last section I used the Euclidean point particle as a simple example of a classical mechanical system. The quantum analog of this system is the wave-mechanical particle in

Euclidean space. An appropriate state space for this system is the Hilbert space $L^2(\mathbb{R}^3)$ of square integrable functions. Components of position $\hat{x}^i$ and canonical momentum $\hat{p}_i$ are observables in $\mathcal{L}(L^2(\mathbb{R}^3))$ satisfying the canonical commutation relation $[x^i, p_j] = i\delta_{ij}$. These operators are said to be canonically conjugate, which means they are related by Fourier transformation. With respect to the position representation of states they have the following Schrödinger picture representations

$$\hat{x}^i\psi(x) = x^i\psi(x), \qquad \hat{p}_i\psi(x) = -i\frac{\partial}{\partial x^i}\psi(x). \tag{1.31}$$

Thus, the canonical momentum generates spatial translations. The position operator likewise generates momentum translations, which can be seen by representing the operators with respect to the momentum representation of states. If the particle moves in a potential V, the Hamiltonian of the system is

$$H = \frac{1}{2m}\sum_i \hat{p}_i^2 + V\{x^j\} \tag{1.32}$$

and the equations of motion read

$$(\dot{\hat{x}}^i(t), \dot{\hat{p}}_i(t)) = \left(\frac{1}{m}\hat{p}_i(t), -\frac{\partial V}{\partial x^i}\right), \tag{1.33}$$

closely mirroring the classical case. We can write states of the system using other representations besides position. For example canonical momentum states $\psi(p)$, and energy states $\varphi_n(x)$ (or equivalently $\varphi_n(p)$) are defined by

$$H\varphi_n(x) = \omega_n\varphi_n(x), \qquad \hat{p}_i\psi(p) = p_i\psi(p) \tag{1.34}$$

where I have assumed V is such that H has a discrete spectrum labelled by n, with $c_n \in \mathbb{C}$. These representations have the following relationships

$$\psi(x) = \sum_n c_n\varphi_n^*(x), \quad c_n = \int d^3x\,\varphi_n(x)\psi(x), \quad \psi(p) = \frac{1}{\sqrt{2\pi^3}}\int d^3x\, e^{ix^ip_i}\psi(x). \tag{1.35}$$

If we define $\hat{\mathbf{x}} = (\hat{x}^1, \hat{x}^2, \hat{x}^3)$ and $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$, then in the heuristic formalism of Dirac (cf. A.3.4) the above are written

$$\begin{gathered}\hat{\mathbf{x}}|\mathbf{x}\rangle = \mathbf{x}|\mathbf{x}\rangle, \qquad H|n\rangle = \omega_n|n\rangle, \qquad \hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle, \\ |\mathbf{x}\rangle = \sum_n \varphi_n^*(\mathbf{x})|n\rangle, \qquad |n\rangle = \int d^3x\,\varphi_n(\mathbf{x})|\mathbf{x}\rangle, \qquad |\mathbf{p}\rangle = \frac{1}{\sqrt{2\pi^3}}\int d^3x\, e^{ix^ip_i}|\mathbf{x}\rangle.\end{gathered} \tag{1.36}$$

1.2.2 Unitary operators

The relationships 1.35 can be thought of as expressions of basis states in terms of another basis. Bases are generally related by unitary transformations, which I consider to be important enough to warrant their own subsection. The crucial fact to remember regarding unitary operators is that

> if initially the associations
>
> $$\begin{aligned} \text{operator } A &\leftrightarrow \text{ physical observable } O, \text{ and...} \\ \text{vector } |\psi\rangle &\leftrightarrow \text{ physical state } S \end{aligned}$$
>
> are made, then precisely the same physical predictions will be obtained if the associations
>
> $$\begin{aligned} \text{operator } UAU^{-1} &\leftrightarrow \text{ physical observable } O, \text{ and...} \\ \text{vector } U|\psi\rangle &\leftrightarrow \text{ physical state } S \end{aligned}$$
>
> are made, where U denotes any unitary operator.

In other words, the associations *observable* $\leftrightarrow$ *operator* and *vector* $\leftrightarrow$ *state* are unique only up to unitary transformation. This is so, because in quantum theory all physical predictions come in the form of inner products and unitary operators are the automorphisms in the category of inner product spaces. I call a particular assignment of vectors to physical states a *representation of states*. Given some representation of states one assigns to each observable a unique operator, which represents the observable *with respect to the given representation of states*. According to the box above unitary operators are the objects relating different representations.

It is easy now to understand why states are in fact *rays* in the Hilbert space rather than just vectors. In the case $U \in U(1)$, U commutes with any $A \in \mathcal{L}(\mathcal{H})$, which means transformation of A by U leaves A invariant. Now according to the rule above any two states such that $|\psi_2\rangle = U|\psi_1\rangle$ must yield the same predictions used in conjunction with A. Since A is arbitrary this implies that physical states are only defined up to such $U(1)$-transformations. Thus, states are equivalence classes of vectors called rays, with two vectors belonging to the same ray if they can be related by a $U(1)$-transformation.

1.2.3 Composite quantum systems

I arrive now at what I most want to discuss - composite quantum systems. The formalism for composite quantum systems relies on the tensor product operation. Given two systems 1 and 2 with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively, the Hilbert space of the composite

system consisting of 1 and 2 is $\mathcal{H}_1 \otimes \mathcal{H}_2$. Any state of the composite system can be written

$$|\psi\rangle = \sum_{i}^{n}\sum_{\mu}^{m} \psi_{i\mu}|i\rangle_1 \otimes |\mu\rangle_2 \tag{1.37}$$

where $\{|i\rangle_1\}$ and $\{|\mu\rangle_2\}$ are bases in $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively, with $\dim\mathcal{H}_1 =: n$ and $\dim\mathcal{H}_2 =: m$. As a notational device product states such as $|\psi\rangle \otimes |\phi\rangle$ are usually abbreviated to $|\psi,\phi\rangle$. A general observable $B \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ of the composite system has the form

$$B = \sum_{i}^{n^2}\sum_{\mu}^{m^2} B_{i\mu} A_1^i \otimes A_2^\mu \tag{1.38}$$

where $\{A_1^i\}$ and $\{A_2^\mu\}$ are bases in $\mathcal{L}(\mathcal{H}_1)$ and $\mathcal{L}(\mathcal{H}_2)$ respectively. An observable O_1 of subsystem 1 is represented by $A_1 \otimes I$, with $A_1 \in \mathcal{L}(\mathcal{H}_1)$ and I denoting the identity on $\mathcal{H}_2$. Thus, subsystem 1 is defined by the collection of operators $\{A_1 \otimes I : A_1 \in \mathcal{L}(\mathcal{H}_1)\} \subset \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$. The eigenstates of the self-adjoint operators A_1 provide bases for the Hilbert space $\mathcal{H}_1$. Similarly subsystem 2 is defined by the set of operators $\{I \otimes A_2 : A_2 \in \mathcal{L}(\mathcal{H}_2)\}$.

There are a couple of reasons that I can identify for extending the basic quantum mechanical formalism in this way. First and perhaps most importantly, operators of the form $A_1 \otimes I$ and $I \otimes A_2$ are trivially compatible, that is, they commute for any $A_1 \in \mathcal{L}(\mathcal{H}_1)$ and $A_2 \in \mathcal{L}(\mathcal{H}_2)$ (Sakurai (1993)). Assume to the contrary that two observables O_1 and O_2 were represented by operators A_1 and A_2 such that $[A_1, A_2] \neq 0$. Suppose in the first instance that consecutive measurements of O_1 were to be performed and the outcomes recorded. Now suppose instead that a measurement of O_2 was to be made *in-between* the measurements of O_1. This time the second measurement of O_1 will not, in general, yield the same result as in the first instance, because of the measurement of O_2 made beforehand. If observables associated with separate subsystems were incompatible a measurement of one subsystem could "disturb" the other subsystem in this way. Now, we want the definition of subsystems to be flexible enough to describe a situation in which two subsystems are space-like separated. If observables associated with separate subsystems were incompatible then one could in principle use measurement disturbances for super-luminal communication. One requires then, that observables associated with separate subsystems are compatible. The second reason for the above composite systems description is that the straightforward extension of the inner product A.25 means that for the system in a product state $|\psi_1, \phi_2\rangle$ the probability that O_1 has value a and O_2 has value a' is simply

$$|\langle a_1, a_2'|\psi_1, \phi_2\rangle|^2 = |\langle a|\psi\rangle_1|^2 |\langle a'|\phi\rangle_2|^2, \tag{1.39}$$

which is just the joint probability of finding $O_1 = a$ and $O_2 = a'$, as one might expect.

Given the definition of composite quantum systems all sorts of strange and exciting states of the composite system e.g. *entangled states* can be constructed. To talk about such things a prerequisite would surely be physically unambiguous definitions of quantum

subsystems. Indeed, to study physics means to study physical systems, and the notion of physical system is surely only useful insofar as it is unique. Since the only physical system that is not a subsystem is the biggest system of all, there is no real distinction between defining subsystems and defining systems in general. Quantum subsystems as they are defined above are not unique, because they are defined in terms of the structural forms of *operators*, and the association of operators with physical observables is not one-to-one.

Suppose, for example, we start off with a representation of states with respect to which an observable O_1 associated with subsystem 1 is represented by the operator $A_1 \otimes I$. It is quite possible that a unitary transformation $U \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ exists, such that $U(A_1 \otimes I)U^{-1}$ is not of the form $A_1' \otimes I$. Therefore, with respect to the initial representation of states, the observable represented by the operator $U(A_1 \otimes I)U^{-1}$ is not, according to our definition, an observable associated with subsystem 1. However, we know that with respect to the new representation of states the operator $U(A_1 \otimes I)U^{-1}$ represents the same physical observable O_1, as the operator $A_1 \otimes I$ represents with respect to the initial representation of states. Conversely, the operator $A_1 \otimes I$ itself represents an altogether different observable with respect to the new representation of states. The subsystem 1 is supposed to be *defined* by the collection of *operators* of the form $A_1 \otimes I$, yet these operators represent different physical observables depending on the representation of states chosen for the composite system. Thus, the definition of a quantum subsystem is a physically *relative* one. A transformation of the *global* system to a physically equivalent representation will not, in general, produce physically equivalent subsystems.

This fact by itself does not necessarily present us with a problem. Provided we can identify the physical degrees of freedom by which subsystems should be defined, and then identify some representation of states of the global system with respect to which the identified observables have the required form i.e. $A_1 \otimes I$ for system 1, and $I \otimes A_2$ for system 2, then we should always be able to keep track of which operators represent the subsystem observables, whatever the representation of states chosen for the global system.

The task of defining quantum subsystems unambiguously, seems to be nothing more than that of identifying the *physical observables*, which should be taken as *defining* the subsystems. In classical physics this seems straightforward and even tacit to some extent. I went to great lengths in the previous section to emphasize that in classical physics the observables in which we are interested are those defined in terms of *motion*. For example, in a system of two classical particles, it is the position and velocity observables of each particle, that constitute the means by which they are identified as individual particle subsystems. By way of the example in the following section I aim to show that for certain interacting composite quantum systems *there is no representation of states for the composite system, in which the velocity observables associated with each subsystem are simultaneously represented by operators of the form* $A_1 \otimes I$ *for subsystem* 1*, and* $I \otimes A_2$ *for subsystem* 2.

1.3 Interacting oscillators: the classical and quantum descriptions

In this section I use the simple example of two interacting harmonic oscillators to try and show how the classical and quantum points of view towards subsystems diverge. Although somewhat long-winded, this example clearly and simply highlights the ambiguity inherent in quantum mechanical subsystems defined in terms of canonical variables. The reason for contrasting this viewpoint with the classical viewpoint is to emphasize how radically the notion of physical system changes when we move to the quantum setting, and to pose the question as to whether or not such a radical departure is really warranted. The example is somewhat artificial, which is the price paid for its simplicity. To try and inject a modicum of actual physics into the proceedings one could imagine that one of the oscillators represents a charged particle in a harmonic trapping potential, while the other one represents a single mode of electromagnetic radiation. The equations of motion of the system are then "single mode versions of Maxwell's equations".

1.3.1 The classical description

For über simplicity I will assume that both oscillators are restricted to one dimension in space, and that they each have mass 1 and oscillate with frequency 1 about the coordinate origin.[5] The classical state space for each oscillator is $\mathbb{R}^2$, which makes the total space $\mathbb{R}^4$. Suppose now that the other day I was fortunate enough to obtain two harmonic oscillators with these exact properties. Suppose also, that in anticipation of writing this section, I took them to my lab, "interacted" them, and found that they obeyed the following equations of motion

$$\ddot{x} = -x + \dot{y}, \qquad \ddot{y} = -y - \dot{x} \tag{1.40}$$

where x and y denote the positions of oscillators 1 and 2 respectively, and $\dot{x}$ and $\dot{y}$ denote the corresponding velocities. These equations are sufficiently simple to be solved exactly, and for the initial conditions $x(0) = y(0) = \dot{x}(0) = 0,\ \dot{y}(0) = 1$, one obtains

$$x(t) = \frac{2}{\sqrt{5}} \sin\left(\frac{t}{2}\right) \sin\left(\frac{\sqrt{5}t}{2}\right), \qquad y(t) = -\frac{2}{\sqrt{5}} \cos\left(\frac{t}{2}\right) \sin\left(\frac{\sqrt{5}t}{2}\right). \tag{1.41}$$

We can find velocities and accelerations by differentiating these expressions. From there we can find forces, energies, momenta and whatever else tickles our fancy. Thus we are essentially done with the classical description. However, I am interested in how this description is encoded into the canonical formalism, so I wish to find a Hamiltonian yielding 1.40. It is

[5] If, as I suggested, the reader wishes to think of one of the oscillators as a charged particle, then we are assuming the charge of this particle is 1.

easy to verify that the Hamiltonian

$$H = \frac{1}{2}(p_x + y)^2 + \frac{1}{2}x^2 + \frac{1}{2}\left(p_y^2 + y^2\right) \tag{1.42}$$

does the job. Here p_x and p_y are the canonical momenta satisfying the canonical Poisson bracket relations B.43 with the coordinates x and y.[6] The velocities according to this Hamiltonian, are identified as

$$\dot{x} = p_x + y, \qquad \dot{y} = p_y. \tag{1.43}$$

Thus, we have encountered a situation whereby the canonical momentum p_x does not coincide with the velocity $\dot{x}$, rather it is the velocity $\dot{x}$ minus the position of the second oscillator y. In the classical setting the oscillators as *physical subsystems* are most naturally defined in terms of their position and velocity observables. Each oscillator occupies a certain position at each point in time. The rate of change of this position is the definition of the oscillator's velocity.

From this point of view the canonical momentum p_x conjugate to x is *not* an observable associated solely with oscillator 1. Is this a problem? In the classical setting it isn't, because there is simply no requirement that p_x *should* be an observable associated with oscillator 1. Sometimes the canonical momenta will represent physically relevant degrees of freedom and sometimes they won't. When they do that's good, and when they don't that's fine too. In the latter case one simply identifies what the physically relevant degrees of freedom are in terms of the canonical coordinates. By solving the dynamics using the canonical coordinates, one can determine the value of any given physical observable at any point in time.

So knowing the dynamics in terms of positions and canonical momenta is strictly equivalent to knowing the dynamics in terms of positions and velocities. It is important to recognise however, that this fact does not imply that canonical momenta $p_i(t)$ and mechanical momenta $mv^i(t)$ are the same. One of the primary reasons for using the canonical formalism is that the canonical dynamics are typically much easier to solve than the second order Euler-Lagrange dynamics.

It is instructive to write the Hamiltonian 1.42 in terms of the velocities, in which case one obtains

$$E = \frac{1}{2}\left(\dot{x}^2 + x^2\right) + \frac{1}{2}\left(\dot{y}^2 + y^2\right), \tag{1.44}$$

which clearly represents the total energy of the system as the sum of energies of the indi-

[6] Recall that in the classical setting observables are represented by functions on the state space. In particular the "projection" functions such as $f_x(x, p_x, y, p_y) := x$ for some $(x, p_x, y, p_y) \in \mathbb{R}^4$ will often be denoted by the same symbol as the component of the point itself; $x(x, p_x, y, p_y) := f_x(x, p_x, y, p_y) := x$. The x, y, p_x, p_y appearing in the Hamiltonian 1.42 are *functions* not components of points. In writing an expression such as $x(t)$ what is meant is $x(\gamma(t))$ where x is the *function* not the point, and $\gamma : \mathbb{R} \to \mathbb{R}^4$ is a curve of motion in the state space.

vidual oscillators. Notice there is no semblance of an "interaction component" appearing explicitly in this expression. The interaction of the subsystems is described by the fact that the velocity $\dot{x}$ is not in involution with the velocity $p_y = \dot{y}$. It is also easy to see from 1.44, that the required Hamiltonian 1.42 is obtained by replacing the "free" canonical momentum $p_x \equiv \dot{x}$ with the canonical momentum $p_x = \dot{x} - y$. This is known as the *minimal coupling prescription*, and here it has been applied to oscillator 1.

At the start I noted that the state space for the system is $\mathbb{R}^4$. It is clear that one can "divide up" this state space in a number of ways. If a state is to be specified in terms of the manifestly physically meaningful positions and velocities, then one has a division

$$\mathbb{R}^4 = \mathbb{R}^2[x,\dot{x}] \times \mathbb{R}^2[y,\dot{y}]. \tag{1.45}$$

The physical state space of oscillator 1 is $\mathbb{R}^2[x,\dot{x}]$, and that of oscillator 2 is $\mathbb{R}^2[y,\dot{y}]$. Similarly we could divide the state space up according to canonical degrees of freedom;

$$\mathbb{R}^4 = \mathbb{R}^2[x,p_x] \times \mathbb{R}^2[y,p_y], \tag{1.46}$$

in which case it is often called *phase space*. The individual factors in the cartesian product here are not the *physical* state spaces of the individual subsystems, so the canonical factorisation 1.46 not only offers an alternative *mathematical* decomposition to 1.45, but also one that is *physically* distinct. One might think that these divisions are the only ones possible, but this is not so, because as I eluded to earlier canonical coordinates are not unique.

Suppose I define new canonical momenta by

$$p'_x := p_x - y, \qquad p'_y := p_y - x. \tag{1.47}$$

It is easy to verify that the primed momenta also satisfy the canonical Poisson bracket relations with the coordinates x and y. If p_x and p_y in 1.42 are replaced by p'_x and p'_y respectively, then one obtains a Hamiltonian

$$H' = \frac{1}{2}\left(p'_x + y\right)^2 + \frac{1}{2}x^2 + \frac{1}{2}\left({p'_y}^2 + y^2\right). \tag{1.48}$$

Obviously H' will produce exactly the same equations of motion when it is used in conjunction with p'_x and p'_y as H does when used in conjunction with p_x and p_y. I could express the Hamiltonian H in terms of the primed quantities, but an equivalent way of doing things (which I prefer) is to keep the momenta the same and change the Hamiltonian. So, suppose now that one expresses H' in terms of the unprimed momenta to give

$$H' = \frac{1}{2}\left(p_x^2 + x^2\right) + \frac{1}{2}\left(p_y - x\right)^2 + \frac{1}{2}y^2. \tag{1.49}$$

This is nothing but the Hamiltonian obtained by applying the minimal coupling prescription (with opposite sign) to the second oscillator instead of the first. The equations of motion for

the coordinates x and y now read

$$\dot{x} = p_x, \qquad \dot{y} = p_y - x, \tag{1.50}$$

so it is now the momentum p_y that doesn't coincide with the velocity $\dot{y}$. Despite this apparent change in the equations of motion, they are exactly the same as they were before when written in terms of velocities and accelerations. This is easy to understand when one expresses H' in terms of the velocities given in 1.50, which yields

$$E' = \frac{1}{2}\left(\dot{x}^2 + x^2\right) + \frac{1}{2}\left(\dot{y}^2 + y^2\right) \equiv E. \tag{1.51}$$

The positions and velocities are invariant under the canonical transformation, but the sets of canonical momenta $\{p_x, p_y\}$ and $\{p'_x, p'_y\}$ have different physical meanings when used in conjunction with the same Hamiltonian. This fact is shown by 1.47 explicitly. Thus, we see that one could also divide the state space up according to

$$\mathbb{R}^4 = \mathbb{R}^2[x, p'_x] \times \mathbb{R}^2[y, p'_y] \tag{1.52}$$

offering yet another physically different decomposition. In the alternative viewpoint in which the Hamiltonian changes rather than the canonical momenta, one can see that the same canonical momenta p_x and p_y have different physical meanings when they are used in conjunction with the two different Hamiltonians. This is because physical meaning is partly determined through dynamical input and the Hamiltonian generates the dynamics. From this point of view the state space decomposition $\mathbb{R}^4 = \mathbb{R}^2[x, p_x] \times \mathbb{R}^2[y, p_y]$ must be understood as being physically different when it is used in conjunction with each different Hamiltonian.[7] The box below summarises the classical perspective.

> The state space of the oscillators can be divided into factors in a number of ways. The decomposition corresponding to a division of the physical degrees of freedom that specify the individual oscillator subsystems uses positions and *velocities*; $\mathbb{R}^4 = \mathbb{R}^2[x, \dot{x}] \times \mathbb{R}^2[y, \dot{y}]$. The *physical* state space of oscillator 1 is $\mathbb{R}^2[x, \dot{x}]$, and that of oscillator 2 is $\mathbb{R}^2[y, \dot{y}]$. There are also many ways to divide the state space based on canonical variables; $\mathbb{R}^4 = \mathbb{R}^2[x, p_x] \times \mathbb{R}^2[y, p_y]$. In such decompositions the factors $\mathbb{R}^2[x, p_x]$ and $\mathbb{R}^2[y, p_y]$ *do not* represent the *physical* state spaces of the individual oscillators. This point of view is sharply contrasted in quantum mechanics as we will see in 1.3.2.

It is worth noting that I could have started with a Lagrangian L for the system and derived the Hamiltonian H in 1.42 from it. Similarly I could have started with a Lagrangian

[7] Of course every Hamiltonian must yield the correct equations of motion when used in conjunction with p_x and p_y.

L' and derived the Hamiltonian H'. These Lagrangians would have been related by the *gauge transformation*

$$L' = L - \frac{d}{dt}xy. \tag{1.53}$$

Thus the primed and unprimed canonical momenta above can be understood as corresponding to different Lagrangians L' and L. The Lagrangians themselves correspond to different choices of gauge. In this sense canonical momenta are manifestly gauge dependent. One often hears the viewpoint expressed that gauge dependent quantities are physically meaningless. It seems to me that such a vague statement is at best an oversimplification, and at worst simply incorrect. *What is certainly true is that certain mathematical objects may have different physical meaning in different gauges*. This does not imply that in any one gauge such objects will be devoid of any physical meaning whatsoever. In our example, when the Hamiltonian H is used the canonical momentum p_x has the unambiguous interpretation as the velocity of oscillator 1, minus the position of oscillator 2. In the second instance when Hamiltonian H' is used p_x simply coincides with the velocity of oscillator 1. The positions and velocities are manifestly gauge-invariant *observables*, whereas the canonical momentum p_x is a manifestly gauge dependent *coordinate*. Nevertheless, the coordinate p_x will always be related in some way to the gauge-invariant observables. What varies between gauges is this relationship itself. One might naturally wonder whether there exists any representation, i.e, choice of Hamiltonian (or Lagrangian, or gauge) in which both canonical momenta coincide with the velocities i.e, $p_x = \dot{x}$ and $p_y = \dot{y}$. If this were the case the Hamiltonian, which represents the total energy would be

$$H = \frac{1}{2}\left(p_x^2 + x^2\right) + \frac{1}{2}\left(p_y^2 + y^2\right). \tag{1.54}$$

This Hamiltonian doesn't yield the correct equations of motion 1.40. The equations of motion it yields are simply the free equations for non-interacting oscillators

$$\ddot{x} = -x, \qquad \ddot{y} = -y. \tag{1.55}$$

Thus, we see that the canonical momenta only coincide with the velocities in the description of the "free" (non-interacting) composite system.

In summary, we have seen that classical subsystems are most naturally defined in terms of gauge-invariant and physically unambiguous *positions and velocities*. As well as these there exist various sets of *canonical coordinates* each having different physical significance when identified in terms of the positions and velocities, but each equally suitable when it comes to describing the dynamics of the composite system. When the subsystems are defined in terms of positions and velocities, the Hamiltonian of the composite system simply represents the sum of energies of the subsystems. The interaction between these subsystems is described by the fact that the velocity observables do not, in general, commute.

1.3.2 The quantum description

Two points I have made so far are that canonical momenta are non-unique, and that the association of quantum observables with linear operators is also non-unique. At the quantum level canonical transformations are unitary transformations and in practice quantum subsystems are often defined in terms of canonical momentum operators. We can obtain the quantum description of the interacting oscillators of 1.3.1 by canonically quantising the classical description, which first of all involves the replacements[8]

$$\mathbb{R}^2[x,p_x] \to L^2(\mathbb{R}), \quad \mathbb{R}^2[y,p_y] \to L^2(\mathbb{R}), \quad \mathbb{R}^2[x,p_x] \times \mathbb{R}^2[y,p_y] \to L^2(\mathbb{R}) \otimes L^2(\mathbb{R}), \tag{1.56}$$

so the quantum state space for the system is $L^2(\mathbb{R}^2) \cong L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$. The classical algebra of observables is replaced according to

$$\mathcal{A}(\mathbb{R}^4) := (F^\infty \mathbb{R}^4, \{\cdot,\cdot\}, \cdot) \to (\mathcal{L}(L^2(\mathbb{R}) \otimes L^2(\mathbb{R})), -i[\cdot,\cdot]). \tag{1.57}$$

In particular the x, y, p_x, p_y as *functions* are replaced by linear operators according to

$$x, \;\; y, \;\; p_x, \;\; p_y \;\; \longrightarrow \;\; x \otimes I, \;\; I \otimes y, \;\; p_x \otimes I, \;\; I \otimes p_y \;\; \in \;\; \mathcal{L}(L^2(\mathbb{R}) \otimes L^2(\mathbb{R})), \tag{1.58}$$

which in terms of the position representation of states, support the Schrödinger picture representations in 1.31. Since both Poisson brackets and commutators are Lie algebras, all of the classical equations of motion are transposed to the quantum level in agreement with the Heisenberg equation of motion used in conjunction with the Hamiltonian

$$H = \frac{1}{2}(p_x \otimes I + I \otimes y)^2 + \frac{1}{2}(x \otimes I)^2 + \frac{1}{2}\left((I \otimes p_y)^2 + (I \otimes y)^2\right). \tag{1.59}$$

The crucial difference in the classical and quantum descriptions is that

> in the classical case the state space decomposition $\mathbb{R}^2[x,p_x] \times \mathbb{R}^2[y,p_y]$ is *not* such that the individual factors are the *physical* subsystem state spaces, whereas in the quantum theory the individual tensor factors of the Hilbert space $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$ *are* supposed to represent the *physical* subsystem state spaces. In the quantum setting, unlike in the classical setting, it appears that it is the *canonical* momenta $p_x \otimes I$ and $I \otimes p_y$ that are supposed to represent the physical momenta of oscillators 1 and 2 respectively.

[8] I should point out that the canonical quantisation procedure is not really an integral part of the point I'm trying to make about subsystems. Regardless of the existence of any classical description the subsystem problem on the quantum level arises as soon as we have quantum mechanical equations of *motion*, that we require the quantum mechanical Hamiltonian to yield, while at the same time we use the standard definition in 1.2.3 of quantum subsystems. The canonical quantisation procedure I'm using here is merely a convenient tool.

In the quantum setting the velocity of oscillator 1

$$\dot{x} := -i[x,H] = p_x \otimes I + I \otimes y \tag{1.60}$$

is not an observable associated with oscillator 1, which seems to be an immediately pathological statement. The interaction between the oscillators is now described by an explicit interaction component H_I in the Hamiltonian, defined according to

$$\begin{aligned} H &\equiv H_0 + H_I, \\ H_0 &:= H_1 + H_2 = \frac{1}{2}\left(p_x^2 + x^2\right) \otimes I + \frac{1}{2} I \otimes \left(p_y^2 + y^2\right), \\ H_I &:= p_x \otimes y + \frac{1}{2}(I \otimes y)^2. \end{aligned} \tag{1.61}$$

In the typical quantum mechanical problem one introduces the so-called *ladder operators*, which are non-Hermitian operators defined by

$$a := \frac{1}{\sqrt{2}}(x + ip_x), \qquad b := \frac{1}{\sqrt{2}}(y + ip_y) \tag{1.62}$$

satisfying the *bosonic* commutation relations

$$[a, a^\dagger] = [b, b^\dagger] = 1. \tag{1.63}$$

If one denotes eigenstates of H_1 by $|n_1\rangle$ such that

$$|n_1\rangle := \frac{1}{\sqrt{n!}}(a^\dagger)^n |0_1\rangle \tag{1.64}$$

where $|0_1\rangle$ denotes the lowest energy eigenstate, then one can show that

$$a^\dagger |n_1\rangle = \sqrt{n_1 + 1}\,|n_1 + 1\rangle, \quad a|n_1\rangle = \sqrt{n_1}\,|n_1 - 1\rangle, \quad a^\dagger a |n_1\rangle = n_1 |n_1\rangle. \tag{1.65}$$

When the frequency of oscillation is 1, as it is in the present case, H_1 can be written

$$H_1 = a^\dagger a + a a^\dagger = a^\dagger a + \frac{1}{2} \cong a^\dagger a \tag{1.66}$$

where to write the second equality I have used 1.63, and in writing the third equality I have neglected the irrelevant constant $\frac{1}{2}$. Thus, the ladder operators $a^\dagger$ and a respectively create and destroy the free energy quanta associated with oscillator 1. The Hamiltonian H can be written in terms of the ladder operators as

$$\begin{aligned} H = H_0 + H_I, \qquad & H_0 := H_1 + H_2 \equiv a^\dagger a \otimes I + I \otimes b^\dagger b \\ & H_I := i(a^\dagger - a) \otimes (b^\dagger + b) + \frac{1}{2}(I \otimes (b^\dagger + b))^2. \end{aligned} \tag{1.67}$$

A typical problem could be that of energy transfer, in which the quantity of interest is the total excitation in oscillator 2 at a time $t > 0$ after oscillator 1 was known to be in the excited state $|1_1\rangle$, and oscillator 2 was known to be in the ground state $|0_2\rangle$. This probability is given according to the rules of quantum mechanics by

$$\langle 1_1, 0_2 | e^{iHt} (b^\dagger b \otimes I) e^{-iHt} | 1_1, 0_2 \rangle. \tag{1.68}$$

Up until now everything seems to be okay, but let's now consider the other route I could have taken to the quantum description, after all I could also have quantised H' in 1.48. In this case I would have obtained the quantum Hamiltonian

$$H' = \frac{1}{2}\left((p_x \otimes I)^2 + (x \otimes I)^2\right) + \frac{1}{2}(I \otimes p_y - x \otimes I)^2 + \frac{1}{2}(I \otimes y)^2. \tag{1.69}$$

At the quantum level the Hamiltonians H and H' are related by a unitary transformation

$$H' = UHU^{-1} \quad \text{where} \quad U := e^{ix \otimes y} \tag{1.70}$$

in which the generator $x \otimes y$ is clearly the quantum analog of the classical generator of the gauge transformation in 1.53. The canonical momenta do not commute with U; using the Baker-Campbell-Hausdorff formula A.17 one finds

$$U(p_x \otimes I)U^{-1} = p_x \otimes I - I \otimes y, \qquad U(I \otimes p_y)U^{-1} = I \otimes p_y - x \otimes I, \tag{1.71}$$

which explains why the Hamiltonians H and H' have different forms in terms of the same canonical momenta. The non-trivial transformations 1.71 mean that the canonical momenta $p_x \otimes I$ and $I \otimes p_y$ have different physical meanings with respect to the two different representations of states related by U. We should already expect this to be true having been through a similar procedure in the classical setting. What is important to note though, is that now all of the operators defined in terms of the momenta i.e, a, b, H_1, H_2, H_I etc., also have different physical meanings with respect to the new representation of states, or equivalently said, with respect to the new Hamiltonian. Suppose we look again at the energy transfer problem and calculate the excitation in oscillator 2 for the initial state $|1_1, 0_2\rangle$, what we obtain this time round is

$$\langle 1_1, 0_2 | e^{iH't} (b^\dagger b \otimes I) e^{-iH't} | 1_1, 0_2 \rangle, \tag{1.72}$$

which is not the same as what we got in 1.68;

$$\begin{aligned} &\langle 1_1, 0_2 | e^{iH't} (b^\dagger b \otimes I) e^{-iH't} | 1_1, 0_2 \rangle = \langle 1_1, 0_2 | U e^{iHt} U^{-1} (b^\dagger b \otimes I) U e^{-iHt} U^{-1} | 1_1, 0_2 \rangle \\ &\neq \langle 1_1, 0_2 | U^{-1} U e^{iHt} U^{-1} U (b^\dagger b \otimes I) U^{-1} U e^{-iHt} U^{-1} U | 1_1, 0_2 \rangle \\ &\equiv \langle 1_1, 0_2 | e^{iHt} (b^\dagger b \otimes I) e^{-iHt} | 1_1, 0_2 \rangle. \end{aligned} \tag{1.73}$$

The reason for the difference is that the quantum mechanical subsystems defined in terms of the canonical momenta are not left invariant by the transformation U. It is important to recognise that the two quantum mechanical formulations *are strictly equivalent*, in the sense that given *any* prediction calculated within one of the representations, precisely the same result can be obtained in the other representation by using the appropriately transformed operators and states. For example, in the case of the first prediction 1.68 above we have

$$\begin{aligned}
&\langle 1_1, 0_2 | e^{iHt} (b^\dagger b \otimes I) e^{-iHt} | 1_1, 0_2 \rangle \\
\equiv &\langle 1_1, 0_2 | U^{-1} U e^{iHt} U^{-1} U (b^\dagger b \otimes I) U^{-1} U e^{-iHt} U^{-1} U | 1_1, 0_2 \rangle \\
= &\langle 1'_1, 0'_2 | e^{iH't} (b'^\dagger b' \otimes I') e^{-iH't} | 1'_1, 0'_2 \rangle
\end{aligned} \tag{1.74}$$

where I have simply *defined* new operators and states by

$$(b'^\dagger b' \otimes I') := U (b^\dagger b \otimes I) U^{-1}, \qquad |1'_1, 0'_2\rangle := U |1_1, 0_2\rangle. \tag{1.75}$$

What we have in 1.68 and 1.72 is two altogether separate predictions pertaining to two physically distinct definitions of quantum subsystems. So which prediction is the correct one? Is it the case that either of the predictions are correct? For in neither of the equivalent descriptions did the canonical momenta $p_x \otimes I$ and $I \otimes p_y$, simultaneously coincide with the gauge-invariant velocities $\dot{x}$ and $\dot{y}$, which constitute the natural degrees of freedom by which classical mechanical systems are defined. While I have only compared two representations of states for the system, there exists an infinitude of other equivalent descriptions, for which the subsystems defined in terms of canonical degrees of freedom are physically different.

1.4 Summary and discussion

In both classical and quantum theories canonical momenta are generally physically different within any two physically equivalent formulations. In the classical setting this does not present a problem with regard to defining subsystems, which defined in terms of velocities, are physically unique and unambiguous. The canonical coordinates x^i, p_i satisfy the canonical Poisson bracket relation $\{x^i, p_j\} = \delta^i_j$, while the physical subsystems are defined in terms of their velocity and position coordinates $x^i, v^i(\{x^j\}, \{p_j\})$. The Hamiltonian of a closed composite system is the sum of energies of the subsystems, and there appears to be no need to introduce anything like an "interaction component". The interaction is described by the fact that the velocities associated with different subsystems *do not commute* (in the sense of the Poisson bracket) while it is the canonical momenta which *do* commute. In classical physics then, dynamical interactions are described using the Lie algebra of Poisson brackets, *with respect to which observables pertaining to different subsystems do not, in general, commute*.

In stark contrast to this, in quantum mechanics dynamical interactions are described using the Lie algebra of commutators, *with respect to which observables pertaining to different*

subsystem are required to commute. If we require non-trivial equations of motion to hold, then it is immediately evident that using the velocities to define physical subsystems is not an option in any theory based on the use of a Hamiltonian—the total energy—together with a Lie algebraic bracket structure with respect to which observables pertaining to different subsystems have to commute. In short, the interacting equations of motion will only follow if the velocities pertaining to separate subsystems don't commute, but it is precisely this fact which in a quantum theory makes the velocities unsuitable candidates when it comes to defining physical subsystems. As a result, in (canonical) quantum theories the canonical operators are used to define physical subsystems instead. Consequently, the Hamiltonian, rather than simply being the sum of subsystem energies, contains an explicit interaction component. This strategy results in a plethora of non-equivalent quantum subsystem decompositions, each associated with a different representation of states of the composite system. This is what I have called the phenomenon of QSR.

It is far from clear that the canonical formalism was ever intended to describe interactions between canonical degrees of freedom through an explicit interaction component in the Hamiltonian. This is nevertheless its primary method of application in quantum physics. If the motional degrees of freedom are no longer to be taken as physically relevant then there seems little point in requiring a Hamiltonian to yield equations of motion in the first place. In this case we are "back at square one" in that we simply have to guess at a Hamiltonian (or some such object), which given the rules of quantum mechanics produces the correct (empirically verified) predictions.

In any case there is an inherent *relativity* in the definition of quantum subsystems. In fact it has been understood for some time that "quantum tensor product structures are observable induced" Zanardi *et al.* (2004). It is natural to assume that what makes one or another particular tensor decomposition preferred, is linked to what is operationally available in the lab. If, for example, the results 1.68 and 1.72 are supposed to predict the number of photons in a single mode of radiation then a comparison of these predictions with the unique experimental result appearing on a dial connected to a photo-detector should reveal which decomposition is best (this is the underlying assumption that will be made in chapter 8).

But even after having determined a Hamiltonian for which the photon number prediction is correct, we would still be far from done. Supposing that oscillator 1 represents an oscillating electron, we would have to check that the outcomes of measurements of the electron's energy (or some such observable) are also correctly predicted. In this instance one is confronted with the question of how experimentally the energy of the electron is actually measured, whether or not any such measurement involves the electron's velocity, and whether or not the equations of motion for the system correctly describe these observables, for if they do, then we require the formalism to yield them as well. In addition to all of this, we would have to ensure that nothing like violations of causality could occur. All in all, we would be faced with a large number of conditions that the formalism would be required to satisfy, and it is not entirely clear how such a theory could be constructed. As the

example above clearly demonstrates one cannot generally use velocities to define physical quantum subsystems in interacting theories. One can of course use canonical operators, but then the question occurs as to *which* of the infinite number of inequivalent sets of canonical operators should be used?

As I set fourth at the beginning of this chapter, the assumption that the *motion* of physical systems in space and time is *definitive* of such systems, seems to be quite fundamental. Indeed, it could be argued that such an assumption holds for any *dynamical* theory of physics whether it be quantum, classical or otherwise. If quantum mechanics forces us to abandon this assumption then we are left with an enormous void to fill in determining how precisely physical systems should be defined. We might even be tempted to entertain the idea that no meaningful division of the (quantum) universe into distinct physical subsystems can actually be given at all?

The following chapters in this thesis explore how subsystems should be defined in quantum optics and quantum electrodynamics, as well as how quantum electrodynamics should be used and what it tells us as a physical theory. The basic question I consider is *how does one separate out material and radiative degrees of freedom?*

CHAPTER 2

Electrodynamics in an arbitrary gauge

Between 1861 and 1862 James Clerk Maxwell unified the known laws of electromagnetism in a set of four elegant equations. To this day Maxwell's equations provide the fundamental underpinnings of electrodynamics, and constitute one of the cornerstones of modern physics. In quantum electrodynamics and quantum optics one models processes involving electromagnetic radiation through the concept of the photon, meaning that Maxwell's equations themselves have less direct involvement. The quantum theory however, is still based upon a theory of fields in which the Hamiltonian is required to yield Maxwell's equations. The photon is defined in terms of the (operator-valued) fields used in this approach, so to understand quantum electrodynamics, the canonical approach to classical electrodynamics is a good place to start.

It is customary to start with a Lagrangian for which the Euler-Lagrange equations are Maxwell's equations, and then derive a Hamiltonian. However, the gauge freedom inherent in Maxwell's equations means that the Lagrangian will be singular (c.f. 1.7), that is, there will be more canonical position variables than corresponding canonical momenta, because the Lagrangian turns out to be independent of the velocity of the scalar potential. For this reason the passage to the canonical formalism won't be as straightforward as we are used to. Ultimately what we will see is that in a similar way to the example in 1.3, gauge freedom leads to a multitude of different ways to decompose the matter-radiation system into matter and radiation subsystems.

The aim of this chapter is to review a canonical quantum theory of nonrelativistic electromagnetism, in which the gauge freedom is kept at the forefront throughout. Following Woolley (1999) (see also Babiker & Loudon (1983)), the gauge freedom will be contained entirely within a (classical) vector Green's function denoted $\mathbf{g}$. At the end, we will be set up nicely to discuss the physical implications of this gauge freedom for the quantum theory. It will be useful to give a brief summary of special relativity and relativistic kinematics before

discussing any electromagnetism.

2.1 Recap of special relativity

Minkowski space-time consists of $\mathbb{R}^4$ with the symmetric bilinear form $g = \eta_{\mu\nu} dx^\mu dx^\nu$, $\eta := \mathrm{diag}(1,-1,-1,-1)$. The study of particles in Minkowski space-time is called relativistic kinematics. The Lorentz group $O(1,3)$ consists of transformations Λ leaving the form g invariant (cf. A.3.5). Physically, Lorentz transformations relate different *inertial frames of reference* in $E^{1,3}$.[9] A *Lorentz invariant quantity* is one which is the same in all inertial frames of reference.[10] A *covariant* equation or law, is one which takes the same form in every inertial frame. These ideas are all that is needed to formulate special relativity in its entirety:

1. There is a maximum speed of propagation c for all physical phenomena.

2. The laws of physics are covariant.

Each point (or *event*) x in Minkowski space-time can be viewed as the mutual apex of two cones, the *backward light cone* and *the forward light cone*. The forward (resp. backward) lightcone consists of points x' such that $x'^0 - x^0 > 0$ (resp, $x'^0 - x^0 < 0$), and for which the (invariant) interval $g(x'-x, x'-x)$ is greater than zero. The intervals between x and the points inside the light cone of x are said to be *timelike* with respect to x. The points inside the lightcone are the ones which can be connected to x by a signal propagating with speed $v < c$. The "present" of the point x consists of all points which lie outside the light cone. According to rule 1 above, points in the present of x can't effect, or be effected by x, and they are said to be *spacelike* to x.

A convenient notion is that of *proper time* τ, which is the time experienced by a particle (observer) in its own rest frame. If a particle[11] has position $\mathbf{r}(t)$ and velocity $\mathbf{v} := d\mathbf{r}/dt$ at time t measured with respect to some inertial frame $\mathcal{O}$, then in an elapsed time $t_2 - t_1$ measured in $\mathcal{O}$, it experiences a proper time interval τ given by

$$\tau = \int_{t_1}^{t_2} dt \gamma^{-1}, \qquad \gamma := (1 - |\mathbf{v}(t)|^2)^{-1/2}. \tag{2.1}$$

[9] By *inertial* frame I mean a frame in uniform relative motion with respect to all other inertial frames, i.e. a non-accelerating frame.

[10] Note the difference between a conserved quantity and an invariant quantity. The former being any quantity which does not change in time as measured in a specific frame of reference, and the latter being a quantity which may or may not be conserved in a given frame, but which takes the same value in each inertial frame.

[11] The term "particle" is really just a label for another inertial frame $\mathcal{O}'$. It could equally well refer to an "observer" rather than to an actual particle.

Unlike ordinary time, proper time is by definition, an invariant quantity. The *proper velocity* and *proper momentum* of a particle are

$$\mathbf{u} := \frac{d\mathbf{r}}{d\tau} = \frac{dt}{d\tau}\frac{d\mathbf{r}}{dt} = \gamma\mathbf{v}, \qquad \mathbf{p} := m\mathbf{u} = \gamma m\mathbf{v}. \tag{2.2}$$

A *covariant quantity* is one which transforms according to a representation (see B.3.7) of the (proper orthochronous) Lorentz group. These include for example, scalars, four-vectors, spinors and four-tensors. Sometimes vectors with four components, which are not covariant are referred to as four-vectors as well, and a clarifier covariant or non-covariant must therefore be added where necessary. The velocities, momenta and other observables of nonrelativistic Newtonian kinematics are not covariant, but one can often define relativistically covariant analogs and extensions of these quantities. For example, one can define (in units such that $c = 1$) the *four-velocity* and *four-momentum* by

$$u := (\gamma, \mathbf{u}), \qquad p := mu = (p^0, \mathbf{p}), \qquad p^0 := m\gamma. \tag{2.3}$$

the quantity p_0 is the relativistic energy $p_0 \equiv E = m\gamma$, which is nonzero even when the particle is at rest; $E_{\text{rest}} = m$. In relativistic kinematics the quantities $\mathbf{p}$ and E are conserved, and so is p. In fact

$$p^\mu p_\mu = (p^0)^2 - \mathbf{p}^2 = m^2\gamma^2(1 - \mathbf{v}^2) = m^2, \tag{2.4}$$

which establishes the well-known relativistic energy momentum relation

$$E^2 = \mathbf{p}^2 + m^2. \tag{2.5}$$

This relation will be the starting point in my consideration of the Dirac field in chapter 3.

2.2 Free electrodynamics

It will be helpful to review free electrodynamics, see how gauge freedom arises and consider how it might be handled. The interacting case of electrodynamics with sources, while more complicated, can be handled in essentially the same way. First in 2.2.1 I identify an appropriate Lagrangian, then in 2.2.2 I consider how to construct the Hamiltonian and deal with the redundant (gauge) degrees of freedom.

2.2.1 Deriving the source free equations of motion

One can express Maxwell's equations in terms of the electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ defined on Euclidean space E^3. However, Maxwell electrodynamics is most naturally formulated on Minkowski space-time $E^{1,3}$ (cf. A.3.5), which supports global coordinates

$\{x^\mu\}$. Maxwell's equations in the absence of any sources read

$$dF = 0, \qquad d*F = 0 \tag{2.6}$$

where $F = \frac{1}{2}F_{\mu\nu}dx^\mu \wedge dx^\nu$ is a two-form called the electromagnetic field strength tensor and the operation $*$ denotes the Hodge dual. The components of F form a matrix

$$(F_{\mu\nu}) = \begin{pmatrix} 0 & E^1 & E^2 & E^3 \\ -E^1 & 0 & -B^3 & B^2 \\ -E^2 & B^3 & 0 & -B^1 \\ -E^3 & -B^2 & B^1 & 0 \end{pmatrix}, \tag{2.7}$$

and the Hodge dual operation has the effect $(\mathbf{E},\mathbf{B}) \to (-\mathbf{B},\mathbf{E})$ in 2.7. To see how F transforms under Lorentz transformations $\Lambda \in \mathcal{L}_+^\uparrow$ (cf. B.93) I denote an inertial frame with coordinates $\{x^\mu\}$ by $\mathcal{O}$, and another frame with coordinates $\{x'^\mu = \Lambda^\mu_\nu x^\nu\}$ by $\mathcal{O}'$. If $F(x) := F_x$ is the field tensor measured in $\mathcal{O}$ then the field tensor measured in $\mathcal{O}'$ is $F'(x') := F'_{x'}$ such that

$$F'_{\mu\nu}(x') = \tilde{\Lambda}^\alpha_\mu \tilde{\Lambda}^\beta_\nu F_{\alpha\beta}(x), \tag{2.8}$$

where $\tilde{\Lambda} := (\Lambda^T)^{-1}$ is the contragradient matrix of the matrix Λ. With the understanding that F is to be evaluated at x and F' is to be evaluated at x', 2.8 is often written simply $F'_{\mu\nu} = \tilde{\Lambda}^\alpha_\mu \tilde{\Lambda}^\beta_\nu F_{\alpha\beta}$. If $\mathcal{O}'$ is obtained from $\mathcal{O}$ by a boost with velocity $\mathbf{v}$ then 2.8 yields the following transformation rules for the electric and magnetic fields[12] (Jackson (1998))

$$\mathbf{E}' = \gamma(\mathbf{E} + \mathbf{v}\times\mathbf{B}) - \frac{\gamma^2}{\gamma+1}\mathbf{v}(\mathbf{v}\cdot\mathbf{E}), \qquad \mathbf{B}' = \gamma(\mathbf{B} - \mathbf{v}\times\mathbf{E}) - \frac{\gamma^2}{\gamma+1}\mathbf{v}(\mathbf{v}\cdot\mathbf{B}). \tag{2.9}$$

Thus, the electric and magnetic fields in $\mathcal{O}'$ are mixtures of the electric and magnetic fields in $\mathcal{O}$. What is interpreted as an electric phenomenon in one frame will be interpreted as partially magnetic in another frame, and vice versa.

One can write F as the exterior derivative of a one-form i.e. $F = dA$ where $A = A_\mu dx^\mu$. In terms of components one has

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{2.10}$$

The vector potential $\mathbf{A}$ and scalar potential ϕ can be defined simply as

$$\mathbf{A} := (A^1, A^2, A^3), \qquad \phi := A_0, \tag{2.11}$$

[12] The physical significance of these transformations will be discussed in 4.3.

which according to equations 2.7 and 2.10 yields

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi, \qquad \mathbf{B} = \nabla \times \mathbf{A} \tag{2.12}$$

where $t \equiv x^0$ and $\nabla := (\partial_1, \partial_2, \partial_3)$.

To derive Maxwell's equations from a Lagrangian one starts by taking a Banach space $FE^{1,3}$ consisting of certain functions on Minkowski space-time vanishing at spatial infinity. The component functions A^μ and $\partial_\mu A^\nu$ are assumed to belong to $FE^{1,3}$. In total there are four components of A^μ and four components of $\dot{A}^\mu := \partial_0 A^\mu$, which means that to actually specify a state of the electromagnetic system the eighth power $Z := (FE^{1,3})^8$ is required.

One can consider the functions A^μ and $\partial_\mu A^\nu$ on a fixed time slice, which means that one fixes their zeroth argument $x^0 \equiv t$, and expresses everything with respect to the specific inertial frame for which t denotes the coordinate time. The space of such restricted functions is denoted $F(\{t\} \times E^3)$, and $Z_t := F(\{t\} \times E^3)^8$ denotes the restricted state space. Similarly one can restrict Z to a single event $(t, \mathbf{x}) \in E^{1,3}$ to yield a space denoted $Z_{(t,\mathbf{x})}$. Coordinates on Z are given by the evaluation functions $e^\mu_{(t,\mathbf{x})} : Z \to \mathbb{R}$ and $\dot{e}^\mu_{(t,\mathbf{x})} : Z \to \mathbb{R}$, which respectively evaluate functions and their zeroth derivatives at the point $(t, \mathbf{x})$. For example, $e^1_{(t,\mathbf{x})}(\{A^\nu\}, \{\dot{A}^\lambda\}) := A^1(t, \mathbf{x}) \in \mathbb{R}$. One can define similar functions on Z_t and $Z_{(t,\mathbf{x})}$. The Lagrangian for the system is a map $L(t) : Z_t \to \mathbb{R}$ defined by

$$L(t) := \int d^3x \, \mathscr{L}(t, \mathbf{x}) \tag{2.13}$$

where the *Lagrangian density* $\mathscr{L}(t, \mathbf{x}) : Z_{(t,\mathbf{x})} \to \mathbb{R}$ is defined by

$$\mathscr{L} := -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} \equiv \frac{1}{2} \left(\mathbf{E}^2 - \mathbf{B}^2 \right). \tag{2.14}$$

In conjunction with this Lagrangian (density) the Euler-Lagrange equations

$$\frac{\partial}{\partial x^\mu} \frac{\partial \mathscr{L}}{\partial (\partial_\mu A^\nu)} = \frac{\partial \mathscr{L}}{\partial A^\nu} \tag{2.15}$$

yield Maxwell's equations 2.6.

2.2.2 Gauge freedom and gauge fixing

Since $F = dA$ and $d(d\lambda) \equiv 0$ for any $\lambda \in F^\infty E^{1,3}$ it follows that $F = d(A \pm d\lambda)$. Thus, Maxwell's equations are unchanged if one substitutes A with A' such that

$$A' := A \pm d\lambda \quad \Leftrightarrow \quad A'_\mu := A_\mu \pm \partial_\mu \lambda \quad \Leftrightarrow \quad \phi' = \phi \pm \frac{\partial \lambda}{\partial t} \text{ and } \mathbf{A}' = \mathbf{A} \mp \nabla\lambda. \tag{2.16}$$

The transformation $A \to A'$ is what is meant by a gauge transformation of A yielding A', and to fix a gauge means to choose a particular potential A. It is useful to try and determine what "part" of A is the gauge dependent part. To do this the three-vector notation seems

best suited.

Any three-vector field $\mathbf{v} \in \chi E^3$ can be uniquely decomposed into so-called *transverse* and *longitudinal* components $\mathbf{v}_\mathrm{T}$ and $\mathbf{v}_\mathrm{L}$, which satisfy

$$\mathbf{v} = \mathbf{v}_\mathrm{T} + \mathbf{v}_\mathrm{L}, \qquad \nabla \cdot \mathbf{v}_\mathrm{T} = 0, \qquad \nabla \times \mathbf{v}_\mathrm{L} = \mathbf{0}. \tag{2.17}$$

The magnetic field is always purely transverse due to the Maxwell equation $\nabla \cdot \mathbf{B} = 0$. This condition is satisfied identically if $\mathbf{B} = \nabla \times \mathbf{A}$, because the curl of a three-vector field is necessarily transverse; $\nabla \cdot \nabla \times \mathbf{v} \equiv 0 \ \forall \mathbf{v} \in \chi E^3$. Similarly the gradient of a function is necessarily longitudinal; $\nabla \times \nabla \lambda \equiv \mathbf{0} \, \forall \lambda \in F E^3$.

In the absence of any sources the other static Maxwell equation

$$\nabla \cdot \mathbf{E} = 0 \tag{2.18}$$

known as Gauss' law, implies that the electric field is also entirely transverse $\mathbf{E} \equiv \mathbf{E}_\mathrm{T}$. According to 2.12 we therefore have in total

$$\dot{\mathbf{A}}_\mathrm{T} = -\mathbf{E}_\mathrm{T}, \quad \nabla \times \mathbf{A}_\mathrm{T} = \mathbf{B}, \quad -\dot{\mathbf{A}}_\mathrm{L} - \nabla \phi = \mathbf{E}_\mathrm{L} = \mathbf{0}. \tag{2.19}$$

The redundant gauge degrees of freedom are characterised entirely by the longitudinal vector potential and scalar potential, for which the only requirement is that the third equation in 2.19 is satisfied. The gauge-invariant physical degrees of freedom are entirely transverse. Thus, there are in fact only four physical degrees of freedom per space-time point rather than eight.[13] Gauss' law is what in the terminology of Dirac (1964) is called a *constraint*.[14]

Dirac (1964) masterfully crafted a way to construct a Hamiltonian version of a Lagrangian theory with constraints, and then quantise it. This approach constitutes the so-called constrained Hamiltonian formalism. The first thing to do is to naively construct the Hamiltonian on Z_t ignoring the constraints to begin with. We have

$$\Pi_\mu := \frac{\partial \mathscr{L}}{\partial \dot{A}_\mu}, \qquad \mathscr{H} := \frac{\partial \mathscr{L}}{\partial \dot{A}_\mu} \dot{A}_\mu - \mathscr{L} \Big|_{\dot{A}_\mu = \dot{A}_\mu(A_\mu, \Pi_\mu)} \tag{2.20}$$

and the corresponding Hamiltonian

$$H := \int d^3x \, \mathscr{H}(t, \mathbf{x}) = \int d^3x \left[\frac{1}{2} \left(\mathbf{\Pi}^2 + (\nabla \times \mathbf{A})^2 \right) - \nabla A_0 \cdot \mathbf{\Pi} \right]. \tag{2.21}$$

Since $\mathscr{L}$ is independent of $\dot{A}_0$ the conjugate momentum Π_0 is identically zero, which poses a problem for the entire construction. It means that the Lagrangian is singular, so we will

[13] One might at first think that since $\mathbf{A}_\mathrm{T}$ and $\dot{\mathbf{A}}_\mathrm{T}$ are three-vectors there should be six rather than four degrees of freedom per space-time point. However, only two components of $\mathbf{A}_\mathrm{T}$ are independent, because the transversality condition implies that the Fourier transform $\boldsymbol{A}_\mathrm{T}$ must lie in the plain orthogonal to its argument.

[14] See Dirac (2003) for the more recent publication.

be unable to give our state space a symplectic form yielding a Hamiltonian system with dynamics equivalent to the Euler-Lagrange equations.

Dirac's strategy in facing this obstacle is as with Gauss' law, to ignore the fact that $\Pi_0 \equiv 0$ at first, and only later impose it as a constraint. Thus, one first defines a naive symplectic form on Z given in definition B.2.7, and one defines a naive Poisson bracket structure on Z as in definition B.2.8. Then one considers the constraint functions

$$\Pi_0, \qquad \nabla \cdot \mathbf{E} = -\nabla \cdot \mathbf{\Pi}, \tag{2.22}$$

which are required to vanish. The first one Π_0 represents a *primary* constraint resulting immediately from the form of the Lagrangian. The second one, Gauss' law, represents a *secondary* constraint resulting from the equations of motion. The secondary constraint arises if we require the first constraint to hold for all times. This is easily verified using the naive Poisson bracket, which yields $\dot{\Pi}_0 = \{\Pi_0, H\} = \nabla \cdot \mathbf{\Pi}$. A constraint is said to be *first class*, if its Poisson brackets with all other constraints are zero. We have only two constraints and each is first class, because their Poisson bracket is zero. The *constraint surface* is defined as the physical subspace of states for which the primary constraint holds throughout all time i.e., $Z_{\text{CS}} \subset Z$ is such that $\Pi_0|_{Z_{\text{CS}}} = \nabla \cdot \mathbf{\Pi}|_{Z_{\text{CS}}} = 0$.

Next one defines the *total Hamiltonian* H_{tot}, which adds to H the primary constraint function Π_0 multiplied by an arbitrary *Lagrange multiplier* $\lambda \in F(\{t\} \times E^3)$

$$H_{\text{tot}} := \int d^3x \left[\frac{1}{2} \left(\mathbf{\Pi}^2 + (\nabla \times \mathbf{A})^2 \right) - \nabla A_0 \cdot \mathbf{\Pi} + \lambda \Pi_0 \right]. \tag{2.23}$$

The naive Poisson bracket now yields $\dot{A}_0 = \lambda$, so according to H_{tot}, the evolution of A_0 is completely arbitrary. One can therefore write $H_{\text{tot}} = H + G$ where

$$H := \frac{1}{2} \int d^3x \left(\mathbf{\Pi}^2 + (\nabla \times \mathbf{A})^2 \right), \qquad G := \int d^3x \left(\dot{\lambda} \Pi_0 + \lambda \nabla \cdot \mathbf{\Pi} \right). \tag{2.24}$$

To write G in this form an integration by parts has been performed.[15] Thus, we see that G is the sum of the constraints each multiplied by arbitrary functions. In the original form

$$G = \int d^3x \left(\dot{\lambda} \Pi_0 - \nabla \lambda \cdot \mathbf{\Pi} \right), \tag{2.25}$$

G can in fact be identified as the *the generator of gauge transformations*. To see this let $\lambda \in F(\{t\} \times E^3)$ and suppose the Lie group $U(1)$, whose Lie algebra is $i\mathbb{R}$ (cf. B.3.3), has right action on Z_t given by

$$(A^\mu, \Pi_\mu) \cdot e^{i\lambda} := \left((A_0 - ie^{-i\lambda} \partial_0 e^{i\lambda}, A^j + ie^{-i\lambda} \partial_j e^{i\lambda}), \Pi_\mu \right), \quad j = 1,2,3. \tag{2.26}$$

[15] Recall that functions in $F(\{t\} \times E^3)$ are assumed to vanish at spatial infinity.

The infinitesimal generator of this action is $X^{i\lambda} \in \chi Z_t$ defined by (cf. B.3.6)

$$X^{i\lambda}(F) := \frac{d}{ds} F\left((A_0 + s\partial_0\lambda, A^j - s\partial_j\lambda), \Pi_\mu\right)\Big|_{s=0}. \tag{2.27}$$

Denoting the evaluation functions on Z_t by $e^\mu_{\mathbf{x}}$ for the A^μ and $\tilde{e}^\mu_{\mathbf{x}}$ for the Π_μ, and considering them as coordinates on Z_t, one obtains

$$X^{i\lambda}(e^0_{\mathbf{x}}) = \partial_0\lambda(t,\mathbf{x}), \qquad X^{i\lambda}(e^j_{\mathbf{x}}) = -\partial_j\lambda(t,\mathbf{x}), \qquad X^{i\lambda}(\tilde{e}^\mu_{\mathbf{x}}) = 0. \tag{2.28}$$

Thus, one can write $X^{i\lambda}$ as

$$X^{i\lambda} = \int d^3x \left(\partial_0\lambda(t,\mathbf{x})\frac{\delta}{\delta A_0} - \partial_j\lambda(t,\mathbf{x})\frac{\delta}{\delta A^j}\right) = X_G \equiv -\{G,\cdot\}. \tag{2.29}$$

The orbits of the $U(1)$ right action on Z_t are called *gauge orbits*. The function G (or equivalently the vector field X_G) generates motion within the gauge orbits, while the function H generates motion from orbit to orbit. The reduced phase space $Z_{\text{RPS}} \subset Z$ is defined as the quotient set $Z_{\text{CS}}/\triangleright$ under the equivalence relation $\triangleright$, which defines the gauge orbits (cf. section A.3.5). Physical observables are functions on Z_{RPS}, which are in one-to-one correspondence with the gauge-invariant functions on Z. To fix a gauge means to choose a particular representative potential A to work with. A gauge fixing criterion in the form of an equation $\mathcal{F}(A) = 0$ provides a third and final constraint to impose. Since according to H_{tot} the dynamics of A_0 are completely arbitrary, having reached the Hamiltonian level one may as well do away with A_0 altogether. This does not completely fix the gauge since it only takes us from eight to six (and not four) degrees of freedom per space-time point. There is still some freedom in choosing the vector potential $\mathbf{A}$. The remaining gauge freedom can be fixed through some condition $\mathcal{F}(\mathbf{A}) = 0$.

Given the total Hamiltonian and our three constraints there are a number of ways in which we might proceed towards the quantum theory[16]:

1. We could try to equip the constraint surface with a suitable bracket structure before imposing all of the constraints at the classical level, and then quantise the theory. This is achieved using Dirac's method of replacing Poisson brackets with so-called *Dirac brackets*, which are consistent with the constraints. The Hamiltonian H together with the Dirac brackets yield the correct equations of motion. Subsequently one can replace functions with operators and the Dirac brackets with commutators to obtain the

[16] According to Dirac one can actually go further at the classical level by defining the so-called *extended Hamiltonian* (Dirac (1964)). The extended Hamiltonian H_{ext} adds to H_{tot} in 2.23 the secondary constraint Gauss' law multiplied by a Lagrange multiplier. For us however, there isn't really anything to be gained by considering H_{ext}.

quantum theory.[17]

2. We could first quantise the theory by replacing Poisson brackets with commutators on some Hilbert space, and then impose the constraints at the quantum level to modify the commutators and obtain the physical space of quantum states as a subspace of the original Hilbert space.

3. We could use some mixture of the above two approaches and impose some constraints at the classical level, then quantise the theory, and impose the rest of the constraints at the quantum level.

These three methods should all give the same results, so which is used is really a matter of personal preference. In the next section I will use the first of the above methods to obtain a quantum description of nonrelativistic electrodynamics with sources. I will return to methods 2 and 3 later on in chapter 3.

2.3 Electrodynamics with sources

I will now consider the case of a single electron $-e$, possibly bound externally, interacting with the electromagnetic field. As in the previous section the first job will be to find a Lagrangian yielding the right equations of motion. For this purpose there is a standard Lagrangian, which will do fine, but it is not gauge-invariant. Following Woolley (1999) I will demonstrate how a gauge-invariant Lagrangian can be constructed. This involves using the non-unique Green's function for the divergence operator on χE^3, denoted $\mathbf{g}$. By writing the total vector potential in terms of its gauge-invariant transverse part the gauge will be fixed up to a choice of $\mathbf{g}$, which then carries the entire gauge freedom of the theory. Fixing the gauge therefore amounts to choosing a particular $\mathbf{g}$, which can be done at the level of the quantum Hamiltonian. Consequently, this method offers a good way of determining the implications of gauge freedom for the quantum theory.

2.3.1 Deriving the equations of motion with sources

The state space for the particle is $Y := (E^{1,3})^2$ and that of the electromagnetic field is Z as defined previously. The total space for the composite system is therefore $Y \times Z$. In terms of proper time $\tau^2 := (x^0)^2 - \mathbf{x}^2$ the particle can be described in terms of coordinates $r^\mu(\tau)$ and $\dot{r}^\mu(\tau)$. Within a fixed frame of reference with time coordinate t the particle space becomes $Y_t := (\{t\} \times E^3)^2$. The particle can then be described by three-vectors $\mathbf{r}(t)$ and $\dot{\mathbf{r}}(t)$. The equations of motion to be found are the inhomogeneous Maxwell equations supplemented

[17] There is another method equivalent to Dirac's, which is attributed to Jackiw (1993), but which I will not discuss. The basics of this method and a demonstration of its equivalence to Dirac's method can be found in Jackiw (1993), Jackiw (1995) and Muller-Kirsten (2006).

with the Lorentz force law

$$dF = 0 \qquad d*F = *j, \qquad -ei_u F = \frac{dp}{d\tau} \tag{2.30}$$

where u, p, E and γ are all defined in 2.1, and i denotes the interior product (cf. B.28). Two of the Maxwell equations are now inhomogeneous due to the source term $j = j_\mu dx^\mu$ called the current, which appears on the right-hand-side. The Hodge star operation produces a three-form from the one-form j. In components the inhomogeneous equations above take the form

$$\partial_\mu F^{\mu\nu} = j^\nu. \tag{2.31}$$

The components $\rho := j_0$ and $\mathbf{J} := (j^1, j^2, j^3)$ make up the *charge density* and the *current density* respectively. The Lagrangian $L(t) : Y_t \times Z_t \to \mathbb{R}$ for the composite system is the sum of three terms, L_P for the particle, L_F for the field and L_I for their interaction;

$$L(t) := -m\gamma^{-1} - \int d^3x\, j^\mu A_\mu - \frac{1}{4}\int d^3x\, F_{\mu\nu}F^{\mu\nu} \equiv L_P + L_I + L_F. \tag{2.32}$$

This Lagrangian together with the Euler Lagrange equations yields the correct equations of motion 2.30. I am primarily interested in the nonrelativistic limit of a particle that might be bound in a potential V. Expanding $-m\gamma^{-1}$ as $-m\gamma^{-1} = -m + \frac{1}{2}m\dot{\mathbf{r}}^2 + \frac{1}{8}m\dot{\mathbf{r}}^4 + \ldots \approx \frac{1}{2}m\dot{\mathbf{r}}^2$ and adding in the external potential V yields the nonrelativistic Lagrangian, which can be written

$$L(t) := \frac{1}{2}m\dot{\mathbf{r}}^2 - V(\mathbf{x}) - \int d^3x\, (\rho A_0 - \mathbf{J}\cdot\mathbf{A}) + \frac{1}{2}\int d^3x\, \left(\mathbf{E}^2 - \mathbf{B}^2\right). \tag{2.33}$$

2.3.2 Gauge freedom and the Lagrangian

Noether's theorem relates symmetries of a variational problem involving an action defined in terms of a Lagrangian, with conservation laws (see, for example, Hassani (1999)). The four-current j is in fact a conserved *Noether current* associated with the *global gauge* symmetry. By "global" gauge symmetry I mean the gauge symmetry for which the gauge function λ is independent of space-time points $(t, \mathbf{x})$.[18] The associated conservation law is the conservation of electric charge, which can be locally expressed through the *continuity equa-*

[18] More precisely, if we were dealing with a matter *field* as in chapter 3, we could say that it is Noether's first theorem that relates the global gauge symmetry of electrodynamics with the conserved current j. Noether's second theorem relates *local* gauge symmetry with the existence of *constraints*, by proving that if there exists a local gauge symmetry then the Euler-Lagrange equations are not independent. This means that the Lagrangian must be singular. At this stage however, we are just dealing with a single classical electron and the material variables are not directly effected by the gauge transformation. Thus, in the present context we actually have to *assume* that the continuity equation holds, but this is fine, because we are assuming Maxwell's equations hold.

tion

$$\partial_\mu j^\mu \equiv \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0. \tag{2.34}$$

where ρ and $\mathbf{J}$ are called the charge density and the current density respectively. One can then define *polarisation* and *magnetisation* fields $\mathbf{P}$ and $\mathbf{M}$ by

$$\rho = -\nabla \cdot \mathbf{P}, \qquad \mathbf{J} = \dot{\mathbf{P}} + \nabla \times \mathbf{M}, \tag{2.35}$$

in terms of which the charge and current densities satisfy 2.34 identically. These definitions do not fix $\mathbf{P}$ and $\mathbf{M}$ uniquely. If they were to be replaced with $\mathbf{P}'$ and $\mathbf{M}'$ defined by

$$\mathbf{P}' := \mathbf{P} + \nabla \times \mathbf{U}, \qquad \mathbf{M}' := \mathbf{M} - \dot{\mathbf{U}} - \nabla U_0, \tag{2.36}$$

where $\mathbf{U}$ and U_0 are arbitrary fields, then the charge and current densities would remain unchanged. Notice that the difference $\mathbf{M}' - \mathbf{M}$ has the form of an electric field $-\dot{\mathbf{U}} - \nabla U_0$, defined in terms of a potential $U = (U_0, \mathbf{U})$. The difference $\mathbf{P}' - \mathbf{P}$ has the form of the corresponding magnetic field $\nabla \times \mathbf{U}$. Since the potential U is only unique up to a gauge transformation, we appear to have introduced an interesting hierarchy of arbitrary fields starting from nothing but the continuity equation 2.34.

One can solve the first equation in 2.35 to give

$$\mathbf{P}(\mathbf{x}) = -\int d^3x' \, \mathbf{g}(\mathbf{x}, \mathbf{x}') \rho(\mathbf{x}') \tag{2.37}$$

where $\mathbf{g}(\mathbf{x}, \mathbf{x}')$ is the Green's function for the divergence operator defined by

$$\nabla \cdot \mathbf{g}(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}'). \tag{2.38}$$

While the longitudinal component of the Green's function $\mathbf{g}$ is fixed according to 2.38 by

$$\mathbf{g}_{\mathrm{L}}(\mathbf{x}, \mathbf{x}') = -\nabla \frac{1}{4\pi |\mathbf{x} - \mathbf{x}'|}, \tag{2.39}$$

its transverse component $\mathbf{g}_{\mathrm{T}}$ is essentially arbitrary, which expresses the arbitrariness of $\mathbf{P}$. Since the magnetisation can also be expressed in terms of ρ, $\mathbf{J}$ and $\mathbf{g}$, the freedom in choosing $\mathbf{P}$ and $\mathbf{M}$ is entirely equivalent to the freedom in choosing $\mathbf{g}_{\mathrm{T}}$.

For a single electron $-e$, the charge and current densities can be written

$$\rho(t, \mathbf{x}) = -e\delta(\mathbf{x} - \mathbf{r}), \qquad \mathbf{J}(t, \mathbf{x}) = -e\dot{\mathbf{r}}\delta(\mathbf{x} - \mathbf{r}). \tag{2.40}$$

in conjunction with which 2.35 gives purely mathematical definitions of polarisation and magnetisation fields. In order to make contact with the conventional physical notions of multipolar polarisation and magnetisation fields that are associated with a globally neutral

system of charges like a hydrogan atom, one must include the contributions of *all* charges within the densities in 2.40. If the (relatively heavy) nucleus of the hydrogen atom for example, is assumed to be fixed at the origin $\mathbf{0}$, one simply adds a term $e\delta(\mathbf{x})$ to ρ in 2.40. The multipolar polarisation and magnetisation fields are then obtained by making a specific choice for the Green's function $\mathbf{g}$. I postpone giving the explicit expression for this Green's function until section 6.1.2 (equation 6.6).

What does any of the above have to do with the Lagrangian? Well the Lagrangian 2.33 is not gauge-invariant, because L_P and L_F are gauge-invariant, while L_I isn't. To make the Lagrangian gauge-invariant one must add to it a term involving $\mathbf{P}$. If one transforms the potential $A \to A + d\lambda =: A'$, then with some integration by parts along with the use of 2.34 one can show that the Lagrangian L transforms into L' such that

$$L' = L + \frac{d}{dt}\int d^3x\, \rho\lambda\,. \tag{2.41}$$

Although L' is certainly equivalent to L, it is clearly not the same as L, so L is not gauge-invariant. On the other hand the Lagrangian

$$L_{\mathrm{GI}} := L - \frac{d}{dt}\int d^3x\, \mathbf{A}\cdot\mathbf{P} \tag{2.42}$$

is gauge-invariant, for now the same gauge transformation produces a Lagrangian

$$L'_{\mathrm{GI}} = L - \frac{d}{dt}\int d^3x\, \mathbf{A}\cdot\mathbf{P} + \frac{d}{dt}\int d^3x\, \lambda\,(\rho + \nabla\cdot\mathbf{P}) = L_{\mathrm{GI}} \tag{2.43}$$

where the first equality follows after an integration by parts, and the second from the definition of $\mathbf{P}$ in 2.35.

2.3.3 *Gauge fixing and quantisation*

The Hamiltonians used in nonrelativistic electromagnetism are usually obtained by starting with a Lagrangian in the form of L in 2.33. Since such a Lagrangian is not gauge-invariant a particular potential is implicitly selected to work with. In other words the gauge is fixed from the outset and the Lagrangian used belongs to a specific gauge. A formulation of electrodynamics, which is sufficiently general so as to include all Lagrangians of this type can be constructed by starting with L, and employing the gauge fixing condition

$$\int d^3x'\, \mathbf{g}(\mathbf{x}',\mathbf{x})\cdot\mathbf{A}(\mathbf{x}') = 0, \tag{2.44}$$

which makes the additional term in 2.42 vanish. Although this condition does not involve A_0, as in the free case the dynamics of A_0 are completely arbitrary, so that it naturally drops out of the formalism altogether. A set of vector potentials satisfying 2.44 identically, are

those such that

$$\mathbf{A}(\mathbf{x}) = \mathbf{A}_{\mathrm{T}}(\mathbf{x}) + \nabla \int d^3x' \, \mathbf{g}(\mathbf{x}', \mathbf{x}) \cdot \mathbf{A}_{\mathrm{T}}(\mathbf{x}') \equiv \mathbf{A}_{\mathrm{T}}(\mathbf{x}) + \mathbf{A}_{\mathrm{L}}(\mathbf{x}). \tag{2.45}$$

Thus, we can use the components of the gauge-invariant transverse vector potential to specify any *total* vector potential in the field configuration space $F(\{t\} \times E^3)^2$ that satisfy 2.44. Notice that the freedom in choosing $\mathbf{g}_{\mathrm{T}}$ implies a concurrent freedom in choosing $\mathbf{A}_{\mathrm{L}}$, but this is necessarily a *gauge* freedom. This means that the gauge can be specified completely by choosing a particular transverse Green's function $\mathbf{g}_{\mathrm{T}}$. Although at the quantum level $\mathbf{A}_{\mathrm{T}}$ will be operator-valued, $\mathbf{g}$ won't be. We will therefore obtain a Hamiltonian written explicitly in terms of the gauge-invariant potential $\mathbf{A}_{\mathrm{T}}$, but in an arbitrary gauge controlled by the "classical" object $\mathbf{g}$.

Starting with the Lagrangian L we can construct the total Hamiltonian, symplectic form and Poisson bracket structure in the usual way (cf. 2.23, B.2.7 and B.2.8 respectively). The total Hamiltonian can be written $H_{\mathrm{tot}} \equiv H + G$ where

$$H := \frac{1}{2m} \left(\mathbf{p} + e\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r}) + \frac{1}{2} \int d^3x \, \left(\mathbf{\Pi} + (\nabla \times \mathbf{A})^2\right) \tag{2.46}$$

and G is the following generator of gauge transformations.

$$G := \int d^3x \left(\dot{\lambda}\Pi_0 + \lambda \left[\rho + \nabla \cdot \mathbf{\Pi}\right]\right). \tag{2.47}$$

In total there are three constraint functions Π_0, $\rho - \nabla \cdot \mathbf{E} = \rho + \nabla \cdot \mathbf{\Pi}$ and $\mathcal{F}(A)$, but as I remarked earlier the time evolution of A_0 is completely arbitrary, so it can be removed from the formalism completely. This leaves us with Gauss' law and a gauge fixing condition $\mathcal{F}(\mathbf{A}) = 0$ as the only two constraints. The generator G is then simply Gauss' law

$$G = \int d^3x \, \lambda \left(\rho + \nabla \cdot \mathbf{\Pi}\right), \tag{2.48}$$

which generates gauge transformations of the vector potential $\mathbf{A}$.

To construct a Lie algebraic bracket structure, which is consistent with the constraints and the equations of motion we can use Dirac's method 1, which was briefly explained at the end of section 2.2.2. Fixing the gauge according to 2.44 means we have two constraint functions

$$C_1 := \rho + \nabla \cdot \mathbf{\Pi}, \qquad C_2 := \int d^3x' \mathbf{g}(\mathbf{x}', \mathbf{x}) \cdot \mathbf{A}(\mathbf{x}') \tag{2.49}$$

whose Poisson brackets $C_{ij}(\mathbf{x}, \mathbf{x}') := \{C_i(\mathbf{x}), C_j(\mathbf{x}')\}$ form a matrix with symplectic inverse

$$C^{-1}(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}') \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{2.50}$$

The equal-time *Dirac bracket* of functions $F, G \in F(Y_t \times Z_t)$ is defined by

$$\{F,G\}_D := \{F,G\} - \int d^3x \int d^3x' \, \{F, C_i(\mathbf{x})\} C^{-1}_{ij}(\mathbf{x},\mathbf{x}') \{C_j(\mathbf{x}'), G\}. \tag{2.51}$$

For a point particle with canonical coordinates $\mathbf{r}$ and $\mathbf{p}$, it is straightforward to check that the nonzero Dirac brackets of the dynamical variables are as follows

$$\{r^i, p_j\}_D = \delta_{ij}, \tag{2.52a}$$

$$\{\mathrm{A}^i(\mathbf{x}), \Pi_j(\mathbf{x}')\}_D = \delta_{ij}\delta(\mathbf{x}-\mathbf{x}') + \frac{\partial}{\partial x^i}\mathrm{g}_j(\mathbf{x}',\mathbf{x}), \tag{2.52b}$$

$$\{p_i, \Pi_j(\mathbf{x})\}_D = e\frac{\partial}{\partial r^i}\mathrm{g}_j(\mathbf{x},\mathbf{r}). \tag{2.52c}$$

If the *Coulomb gauge* $\mathbf{g}_\mathrm{T} \equiv \mathbf{0}$ is chosen then $\mathbf{A} \equiv \mathbf{A}_\mathrm{T}$, which along with 2.39 yields

$$\{\mathrm{A}^i_\mathrm{T}(\mathbf{x}), \Pi_j(\mathbf{x}')\}_D = \delta_{ij}\delta(\mathbf{x}-\mathbf{x}') + \frac{\partial^2}{\partial x^i \partial x^j}\frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|} \equiv \delta^\mathrm{T}_{ij}(\mathbf{x}-\mathbf{x}'), \tag{2.53a}$$

$$\{p_i, \Pi_j(\mathbf{x})\}_D = -\frac{\partial^2}{\partial r^i \partial x^j}\frac{e}{4\pi|\mathbf{x}-\mathbf{r}|} \tag{2.53b}$$

where $\delta^\mathrm{T}_{ij}(\mathbf{x}-\mathbf{x}')$ is called the *transverse delta function*.

Rather than setting $\mathbf{g}_\mathrm{T} \equiv \mathbf{0}$, we are now free, having constructed the Dirac brackets, to implement our constraints $C_1 = C_2 = 0$. The first constraint C_1 implies that

$$\mathbf{\Pi}_\mathrm{L} = -\mathbf{E}_\mathrm{L} = \mathbf{P}_\mathrm{L} \tag{2.54}$$

up to a constant vector. The second constraint C_2 implies that $\mathbf{A}$ can be written as in 2.45. In view of the fact that $\mathbf{\Pi} = -\mathbf{E}$, the transverse component of $\mathbf{\Pi}$ must be $-\mathbf{E}_\mathrm{T}$. In the Coulomb gauge $\mathbf{\Pi}$ is entirely transverse; $\mathbf{\Pi} \equiv \mathbf{\Pi}_\mathrm{T} \equiv -\mathbf{E}_\mathrm{T}$, and one has the *transverse canonical Dirac bracket relation*

$$\{\mathrm{A}_{\mathrm{T,i}}(\mathbf{x}), \Pi_{\mathrm{T,j}}(\mathbf{x}')\}_D = \delta^\mathrm{T}_{ij}(\mathbf{x}-\mathbf{x}'). \tag{2.55}$$

For this reason $\mathbf{\Pi}_\mathrm{T}$ can be viewed as the momentum conjugate to the *transverse* vector potential. The field that satisfies the same Dirac bracket relations as $\mathbf{\Pi}_\mathrm{T}$ in *all* gauges (including the Coulomb gauge) will henceforth be denoted using the same symbol $\mathbf{\Pi}_\mathrm{T}$, and it is defined as

$$\mathbf{\Pi}_\mathrm{T} := -\mathbf{D}_\mathrm{T} := -\mathbf{E}_\mathrm{T} - \mathbf{P}_\mathrm{T}. \tag{2.56}$$

This is nothing but (the negative of) the transverse component of the *electric displacement field* $\mathbf{D} := \mathbf{E} + \mathbf{P}$.

The Hamiltonian 2.46 can be written

$$H \equiv H = \frac{1}{2m}\left(\mathbf{p} + e\left[\mathbf{A}_{\mathrm{T}}(\mathbf{r}) + \nabla \int d^3x' \mathbf{g}(\mathbf{x}', \mathbf{r}) \cdot \mathbf{A}_{\mathrm{T}}(\mathbf{x}')\right]\right)^2 + V(\mathbf{r}) + V_{\mathrm{self}} + \frac{1}{2}\int d^3x \left[(\mathbf{\Pi}_{\mathrm{T}} + \mathbf{P}_{\mathrm{T}})^2 + (\nabla \times \mathbf{A}_{\mathrm{T}})^2\right] \tag{2.57}$$

where

$$V_{\mathrm{self}} := \frac{1}{2}\int d^3x \mathbf{E}_{\mathrm{L}}(\mathbf{x})^2 = \frac{1}{2}\int d^3x \mathbf{P}_{\mathrm{L}}(\mathbf{x})^2 \tag{2.58}$$

represents the divergent Coulomb self-energy of the electron, due to its own static longitudinal electric field. For a point particle $\rho(\mathbf{x}) = -e\delta(\mathbf{x} - \mathbf{r})$ one has

$$V_{\mathrm{self}} = \frac{e^2}{2}\int d^3x \mathbf{g}_{\mathrm{L}}(\mathbf{x}, \mathbf{r})^2. \tag{2.59}$$

The Dirac bracket $\{p_i, \Pi_{\mathrm{T,j}}(\mathbf{x})\}_D$ vanishes identically, so equation 2.57 gives a Hamiltonian in terms of transverse fields *that are in involution with the particle variables* $\mathbf{r}$ *and* $\mathbf{p}$ (with respect to the Dirac bracket). The vector potential $\mathbf{A}_{\mathrm{T}}$ belongs to the Coulomb gauge, but the Hamiltonian itself has been expressed in an arbitrary gauge, which is determined by $\mathbf{g}_{\mathrm{T}}$. The Coulomb gauge Hamiltonian is obtained by setting $\mathbf{g}_{\mathrm{T}} \equiv \mathbf{0}$. The conjugate momenta can be identified in the gauge g as

$$\mathbf{p} = m\dot{\mathbf{r}} - e\left(\mathbf{A}_{\mathrm{T}}(\mathbf{r}) + \nabla \int d^3x' \mathbf{g}(\mathbf{x}', \mathbf{r}) \cdot \mathbf{A}_{\mathrm{T}}(\mathbf{x}')\right). \tag{2.60}$$

Thus, as in the example in section 1.3 both $\mathbf{p}$ and $\mathbf{\Pi}_{\mathrm{T}}$ are manifestly gauge-dependent, while the velocities $\dot{\mathbf{r}}$ and $\dot{\mathbf{A}}_{\mathrm{T}} = -\mathbf{E}_{\mathrm{T}}$ are gauge-invariant. The Hamiltonian in *any* gauge can be written

$$\begin{aligned} &H = H_A + V_{\mathrm{self}} + H_{\mathrm{TF}} = H_A + H_{\mathrm{EM}}, \\ &H_A := \frac{1}{2}m\dot{\mathbf{r}}^2 + V(\mathbf{r}), \qquad H_{\mathrm{TF}} := \frac{1}{2}\int d^3x \left(\mathbf{E}_{\mathrm{T}}^2 + \mathbf{B}^2\right), \qquad H_{\mathrm{EM}} := \frac{1}{2}\int d^3x \left(\mathbf{E}^2 + \mathbf{B}^2\right). \end{aligned} \tag{2.61}$$

The term H_A represents the electron's energy, while the terms H_{TF} and H_{EM} represent the energy of the *transverse* electromagnetic field and the *total* electromagnetic field respectively. As usual the Hamiltonian for the system represents the total energy as the sum of energies of the subsystems, which can be naturally defined in terms of gauge invariant observables.

To quantise the theory we will need to define the so-called *normal variables* (Cohen-Tannoudji *et al.* (1997)). This is done using the spatial Fourier transform $\mathfrak{F} : \chi E^3 \to \chi E^3$

defined for $\mathbf{v} \in \chi E^3$ by

$$\boldsymbol{v}(\mathbf{k}) := [\mathfrak{F}(\mathbf{v})](\mathbf{k}) := \frac{1}{\sqrt{(2\pi)^3}} \int d^3x\, \mathbf{v}(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}}. \tag{2.62}$$

Since any transverse $\mathbf{v}_{\mathrm{T}} \in \chi E^3$ satisfies

$$\mathbf{k} \cdot \boldsymbol{v}_{\mathrm{T}}(\mathbf{k}) = 0, \tag{2.63}$$

the Fourier transform $\boldsymbol{v}_{\mathrm{T}}$ can be written

$$\boldsymbol{v}_{\mathrm{T}}(\mathbf{k}) = \sum_{\lambda=1,2} \mathbf{e}_\lambda(\mathbf{k}) v_{\mathrm{T},\lambda}(\mathbf{k}) \tag{2.64}$$

where $\{\mathbf{e}_1(\mathbf{k}), \mathbf{e}_2(\mathbf{k}), \hat{\mathbf{k}}\}$ is an orthogonal triad of unit three-vectors. In other words the vector $\boldsymbol{v}_{\mathrm{T}}(\mathbf{k})$ lies in the plane orthogonal to $\mathbf{k}$, within which $\{\mathbf{e}_1(\mathbf{k}), \mathbf{e}_2(\mathbf{k})\}$ denotes an orthogonal basis. The normal variable $\boldsymbol{\alpha}(\mathbf{k})$ is defined as

$$\boldsymbol{\alpha}(\mathbf{k}) = \sum_{\lambda=1,2} \mathbf{e}_\lambda(\mathbf{k}) \alpha_\lambda(\mathbf{k}), \qquad \alpha_\lambda(\mathbf{k}) := \sqrt{\frac{1}{2\omega}} \Big(\omega A_{\mathrm{T},\lambda}(\mathbf{k}) + i\Pi_{\mathrm{T},\lambda}(\mathbf{k}) \Big) \tag{2.65}$$

where $\omega := |\mathbf{k}|$. The bosonic Dirac bracket relation

$$\{\alpha_\lambda(\mathbf{k}), \alpha^*_{\lambda'}(\mathbf{k}')\}_D = -i\delta_{\lambda\lambda'}\delta(\mathbf{k}-\mathbf{k}'), \tag{2.66}$$

follows from 2.55 and the fact that the canonical fields $\mathbf{A}_{\mathrm{T}}$ and $\boldsymbol{\Pi}_{\mathrm{T}}$ are real. It is common to consider the fields as being contained within a cube of volume $V = L^3$, and as satisfying periodic boundary conditions at the sides of the cube. One can let L go to infinity at the end of the calculation of some physical prediction. The components of the vector $\mathbf{k}$ then take discrete values $k_{x,y,z} = 2\pi n_{x,y,z}/L$, $n_j \in \mathbb{Z}$. This allows one to substitute Fourier integrals with discrete sums as follows

$$\frac{1}{(2\pi)^3} \int d^3k \to \frac{1}{V} \sum_{\mathbf{k}}. \tag{2.67}$$

Quantities dependent on $\mathbf{k}$ are subsequently labelled with a discrete index $_{\mathbf{k}}$.

We can now quantise the theory by firstly replacing the classical state space $Y \times Z|_{\mathrm{CS}}$ with some suitable Hilbert space $\mathcal{H}$, by secondly replacing the classical canonical variables in $F(Y \times Z)|_{\mathrm{CS}}$ with canonical operators in $\mathcal{L}(\mathcal{H})$, and by finally replacing the Dirac bracket $\{\cdot,\cdot\}_D$ on $F(Y \times Z)|^2_{\mathrm{CS}}$ with the commutator $-i[\cdot,\cdot]$ on $\mathcal{L}(\mathcal{H})^2$. To carry out this procedure it is actually the normal variables which are replaced with operators satisfying the commutation relation of bosonic creation and annihilation operators; $\alpha_{\mathbf{k}\lambda} \to a_{\mathbf{k}\lambda}$, $\alpha^*_{\mathbf{k}\lambda} \to a^\dagger_{\mathbf{k}\lambda}$

with

$$[a_{\mathbf{k}\lambda}, a^\dagger_{\mathbf{k}'\lambda'}] = \delta_{\lambda\lambda'}\delta_{\mathbf{k}\mathbf{k}'}. \tag{2.68}$$

We can therefore take the Hilbert space for the canonical field degrees of freedom to be the bosonic Fock space $\mathcal{F}_B\left(L^2(\mathbb{R}^3,\mathbb{C}^2)\right)$, built out of the single particle space $L^2(\mathbb{R}^3,\mathbb{C}^2) = L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3) = L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ (cf. section A.3.6). Two lots of $L^2(\mathbb{R}^3)$ are required to cater for the two values of λ, which is now taken to label the polarisation state of the *photon*. The single particle eigenstate $|\mathbf{k}\lambda\rangle$ of the number operator $a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}$ is the state of one photon with definite momentum $\mathbf{k}$ and polarisation λ. As operators the canonical fields in real space $\mathbf{A}_\mathrm{T}$ and $\mathbf{\Pi}_\mathrm{T}$ support the following *mode expansions*

$$\begin{aligned}\mathbf{A}_\mathrm{T}(\mathbf{x}) &= \sum_{\mathbf{k}\lambda} g\mathbf{e}_{\mathbf{k}\lambda}\left(a^\dagger_{\mathbf{k}\lambda}e^{-i\mathbf{k}\cdot\mathbf{x}} + a_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{x}}\right),\\ \mathbf{\Pi}_\mathrm{T}(\mathbf{x}) &= i\sum_{\mathbf{k}\lambda}\omega g\mathbf{e}_{\mathbf{k}\lambda}\left(a^\dagger_{\mathbf{k}\lambda}e^{-i\mathbf{k}\cdot\mathbf{x}} - a_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{x}}\right)\end{aligned} \tag{2.69}$$

where

$$g := \frac{1}{\sqrt{2\omega V^3}}. \tag{2.70}$$

The electron's canonical Hilbert space can be taken to be $L^2(\mathbb{R}^3)$ as usual, which means the total Hilbert space of the composite electron-field system is $\mathcal{H} := L^2(\mathbb{R}^3)\otimes\mathcal{F}_B\left(L^2(\mathbb{R}^3,\mathbb{C}^2)\right)$. Since the entire construction is defined in terms of the canonical degrees of freedom, as with the example in section 1.3, the quantum mechanical subsystems are manifestly gauge dependent and generally physically distinct for each different choice of $\mathbf{g}_\mathrm{T}$. The quantum Hamiltonian consists of three gauge dependent components

$$\begin{aligned}H \equiv H &:= H_A + H_F + V,\\ H_A &:= \left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + V_\mathrm{self} + \frac{1}{2}\int d^3x\,\mathbf{P}_\mathrm{T}(\mathbf{x})^2\right]\otimes I\\ V &:= \frac{e}{m}\left[\mathbf{p}\otimes I\right]\cdot\mathbf{A}(\mathbf{r}) + \frac{e^2}{2m}\mathbf{A}(\mathbf{r})^2 + \int d^3x\,\left[\mathbf{P}_\mathrm{T}\otimes I\right]\cdot\left[I\otimes\mathbf{\Pi}_\mathrm{T}\right]\\ H_F &:= I\otimes\left[\frac{1}{2}\int d^3x\,\left(\mathbf{\Pi}_\mathrm{T}^2 + (\nabla\times\mathbf{A}_\mathrm{T})^2\right)\right] \equiv I\otimes\left[\sum_{\mathbf{k}\lambda}\omega\left(a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda} + \frac{1}{2}\right)\right]\end{aligned} \tag{2.71}$$

where

$$\mathbf{A}(\mathbf{r}) := \mathbf{A}_\mathrm{T}(\mathbf{r}) + \nabla_\mathbf{r}\int d^3x'\,\mathbf{g}(\mathbf{x}',\mathbf{r})\cdot\mathbf{A}_\mathrm{T}(\mathbf{x}'). \tag{2.72}$$

Since $\mathbf{r}$ is an electronic operator in $\mathcal{L}(L^2(\mathbb{R}^3))$, any products of the field operators $a_{\mathbf{k}\lambda}, a^\dagger_{\mathbf{k}\lambda}$ with functions of $\mathbf{r}$ such as the plane wave terms $e^{\pm i\mathbf{k}\cdot\mathbf{r}}$ in 2.69, must be interpreted as tensor products. The operators $\mathbf{A}_\mathrm{T}(\mathbf{r})$ and $\mathbf{\Pi}_\mathrm{T}(\mathbf{r})$ therefore act nontrivially in the entire composite

space $\mathcal{H}$. From here on I will employ the standard practice of omitting tensor products with the identity, so for example, $H_A \otimes I$ will be written simply H_A, and "interaction" terms like $[\mathbf{P}_\mathrm{T} \otimes I] \cdot [I \otimes \mathbf{\Pi}_\mathrm{T}]$ will be written simply $\mathbf{P}_\mathrm{T} \cdot \mathbf{\Pi}_\mathrm{T}$.

I will end this section with a note of caution regarding the Hamiltonian 2.71, which has been obtained using the somewhat ad hoc ideas of canonical quantisation. Having crudely supplanted classical structure with quantum structure we might anticipate having created certain problems. In particular the Hamiltonian is certain to require regularisation through momentum cut-offs in order that it is well defined and self-adjoint on some domain in $\mathcal{H}$. The divergences associated with relativistic modes are actually also found at the classical level, where they arise due to difficulties with the notion of a point particle. In any case, the spectral properties of the Coulomb gauge Hamiltonian with cut-offs have been studied thoroughly, and in particular it is known that a ground state exists (see Bach (2001), Fröhlich *et al.* (2008), Sigal (2009), Dimassi & Guillot (2003), and references therein). In what follows throughout this thesis I will assume that similar results hold in gauges other than the Coulomb gauge, and when discussing the physical content of the theory developed so far, I will rely heavily on the formal ideas of nonrelativistic quantum field theory predominant in the physics literature (see for example, Cohen-Tannoudji *et al.* (1997)).

2.4 Summary and discussion

We have arrived at an arbitrary gauge quantum theory of a bound electron interacting with electromagnetic radiation, and along the way encountered the photon concept. A common impression of photons is that they are unique particle-like globules of radiant energy. However, we have seen that photons are defined using gauge dependent and physically ambiguous canonical degrees of freedom. There is in fact an infinitude of physically distinct "photons", just as there is an infinitude of physically distinct "bound electrons", whenever these things are defined in terms of canonical degrees of freedom.

Only in the case of *free* quantum electrodynamics can photons be uniquely defined. This is possible, because in free space the electric and magnetic fields are entirely transverse, and coincide with the transverse canonical field operators i.e., in free space $\mathbf{E} = \mathbf{E}_\mathrm{T} = -\mathbf{\Pi}_\mathrm{T}$ and $\mathbf{B} = \nabla \times \mathbf{A}_\mathrm{T}$. Similarly, there is no ambiguity in defining the non-interacting quantum mechanical electron for which $\mathbf{p} = m\dot{\mathbf{r}}$. However, while the non-interacting electron is relatively uncontentious, the notion of photon has to be handled with care even in free space. As Lamb (1995) put it;

> *"photons cannot be localized in any meaningful manner, and they do not behave at all like particles."*

CHAPTER 3

Quantum-mechanical gauge fixing and QED

In this chapter I will adapt the methods used in chapter 2, to describe the relativistic Dirac field interacting with electromagnetic radiation. The results of section 3.3 of this chapter are summarised in the paper Stokes (2012). The main new result presented in this chapter is the arbitrary gauge Hamiltonian to be found in 3.96.

In the late 1920s Dirac was unhappy with the viewpoint that the *Klein-Gordon equation* was the correct relativistic version of the wave-mechanical Schrödinger equation, because it suffered from quite severe interpretational problems. He viewed these problems as symptoms of its second order nature and so sought a relativistic wave equation, which was first order in time. *The Dirac equation* was the fruit of this labour. While it immediately solves some of the problems associated with the Klein-Gordon equation, the Dirac equation still incurs problematic negative-energy solutions. This problem is seen to dissolve if the Dirac wavefunction is treated as a quantum *field*. The interacting Dirac-Maxwell quantum system is the system of study in quantum electrodynamics.

In the last chapter I quantised the composite charge-electromagnetic system, by treating the material degrees of freedom as those of a single wave-mechanical particle. In this chapter I will treat the material degrees of freedom using the quantised Dirac field instead.[19]

[19] One can also describe the nonrelativistic theory of chapter 2 in purely field-theoretic language by way of the *Schrödinger matter field* (Babiker *et al.* (1973)). In practice this is quite common, and can be useful in describing many-body systems such as complex atoms and molecules. However, the total number of electrons is necessarily conserved in such a theory (in contrast to the relativistic theory), because the electronic number operator commutes with the Hamiltonian (Cohen-Tannoudji *et al.* (1997)). Thus, if one is only interested in describing a single electron system there is no need to use the field-theoretic description, which reduces to the ordinary wave-mechanical description when restricted to the one-electron subspace.

3.1 The Dirac field

I begin by briefly reviewing the free Dirac field and its quantisation. More detailed accounts can be found in a number of textbooks (see for example Thaller (1992), Peskin & Schroeder (1995), Ryder (1996)). Afterwards I will add an external Coulomb potential appropriate for the description of bound systems of charges.

3.1.1 The free Dirac field

Consider relativistic wavefunctions ψ defined on Minkowski space-time A.3.5. Taking the relativistic energy-momentum relation 2.5 and making the naive substitutions

$$\mathbf{p} \to -i\nabla, \qquad E \to i\frac{\partial}{\partial t} \tag{3.1}$$

one immediately arrives at the Klein-Gordon equation

$$(\Box + m^2)\psi = 0, \qquad \Box := \partial_\mu \partial^\mu. \tag{3.2}$$

Since this second order equation doesn't work very well Dirac decided to "linearise" it by first taking the square root of 2.5, and only then making the substitutions 3.1. He assumed that the required linear version of 2.5 took the natural form $E = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m$. Upon using 3.1, the Dirac equation

$$i\dot{\psi} = h_D \psi, \qquad h_D := -i\boldsymbol{\alpha} \cdot \nabla + \beta m. \tag{3.3}$$

follows. For the idea to make sense we need to get back 2.5, which means the α_i and β have to satisfy

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \qquad \{\alpha_i, \beta\} = 0, \qquad \beta^2 = 1. \tag{3.4}$$

where $\{\cdot,\cdot\}$ denotes the anti-commutator. It follows immediately from this, that the α_i and β must be at least 4×4 matrices, and therefore that the Dirac wavefunctions are (at least) $\mathbb{C}^4$-valued. These wavefunctions are actually called Dirac spinors, and they quite naturally support a representation of the Lorentz group. The *standard representation* of the Dirac matrices is

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \tag{3.5}$$

where I is the 2×2 identity matrix and the Pauli matrices σ_i are defined in B.79. Defining the γ-matrices by

$$\gamma^0 := \beta, \qquad \gamma^i = \gamma_0 \alpha_i, \tag{3.6}$$

the Dirac equation 3.3 can be written

$$(i\gamma^\mu \partial_\mu - m)\psi = 0. \tag{3.7}$$

In actual fact the defining property of the γ-matrices can be taken as the (*Clifford*) algebraic relation

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}. \tag{3.8}$$

where η is defined in A.3.5. The relations 3.4 along with 3.5 and 3.6 merely constitute a particular manifestation of 3.8. The Dirac equation 3.7 will also be satisfied if we transform the γ-matrices and wavefunctions using a similarity transformation R as

$$\gamma'^\mu = R\gamma^\mu R^{-1}, \qquad \psi' = R\psi. \tag{3.9}$$

A useful second representation of the γ-matrices is the *Weyl* representation, which is related to the standard representation via the matrix

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix}. \tag{3.10}$$

where I denotes the 2×2 identity matrix. In the Weyl representation the γ-matrices take the form

$$\gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}. \tag{3.11}$$

and the Dirac spinors can be viewed as being composed of left and right Weyl spinors (cf. B.101 and B.110);

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}. \tag{3.12}$$

Within this representation the effect of a Lorentz transformation is particularly simple with the left and right Weyl spinors individually transforming according to B.110. An isomorphic representation of the Lie algebra of the Lorentz group $so(1,3)$ given by the relations B.96 is given in terms of the γ-matrices by

$$l_i \leftrightarrow \Sigma_i := \frac{1}{4}\varepsilon_{ijk}\gamma^j\gamma^k = -\frac{i}{2}\begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}, \qquad b_i \leftrightarrow \kappa_i := \frac{1}{2}\gamma_0\gamma^i = \frac{1}{2}\begin{pmatrix} \sigma_i & 0 \\ 0 & -\sigma_i \end{pmatrix}, \tag{3.13}$$

which is clearly just the natural adaptation of the representations B.100 on $\mathbb{C}^2$, to the $\mathbb{C}^4$-valued wavefunctions in 3.12. The representation $D : \mathcal{L}_+^\uparrow \to GL(L_2(E^{1,3}, \mathbb{C}^4))$ of a general

Lorentz transformation $\Lambda = e^{\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})}$ (cf. B.3.5) on the Dirac spinor ψ is given through exponentiation of 3.13 (cf. B.110).[20] It is constructed out of two maps, $\hat{D} : \mathcal{L}_+^\uparrow \to \mathbb{C}^4$, which is a representation in the sense of B.3.7, and $\bar{D} : \mathcal{L}_+^\uparrow \to GL(L_2(E^{1,3}))$, which is a representation in the sense of B.3.10. Letting $\{E_a\}$ denote the canonical basis in $\mathbb{C}^4$ and writing $\psi \equiv \psi^a E_a$, we have that under a Lorentz transformation

$$\begin{aligned}\psi(x) \to D(\Lambda)\psi(x) \equiv \hat{D}(\Lambda)\psi(\Lambda^{-1}x) \equiv \left[\hat{D}(\Lambda)E_a\right]\psi^a(\Lambda^{-1}x)\\ := e^{\hat{n}_i(\theta\Sigma_i+\phi\kappa_i)}\psi(e^{-\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})}x)\end{aligned} \tag{3.14}$$

where the representation $\bar{D}$ is evidently defined by $\bar{D}(\Lambda)\psi^a(x) := \psi^a(\Lambda^{-1}x)$.

Often (see for example Peskin & Schroeder (1995)), the generators of $so(1,3)$ in B.96 are combined into a set of anti-symmetric generators $\ell^{\alpha\beta}$, $\alpha,\beta = 0,1,2,3$ for which I choose the convention

$$\ell^{ij} := -i\varepsilon^{ijk}l_k, \quad \ell^{0i} := -ib_i. \tag{3.15}$$

These definitions imply that

$$[\ell^{\alpha\beta},\ell^{\mu\nu}] = i(\eta^{\beta\mu}\ell^{\alpha\nu} - \eta^{\alpha\mu}\ell^{\beta\nu} - \eta^{\beta\ni}\ell^{\alpha\mu} + \eta^{\alpha\nu}\ell^{\beta\mu}). \tag{3.16}$$

Defining now the anti-symmetric generators $S^{\alpha\beta}$ by

$$S^{\alpha\beta} = -\frac{i}{4}[\gamma^\alpha,\gamma^\beta] = -\frac{i}{2}(1-\delta_{\alpha\beta})\gamma^\alpha\gamma^\beta \tag{3.17}$$

it follows that

$$S^{jk} = -i\varepsilon_{ijk}\Sigma_i, \qquad S^{0i} = -i\kappa_i, \qquad [S^{\alpha\beta},S^{\mu\nu}] = [\ell^{\alpha\beta},\ell^{\mu\nu}], \tag{3.18}$$

and that the representation defined in 3.13 is simply

$$\ell^{\alpha\beta} \leftrightarrow S^{\alpha\beta}. \tag{3.19}$$

We can therefore express a Lorentz transformation as

$$\Lambda = e^{\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})} = e^{i\omega_{\alpha\beta}\ell^{\alpha\beta}}, \qquad \omega_{\alpha\beta} = -\omega_{\beta\alpha}, \quad \varepsilon^{ijk}\omega_{ij} = \theta\hat{n}_k, \quad \omega_{i0} = \phi\hat{n}_i, \tag{3.20}$$

so that according to 3.14 we obtain the representation

$$D(\Lambda)\psi(x) = \hat{D}(\Lambda)\psi(\Lambda^{-1}x) = e^{i\omega_{\alpha\beta}S^{\alpha\beta}}\psi(e^{-i\omega_{\alpha\beta}\ell^{\alpha\beta}}x). \tag{3.21}$$

[20] In B.3.4 I use the symbol ρ to denote representations in keeping with the common practice in some of the maths literature. Here I adopt the symbol D instead as this seems to be the convention used throughout the physics literature.

It is easy to verify using $[\gamma, S^{\alpha\beta}] = (\ell^{\alpha\beta})^{\mu}_{\nu}\gamma^{\nu}$ that

$$\hat{D}^{-1}(\Lambda)\gamma^{\mu}\hat{D}(\Lambda) = \Lambda^{\mu}_{\nu}\gamma^{\nu}. \tag{3.22}$$

It follows from this that the Dirac equation is covariant under a Lorentz transformation $x \to x' := \Lambda x$;

$$\begin{aligned}[i\gamma^{\mu}\partial'_{\mu} - m]\psi'(x') &= \left[i\gamma^{\mu}(\Lambda^{-1})^{\nu}_{\mu}\partial_{\nu} - m\right]\hat{D}(\Lambda)\psi(x) \\ &= i\left[\hat{D}(\Lambda)\gamma^{\nu}\hat{D}^{-1}(\Lambda)\partial_{\nu} - \hat{D}(\Lambda)\hat{D}^{-1}(\Lambda)m\right]\hat{D}(\Lambda)\psi(x) \\ &= \hat{D}(\Lambda)i\left[\gamma^{\nu}\partial_{\nu} - m\right]\psi(x) = 0\end{aligned} \tag{3.23}$$

where I have used $\partial'_{\mu} = (\partial x^{\nu}/\partial x'^{\mu})\partial_{\nu} = (\Lambda^{-1})^{\nu}_{\mu}\partial_{\nu}$.

The scalar quantity $\psi^{\dagger}\psi$ is not a Lorentz scalar meaning that it isn't covariant. For this reason one defines the relativistic adjoint $\bar{\psi}$ by

$$\bar{\psi} := \psi^{\dagger}\gamma^{0}, \tag{3.24}$$

which can be used to define the covariant scalar $\bar{\psi}\psi$. One can define a *covariant conserved current* of the Dirac field by

$$j^{\mu} := \bar{\psi}\gamma^{\mu}\psi \equiv (\psi^{\dagger}\psi, \psi^{\dagger}\boldsymbol{\alpha}\psi) =: (\rho, \mathbf{j}), \tag{3.25}$$

and it is easy to verify using 3.7 that j^{μ} does indeed satisfy $\partial_{\mu}j^{\mu} = 0$.

To understand the significance of the three-current $\mathbf{j}$ it is instructive to look at the time evolution of the *standard position operator* $\mathbf{r}(t)$ (Thaller (1992)).[21] According to 3.3 we have

$$\dot{\mathbf{r}}(t) = -i[\mathbf{r}(t), h_D] = \boldsymbol{\alpha}(t), \tag{3.26}$$

which means $\mathbf{j}(t) = \psi^{\dagger}\dot{\mathbf{r}}(t)\psi$ in direct analogy with the nonrelativistic theory. However, in contrast to the nonrelativistic theory $m\dot{\mathbf{r}} \neq \mathbf{p}$ with $\mathbf{p} = -i\nabla$ denoting the *canonical* momentum. This is perhaps not surprising, because in relativity the proper momentum $\mathbf{p}$ is related to the velocity by 2.3, which along with 2.5 implies $\dot{\mathbf{r}} \equiv \mathbf{v} = \mathbf{p}/E$. We might therefore expect the velocity operator to be $\mathbf{p}/h_D$. This "classical-type" velocity is related physically to the operator $\dot{\mathbf{r}} = \boldsymbol{\alpha}$ in the following simple way. According to 3.3

$$\dot{\boldsymbol{\alpha}}(t) = 2ih_D e^{2ih_D t}\left(\alpha(0) - \frac{\mathbf{p}}{h_D}\right), \tag{3.27}$$

[21] The clarifier "standard" is necessary here, because the position observable is somewhat contentious within the relativistic quantum mechanical theory described by the Dirac equation. According to this theory, it is far from clear that localised single particles exist at all. As such there are several candidates for operators that could each reasonably be called "position" operators (Thaller (1992)).

which upon integrating yields

$$\dot{\mathbf{r}}(t) = \boldsymbol{\alpha}(t) = \frac{\mathbf{p}}{h_D} + e^{2iH_0 t}\left(\boldsymbol{\alpha}(0) - \frac{\mathbf{p}}{h_D}\right) \tag{3.28}$$

meaning that the velocity oscillates about the classical velocity $\mathbf{p}/h_D$. This peculiar behaviour is related to the existence of negative energy solutions, and to the lack of a satisfactory position operator within the relativistic theory. We can nevertheless go ahead and define the current $\mathbf{j} = \psi^\dagger \boldsymbol{\alpha} \psi$. Moreover, in a way analogous to the nonrelativistic theory, when we couple the Dirac field to the Maxwell field the canonical momentum $\mathbf{p}$ is replaced using a minimal coupling prescription.

Solutions of the free Dirac equation

To quantise the theory we need to find solutions of the Dirac equation. This is most easily done in momentum space. The Fourier transform of the Dirac spinor $\psi = \psi^\alpha E_\alpha$ is defined componentwise as in 2.62;

$$\psi^\alpha(\mathbf{p}) := [\mathfrak{F}\psi^\alpha](\mathbf{p}) := \frac{1}{\sqrt{(2\pi)^3}} \int d^3x\, \psi^\alpha(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}}. \tag{3.29}$$

The Dirac Hamiltonian h_D (in the standard representation) is in momentum space given by

$$H_0(\mathbf{p}) := \mathfrak{F} h_D \mathfrak{F}^{-1} = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta m, \tag{3.30}$$

This just means that acting on momentum spinors the operator p_i multiplies by the i'th component of the vector $\mathbf{p}$, so that we simply need to make the familiar substitution $-i\nabla \to \mathbf{p}$ in 3.3. If we square $h_D(\mathbf{p})$ and use the relations 3.4 then we see that

$$h_D(\mathbf{p})^2 = (p^2 + m^2) I \tag{3.31}$$

where for convenience I have introduced the notation $p := |\mathbf{p}|$, which mustn't be confused with $p^2 = p_\mu p^\mu$ sometimes used for the four-momentum. It follows from 3.31 that $h_D(\mathbf{p})$ possesses two energy eigenvalues

$$E = \pm\varepsilon(\mathbf{p}) := \pm\sqrt{p^2 + m^2}. \tag{3.32}$$

Since we expect there to be four eigenspinors for each value of $\mathbf{p}$, the eigenspinors must be degenerate. We need therefore, to find an operator commuting with $h_D(\mathbf{p})$, which we can use to label the degenerate eigenspinors. A suitable choice is the *helicity* operator

$$h(\mathbf{p}) := i\vec{\Sigma}\cdot\hat{\mathbf{p}} \tag{3.33}$$

with $\vec{\Sigma} := (\Sigma_1, \Sigma_2, \Sigma_3)$ defined in 3.13. The four eigenspinors we seek are given in numerous textbooks (see for example Sakurai (1967), Peskin & Schroeder (1995), Ryder (1996), Ticciati (2008)). They are usually found by boosting the trivial rest frame solutions for which $\mathbf{p} = \mathbf{0}$ to a general frame (Peskin & Schroeder (1995), Ryder (1996), Ticciati (2008)). I will use Thaller (1992) to simply state general solutions for which it can be checked easily that the Dirac equation is satisfied. In total there are two mutually degenerate positive energy solutions $u^r(\mathbf{p})$, $r = +,-$, and two mutually degenerate negative energy solutions $v^r(\mathbf{p})$. Both positive and negative energy sets consist of simultaneous eigenspinors of energy and helicity, with the label $r = +,-$ corresponding to the two distinct eigenvalues of helicity $\pm p/2$. Explicitly the solutions are (Thaller (1992))

$$u^{\pm}(\mathbf{p}) = \begin{pmatrix} a_+ h_\pm \\ \pm a_- h_\pm \end{pmatrix}, \tag{3.34a}$$

$$v^{\pm}(\mathbf{p}) = \begin{pmatrix} \mp a_- h_\pm \\ a_+ h_\pm \end{pmatrix} \tag{3.34b}$$

where

$$h_+(\mathbf{p}) := \frac{1}{\sqrt{2p(p-p_z)}} \begin{pmatrix} p_x - ip_y \\ p_z - p \end{pmatrix}, \qquad h_-(\mathbf{p}) := \frac{1}{\sqrt{2p(p-p_z)}} \begin{pmatrix} p_z - p \\ p_x + ip_y \end{pmatrix} \tag{3.35}$$

and

$$a_\pm(\mathbf{p}) := \sqrt{\frac{1}{2}\left(1 \pm \frac{m}{\varepsilon(\mathbf{p})}\right)}. \tag{3.36}$$

The relativistic adjoints are defined as in 3.24 by

$$\bar{u}^{\pm}(\mathbf{p}) = u^{\pm}(\mathbf{p})^\dagger \gamma^0, \qquad \bar{v}^{\pm}(\mathbf{p}) = v^{\pm}(\mathbf{p})^\dagger \gamma^0. \tag{3.37}$$

With the appropriate normalisation, the solutions together with their adjoints will satisfy the normalisation conditions

$$\bar{u}^r(\mathbf{p})u^{r'}(\mathbf{p}) = 2m\delta_{rr'}, \quad \bar{v}^r(\mathbf{p})v^{r'}(\mathbf{p}) = -2m\delta_{rr'}, \quad \bar{v}^r(\mathbf{p})u^{r'}(\mathbf{p}) = \bar{u}^r(\mathbf{p})v^{r'}(\mathbf{p}) = 0, \tag{3.38a}$$

$$u^r(\mathbf{p})^\dagger u^{r'}(\mathbf{p}) = v^r(\mathbf{p})^\dagger v^{r'}(\mathbf{p}) = 2\varepsilon(\mathbf{p})\delta_{rr'}, \quad u^r(\mathbf{p})^\dagger v^{r'}(-\mathbf{p}) = v^r(-\mathbf{p})^\dagger u^{r'}(\mathbf{p}) = 0. \tag{3.38b}$$

Useful projection operators onto the positive and negative subspaces can be defined as (Peskin & Schroeder (1995), Ryder (1996))

$$P_+ = \sum_{r=+,-} u^r(\mathbf{p})\bar{u}^r(\mathbf{p}) = \gamma^\mu p_\mu + m, \qquad P_- = \sum_{r=+,-} v^r(\mathbf{p})\bar{v}^r(\mathbf{p}) = -\gamma^\mu p_\mu + m. \tag{3.39}$$

Quantisation

The fields ψ and $\bar{\psi}$ can be expanded in plane wave components as follows (Peskin & Schroeder (1995), Ryder (1996), Ticciati (2008))

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^3}\int d^3p\,\frac{1}{\sqrt{\varepsilon(\mathbf{p})}}\sum_{r=+,-}\left[a_r(\mathbf{p})u^r(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}} + b_r^*(\mathbf{p})v^r(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}}\right] \tag{3.40a}$$

$$\bar{\psi}(\mathbf{x}) = \frac{1}{(2\pi)^3}\int d^3p\,\frac{1}{\sqrt{\varepsilon(\mathbf{p})}}\sum_{r=+,-}\left[a_r^*(\mathbf{p})\bar{u}^r(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} + b_r(\mathbf{p})\bar{v}^r(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}\right]. \tag{3.40b}$$

In the quantised theory these fields along with the a_r and b_r are interpreted as operators. To quantise the theory we need to impose specific commutation or anti-commutation relations between the ψ^α and their conjugates, or between the a_r and b_r and their conjugates. To find suitable conjugate momenta we need a Lagrangian (density) whose equation of motion is the Dirac equation. The classical free Dirac Lagrangian density can be taken simply as

$$\mathscr{L}_D = \bar{\psi}(i\gamma^\mu \overset{\leftrightarrow}{\partial}_\mu - m)\psi \tag{3.41}$$

where in the classical setting the ψ are square-integrable $\mathbb{C}^4$-valued wavefunctions and it is understood that the derivative "acts in both directions" on the (classical) field ψ and its adjoint $\bar{\psi}$;

$$\psi_1 \overset{\leftrightarrow}{\partial}_\mu \psi_2 := \frac{1}{2}\left(\psi_1\partial_\mu\psi_2 - (\partial_\mu\psi_1)\psi_2\right). \tag{3.42}$$

According to 3.41 the momentum π conjugate to ψ is

$$\pi := \frac{\partial\mathscr{L}}{\partial\dot{\psi}} = i\psi^\dagger. \tag{3.43}$$

In order to get an energy operator $\mathscr{H} = \pi\dot{\psi} - \mathscr{L}$, which is bounded from below, we must impose anti-commutation relations between the a_r and b_r and their conjugates. We therefore demand that

$$\begin{aligned}\{a_r(\mathbf{p}), a_{r'}^\dagger(\mathbf{p}')\} = \{b_r(\mathbf{p}), b_{r'}^\dagger(\mathbf{p}')\} = (2\pi)^3\delta_{rr'}\delta(\mathbf{p}-\mathbf{p}'),\\ \{a_r(\mathbf{p}), a_{r'}(\mathbf{p}')\} = \{b_r(\mathbf{p}), b_{r'}(\mathbf{p}')\} = 0.\end{aligned} \tag{3.44}$$

We interpret the $a_r^\dagger(\mathbf{p})$ and $a_r(\mathbf{r})$ as creation and annihilation operators of electrons with momentum $\mathbf{p}$ and helicity labelled by r. The $b_r^\dagger(\mathbf{p})$ and $b_r(\mathbf{r})$ are creation and annihilation operators of *positrons*, the anti-particles of electrons. The Hilbert space $\mathcal{H}$ of the free Dirac field can therefore be taken as the tensor product of fermionic Fock spaces built out of $L^2(\mathbb{R}^3,\mathbb{C}^4)$; $\mathcal{H} = \mathcal{F}_F(L^2(\mathbb{R}^3,\mathbb{C}^4)) \otimes \mathcal{F}_F(L^2(\mathbb{R}^3,\mathbb{C}^4))$ (cf. A.3.6).[22] The field $\psi(\mathbf{x})$ at a

[22] The single particle space for both electrons and positrons is in fact a subspace of $L^2(\mathbb{R}^3,\mathbb{C}^4)$ on which h_D is self-adjoint.

specific point $\mathbf{x}$ is clearly a superposition of positron and electron terms. Using 3.39, 3.40 and 3.44, the fields ψ and $\psi^\dagger$ are found to satisfy (Ryder (1996))

$$\{\psi^\alpha(\mathbf{x}), \psi^\beta(\mathbf{x}')\} = \delta^{\alpha\beta}\delta(\mathbf{x}-\mathbf{x}'). \tag{3.45}$$

The conserved four-current operator such that $\partial_\mu j^\mu = 0$ is defined as

$$j^\mu = e : \bar{\psi}\gamma^\mu\psi := (\rho, \mathbf{j}), \qquad \rho := e : \psi^\dagger\psi :, \qquad \mathbf{j} := e : \psi^\dagger \boldsymbol{\alpha}\psi : \tag{3.46}$$

with e the elementary charge. The notation $: \cdot :$ indicates that normal-ordering of the creation and annihilation operators is to be carried out once the fields $\bar{\psi}$ and ψ have been multiplied out in terms of these operators. The four-current is related to the operator representing the total charge by

$$Q = -\int d^3x\,\rho = -\frac{e}{(2\pi)^3}\int d^3p \sum_r \left[a_r^\dagger(\mathbf{p})a_r(\mathbf{p}) - b_r^\dagger(\mathbf{p})b_r(\mathbf{p})\right]. \tag{3.47}$$

The Hamiltonian is found to be

$$H = \int d^3x\,\mathscr{H} = \int d^3x\,\psi^\dagger h_D \psi = \frac{1}{(2\pi)^3}\int d^3p\,\varepsilon(\mathbf{p}) \sum_r \left[a_r^\dagger(\mathbf{p})a_r(\mathbf{p}) + b_r^\dagger(\mathbf{p})b_r(\mathbf{p})\right], \tag{3.48}$$

and the total momentum operator is as one would expect, given by 3.48 with the energy $\varepsilon(\mathbf{p})$ replaced by $\mathbf{p}$ itself.

3.1.2 The Dirac field with an external Coulomb potential

A complete discussion of the Dirac equation in the presence of an external Coulomb potential would be too lengthy for me to give. I will review only the elements necessary to proceed with quantisation. The Dirac equation with an attractive single proton nucleus is

$$i\dot{\psi} = h_D'\psi, \qquad h_D' := -i\boldsymbol{\alpha}\cdot\nabla + \beta m + \frac{e^2}{|\mathbf{x}|}. \tag{3.49}$$

In this situation the spectrum of h_D' has a discrete component corresponding to bound states with energy between 0 and m. The energies within the continuous spectrum remain $\pm\varepsilon(\mathbf{p}) \equiv \pm\varepsilon(p) = \pm\sqrt{p^2+m^2}$. The eigenspinors of the Dirac operator h_D' are labelled by the quantum numbers $j = \frac{1}{2}, \frac{3}{2}, \ldots$, $m_j = -j, -j+1, \ldots, j-1, j$ and $\kappa_j = \pm(j+\frac{1}{2})$, which correspond to angular momentum operators commuting with h_D' (Thaller (1992)). It is convenient to collect these quantum numbers into a single label τ. As well as τ there is also the principal quantum number n labelling the bound states. One can divide the single particle space $L^2(\mathbb{R}^3, \mathbb{C}^4)$ into three components corresponding to the positive and negative, discrete and continuous spectrum of h_D', and one can find corresponding eigenspinors of h_D'

satisfying

$$h'_D u^\tau(\mathbf{x},p) = \varepsilon(p)u^\tau(\mathbf{x},p), \qquad h'_D v^\tau(\mathbf{x},p) = -\varepsilon(p)v^\tau(\mathbf{x},p), \qquad h'_D \psi^\tau_n(\mathbf{x}) = \omega_n \psi^\tau_n(\mathbf{x}) \tag{3.50}$$

together with the normalisation conditions

$$\begin{aligned} &\int d^3x\, u^\tau(\mathbf{x},p)^\dagger u^{\tau'}(\mathbf{x},p') = \int d^3x\, v^\tau(\mathbf{x},p)^\dagger v^{\tau'}(\mathbf{x},p') = \delta^{\tau\tau'}\delta(p-p'), \\ &\int d^3x\, \psi^\tau_n(\mathbf{x})^\dagger \psi^{\tau'}_{n'}(\mathbf{x}) = \delta_{nn'}\delta^{\tau\tau'} \end{aligned} \tag{3.51}$$

with the integrals of all other combinations of an adjoint spinor multiplied by a spinor being zero. With due care one can then build three separate Fock spaces over each of the three components of $L^2(\mathbb{R}^3,\mathbb{C}^4)$ (Dimassi & Guillot (2003)). The total Fock space for electrons and positrons including bound states is then the tensor product of these three. One can define three types of creation and annihilation operators corresponding to positrons, bound electrons and free electrons each satisfying canonical anti-commutation relations. Finally, one can expand the fields ψ and $\psi^\dagger$ satisfying the anti-commutation relation 3.45 in terms of the creation and annihilation operators. One can then define the conserved four current as in 3.46, along with the Hamiltonian, total momentum and total charge operators.

3.2 Non-covariant QED in an arbitrary gauge

Having reviewed the free Dirac field I now turn my attention to QED. First I will derive the QED Lagrangian and then look at how redundant gauge degrees of freedom can be eliminated at the quantum level. Finally, I will adapt the quantisation method of the last chapter in order to construct a formulation of the theory in an arbitrary gauge.

3.2.1 The QED Lagrangian

Following the procedure laid out in B.4.3, we can view the spinor wavefunctions ψ as sections of a trivial bundle $E^{1,3}\times\mathbb{C}^4$ equipped with a $U(1)$ right action. The associated transition maps $c_{UV}(x)$ between open regions $U,V\subset E^{1,3}$ are given by

$$c_{UV}(x) = e^{ie\lambda(x)}I, \tag{3.52}$$

where $\lambda : E^{1,3}\to\mathbb{R}$ and I denotes the 4×4 identity matrix. Since the transition maps are proportional to the identity one can simply write $c_{UV}(x) = e^{ie\lambda(x)}$. Requiring that the connection defined in B.4.5 be unique on an overlap $U\cap V$ gives rise to a connection one-form, which according to B.4.5, can in each region U be written

$$A^U = A^U_\mu(x)dx^\mu I \equiv A^U_\mu(x)dx^\mu \tag{3.53}$$

where again we can simply omit the identity. Furthermore, since on an overlap $U \cap V$ the connection one-form 3.53 obeys the transformation law B.129, we can interpret it as the gauge potential defined in 2.16. The so-called *gauge-covariant derivative* acting on the components of the Dirac spinors is given by B.126;

$$D_\mu^U \psi_U(x) := (\partial_\mu + ieA_\mu^U)\psi_U(x). \tag{3.54}$$

The QED Lagrangian density is obtained by adding to $\mathscr{L}_D$ in 3.41 the field Lagrangian density in 2.14, and replacing the ordinary four-derivative ∂_μ in 3.41 with the gauge covariant derivative in 3.54;[23]

$$\mathscr{L} = \bar{\psi}(i\gamma^\mu \overset{\leftrightarrow}{D}_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{3.55}$$

The Lagrangian density 3.55 yields as Euler-Lagrange equations Maxwell's equations containing the classical analog of the four-current 3.46, and the Dirac equation

$$(i\gamma^\mu D_\mu - m)\psi = 0, \tag{3.56}$$

which is the generalisation of the free Dirac equation, so that it includes electromagnetic interactions. Note that this equation is obtained if one simply replaces the normal derivative in 3.7 with the gauge-covariant derivative from 3.54. We obtain in this way an electromagnetic field for which any two potentials A and A' such that

$$A(x) := A^U(x), \qquad A'(x) := A^V(x) = A^U(x) + c_{UV}(x)^{-1}dc_{UV}(x) = A(x) + d\lambda(x), \tag{3.57}$$

are viewed as physically equivalent. This is necessary (and sufficient) to ensure *local phase invariance* of the Dirac equation. By local phase invariance I mean invariance under the replacement $\psi \to \psi'$ such that

$$\psi(x) := \psi_U(x) \to \psi_V(x) = c_{VU}(x)\psi_U(x) = e^{-ie\lambda(x)}\psi_U(x) =: \psi'(x), \tag{3.58}$$

which will only follow if the covariant derivative is used rather than the ordinary derivative.

3.2.2 Eliminating redundancies through symmetries

To quantise the interacting Dirac-Maxwell field theory we must try to construct an irreducible representation of the field operator algebras on the tensor product space $\mathcal{H}_D \otimes \mathcal{H}_M$, in which $\mathcal{H}_D$ is the Dirac field Hilbert space and $\mathcal{H}_M$ is the Maxwell field Hilbert space. To achieve this I will use a similar procedure to the one used in chapter 2, but instead of implementing the constraints at the classical level I will quantise the theory first and then

[23] I have omitted the label U from the covariant derivative and spinors in 3.55 in order to indicate that the gauge is not fixed in the Lagrangian. To fix the gauge would be to choose a specific set $\{\psi_U, A^U\}$ to work with.

implement the constraints to obtain the physical subspace of states. In order to do this I will fix the gauge, i.e., eliminate the redundant degrees of freedom, by using unitary transformations. This method of gauge fixing has been called *quantum-mechanical gauge-fixing* in the past (Lenz *et al.* (1994)). It bares a close resemblance to the method of *symplectic reduction* used in classical mechanics, which relies on the identification of symmetries. To see how the idea works I will go through the simple example of a two particle system (e.g. a hydrogen atom), which is assumed to have an initially stationary centre-of-mass. It is this stationary centre-of-mass *constraint*, that effectively halfs the number of physically relevent degrees of freedom.

I will denote the canonical variables of the first particle $\mathbf{r}_1, \mathbf{p}_1$ and those of the second $\mathbf{r}_2, \mathbf{p}_2$. I take the Hamiltonian for the system to be

$$H = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + V(|\mathbf{r}_1 - \mathbf{r}_2|). \tag{3.59}$$

In the classical theory the state space is $\mathbb{R}^{12}[\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}_1, \mathbf{p}_2] \cong T^*\mathbb{R}^6[\mathbf{r}_1, \mathbf{r}_2]$ (cf. B.9 and 1.1.3). It is equipped with the symplectic form $\omega = d\mathbf{p}_1 \wedge \cdot d\mathbf{r}_1 + d\mathbf{p}_2 \wedge \cdot d\mathbf{r}_2$ where $\mathbf{a} \wedge \cdot \mathbf{b} := a^i \wedge b_i$ (cf. B.2.1 and 1.21) and there is a natural action of the translation group on the position variables which reads

$$R_{\mathbf{a}}\mathbf{r}_i = \mathbf{r}_i + \mathbf{a}. \tag{3.60}$$

Moving to centre-of-mass/relative coordinates defined by

$$\mathbf{R} := \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \qquad \mathbf{P} := \mathbf{p}_1 + \mathbf{p}_2 \tag{3.61}$$

$$\mathbf{r} := \mathbf{r}_1 - \mathbf{r}_2, \qquad \mathbf{p} := \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{m_1 + m_2} \tag{3.62}$$

leaves the symplectic form invariant; $\omega = d\mathbf{P} \wedge \cdot d\mathbf{R} + d\mathbf{p} \wedge \cdot d\mathbf{r}$, which means the transformation is canonical. Moreover, the translation group only alters $\mathbf{R}$ without changing $\mathbf{r}$, and the Hamiltonian

$$H = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2m} + V(|\mathbf{r}|), \qquad M := m_1 + m_2, \qquad m := \frac{m_1 m_2}{m_1 + m_2} \tag{3.63}$$

is invariant under translations, because it doesn't depend on $\mathbf{R}$. The centre-of-mass momentum $\mathbf{P}$ is seen to be a symmetry of the Hamiltonian. Since by assumption the atom is initially stationary $\mathbf{P} = \mathbf{0}$, it remains stationary for all time. The dynamically invariant constraint $\mathbf{P} = \mathbf{0}$, therefore defines the physical subspace of classical states as those having zero components of centre-of-mass motion. Considering only the physical states amounts to ignoring $\mathbf{P}$ altogether, which gives for the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(|\mathbf{r}|). \tag{3.64}$$

We have therefore arrived at the reduced phase space $\mathbb{R}^6[\mathbf{r},\mathbf{p}]$ of a one particle system having half the dimension of the original space. The (reduced) symplectic form on this reduced phase space is simply $\omega = d\mathbf{p}\wedge\cdot d\mathbf{r}$. To summarise, we have identified the *physical subspace of states* by way of a constraint function $\mathbf{P}$, which is a symmetry of the Hamiltonian.[24]

On the quantum level the state space for the system is $L^2(\mathbb{R}^6,\mathbb{C}) \cong L^2(\mathbb{R}^3,\mathbb{C})\otimes L^2(\mathbb{R}^3,\mathbb{C})$ and the $\mathbf{r}_i,\mathbf{p}_i$ are canonical operators. We can *define* the physical subspace of states as the subspace consisting of states $|\psi\rangle$ which vanish under the action of the constraint $\mathbf{P}$;

$$(\mathbf{p}_1+\mathbf{p}_2)|\psi\rangle \equiv \mathbf{P}|\psi\rangle = 0. \tag{3.65}$$

Since $\mathbf{P}$ is a symmetry of H (now an operator, but still as in 3.59), the physical subspace is dynamically invariant. Moreover, the constraint $\mathbf{P}$ is the generator of translations by $\mathbf{R}$ under which H is invariant. The translation group here is the analog of the gauge group $U(1)$ in QED, and $\mathbf{P}$ is the analog of Gauss' law G. The unitary transformation

$$\Omega[\mathbf{a}] := e^{i\mathbf{P}\cdot\mathbf{a}} \tag{3.66}$$

generates translations, and we will see in 3.3 that this is analogous to the generator of gauge transformations in QED (c.f. 3.77);

$$\Omega[\lambda] := e^{-i\int d^3x G(x)\lambda(x)} \tag{3.67}$$

where G is the *Gauss law* operator constraint.

To eliminate the unphysical degrees of freedom we can do exactly what we did in the classical setting. We define the physical subspace $\mathcal{H}_p$ by $\mathbf{P}|\psi\rangle = 0\ \forall|\psi\rangle\in\mathcal{H}_p$ and obtain the Hamiltonian 3.64 on $\mathcal{H}_p$. To implement the elimination we can use the transformation (Lenz *et al.* (1994))

$$U := e^{-i\frac{m_1}{m_1+m_2}\mathbf{r}_1\mathbf{p}_2}e^{i\mathbf{r}_2\mathbf{p}_1}, \tag{3.68}$$

such that

$$U\mathbf{r}U^{-1} = \mathbf{r}_1, \quad U\mathbf{R}U^{-1} = \mathbf{r}_2, \quad U\mathbf{p}U^{-1} = \mathbf{p}_1, \quad U\mathbf{P}U^{-1} = \mathbf{p}_2. \tag{3.69}$$

With respect to the new representation of states $|\psi'\rangle = U|\psi\rangle$, the same operators now take on a different physical meaning. For example, with respect to the new representation the operator $\mathbf{r}_1$ has the same physical meaning as the operator $\mathbf{r}_1-\mathbf{r}_2$ had with respect to the original representation; $\mathbf{r}_1$ therefore denotes the *relative* position. Furthermore, we have

$$H = \frac{\mathbf{p}_2}{2M} + \frac{\mathbf{p}_1}{2m} + V(|\mathbf{r}_1|) \tag{3.70}$$

[24] Recall that as a classical *observable* $\mathbf{P}$ is viewed as a function on phase space defined by $\mathbf{P}(\mathbf{R},\mathbf{P},\mathbf{r},\mathbf{p}) := \mathbf{P}$.

which can be simplified further by noting that the physical states are subject to the constraint $0 = U(\mathbf{p}_1 + \mathbf{p}_2)U^{-1}U|\psi\rangle = \mathbf{p}_2|\psi'\rangle$. Thus, on the physical subspace $\mathcal{H}'_p = U\mathcal{H}_p$, 3.70 can be written

$$H = \frac{\mathbf{p}_1}{2m} + V(|\mathbf{r}_1|). \tag{3.71}$$

One can obtain from 3.71 the classical functional form 3.64 for the quantum Hamiltonian by simply relabelling the physical operators as follows $\mathbf{p}_1 \to \mathbf{p}$ and $\mathbf{r}_1 \to \mathbf{r}$. This notation reflects the *physical* observables that the operators in 3.71 represent with respect to the new representation of states. Of course, we could have gotten this reduced formulation by simply writing down the initial Hamiltonian 3.59 in the form 3.63, and by then identifying the physical subspace through $\mathbf{P}|\psi\rangle = 0$. What the transformation 3.69 gives us is the explicit relationship between the old and new representations of states.

3.3 Quantisation of the composite Dirac-Maxwell system

I turn my attention now to quantising the Dirac-Maxwell system. The new results presented here are summarised in the paper Stokes (2012). First I identify the states of the system as *Schrödinger wave functionals* and determine the general form of a physical state using the "coordinate" representation for the canonical operators of the Maxwell field and the Gauss law constraint. From there I identify a general unitary gauge fixing transformation U_g as a map from the physical space of states $\mathcal{H}_p$ to a space $\mathcal{H}_g$, which is the space of states for the gauge g. Next I determine the effect of this transformation on the various operators of the theory and express the Hamiltonian in the arbitrary gauge g. I conclude by using the Hamiltonian to calculate the Dirac equation in the gauge g.

3.3.1 The Weyl gauge Lagrangian and residual gauge symmetry

I start formally with the QED Lagrangian density 3.55 with an external Coulomb potential ϕ_e added;[25]

$$\mathscr{L} = i\psi^\dagger\gamma_0\gamma^\mu\overleftrightarrow{D}_\mu\psi - \psi^\dagger(\gamma_0 m + e\phi_e)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{3.72}$$

Since the Lagrangian is independent of the velocity of the scalar potential its conjugate momentum is identically zero. As a result it is natural to quantize the theory within the Weyl

[25] This Lagrangian (density) is clearly gauge-invariant and can therefore be considered the relativistic analog of 2.42. The reader may have been curious as to why in chapter 2 I went to the trouble of giving 2.42, but then proceeded to use the gauge dependent Lagrangian 2.33. The reason is that due to the constraint 2.44 the gauge-dependent and gauge-invariant Lagrangians of chapter 2 both yield the same results, because whenever the constraint is satisfied the two Lagrangians are identical. The quantisation procedure to be followed in this chapter is the relativistic analog of the quantisation procedure used in chapter 2 *in which one starts with the gauge-invariant Lagrangian 2.42* (this of course, is true with the proviso that this time I am going to implement the constraints at the quantum level rather than the classical level).

gauge corresponding to the choice $\phi := A_0 \equiv 0$.[26] The remaining redundant degrees of freedom are eliminated by defining the physical subspace of states $\mathcal{H}_p$ consisting of those states, which vanish under the action of the Gauss law constraint; $G|\varphi_p\rangle \equiv (\nabla\cdot\mathbf{E}-\rho)|\varphi_p\rangle = 0$. The Hamiltonian density is obtained from the Lagrangian density via a Legendre transformation;

$$\mathscr{H} = -i\psi^\dagger \boldsymbol{\alpha}\cdot(\nabla - ie\mathbf{A})\psi + \psi^\dagger(\beta m + e\phi_e)\psi + \frac{1}{2}\left(\boldsymbol{\Pi}^2 + (\nabla\times\mathbf{A})^2\right). \tag{3.73}$$

Quantum mechanically ψ and its conjugate $\psi^\dagger$ are Dirac field operators satisfying the anti-commutation relation 3.45, while $\mathbf{A}$ and $\boldsymbol{\Pi} = -\mathbf{E}$ are the canonical operators of the Maxwell field satisfying the commutation relation

$$[A_i(\mathbf{x}), \Pi_j(\mathbf{x}')] = i\delta_{ij}\delta(\mathbf{x}-\mathbf{x}'). \tag{3.74}$$

The polarization field $\mathbf{P}_g$ can be defined as in 2.37 and Gauss' law G can be written

$$G = \nabla\cdot\boldsymbol{\Pi} + \rho = \nabla\cdot(\boldsymbol{\Pi} - \mathbf{P}_g). \tag{3.75}$$

As an operator G is a symmetry of the Hamiltonian; $[G,H]=0$, and is responsible for generating time-independent gauge transformations of the vector potential and Dirac field operators. Identifying a group $(\{\lambda(\mathbf{x})\},+)$ consisting of real valued functions on $\mathbb{R}^3$ and group operation of addition, we define a group action Φ (cf. A.3.5) acting on the vector potential and Dirac fields by

$$\Phi[\psi,\lambda] = e^{-ie\lambda}\psi, \qquad \Phi[\mathbf{A},\lambda] = \mathbf{A} + \nabla\lambda. \tag{3.76}$$

A unitary representation of this action on the Hilbert space $\mathcal{H}$ is given by $\Omega\psi\Omega^{-1} = \Phi[\psi,\lambda]$ and $\Omega\mathbf{A}\Omega^{-1} = \Phi[\mathbf{A},\lambda]$ where

$$\Omega[\lambda] = \exp\left(-i\int \mathrm{d}^3x\,(\nabla\cdot\boldsymbol{\Pi}+\rho)\lambda(\mathbf{x})\right) = \exp\left(i\int \mathrm{d}^3x\,(\boldsymbol{\Pi}\cdot\nabla-\rho)\lambda(\mathbf{x})\right). \tag{3.77}$$

The second equality follows after an integration by parts has been performed and as usual use has been made of the fact that the fields vanish at infinity. These transformations are called *residual gauge transformations*, with the word residual intended to signify that the above time independent symmetry is what remains of the local gauge-symmetry (local phase-invariance) present in the original formulation Lenz *et al.* (1994).

[26] One could impose as an additional constraint $A_0|\psi\rangle = 0$ at the quantum level, but then the physical states would be completely independent of A_0, and the dynamics of A_0 would be permanently restricted to the non-physical subspace. As such we may as well get rid of A_0 at the beginning.

3.3.2 Unitary gauge fixing transformations

In order to determine the form of a general gauge fixing transformation we first need to identify the form of a physical state. To do this I take as a Hilbert space $\mathcal{H}$ for the composite system wave functionals $\varphi : FE^3 \to \mathbb{C}$ of the classical vector potential $\mathbf{A} \in FE^3$ (cf. 2.2.1). I denote the space of such wave-functionals $\mathscr{F}(FE^3)$. The inner-product required to make $\mathscr{F}(FE^3)$ a Hilbert space is defined in terms of functional integration (Jackiw (1995)). These wave functionals are supposed to take values in the Hilbert space $\mathcal{H}_D$ of the Dirac field operators, which can be taken as the usual Fock space for electrons and positrons as in 3.1.1. Alternatively one can use functionals to represent the states of the Dirac field as well. Regarding this I refer the reader to Jackiw (1995) and Hatfield (1998). The Hilbert space $\mathcal{H}$ of the composite system can be written $\mathscr{F}(FE^3, \mathcal{H}_D) \supset \mathscr{F}(FE^3) \otimes \mathcal{H}_D$.

A realization of the algebra of the Maxwell field operators $\mathbf{A}$ and $\mathbf{\Pi}$ is given on $\mathcal{H}$ using the "coordinate" representation

$$(\hat{\mathbf{A}}\varphi)[\mathbf{A}] = \mathbf{A}\varphi[\mathbf{A}], \qquad (\hat{\mathbf{\Pi}}\varphi)[\mathbf{A}] = -i\frac{\delta\varphi[\mathbf{A}]}{\delta\mathbf{A}} \tag{3.78}$$

where the functional derivative is defined in B.2.6, and I have introduced hats to distinguish between operators and classical vector fields. Defining a scalar function α by $\nabla\alpha = \mathbf{A}_{\mathrm{L}}$, we can vary the wave functional φ with respect to α and make use of 3.78 to obtain (cf. B.2.1)

$$i\frac{\delta\varphi}{\delta\alpha} = -i\nabla\cdot\frac{\delta\varphi}{\delta\nabla\alpha} = -i\nabla\cdot\frac{\delta\varphi}{\delta\mathbf{A}_{\mathrm{L}}} = \nabla\cdot\hat{\mathbf{\Pi}}_{\mathrm{L}}\varphi = \nabla\cdot\hat{\mathbf{\Pi}}\varphi. \tag{3.79}$$

Using the constraint G in 7.38 we get for a physical state φ_p

$$i\frac{\delta\varphi_p}{\delta\alpha} = -\rho\varphi_p \tag{3.80}$$

and finally solving this equation gives the general form of a physical state;

$$\varphi_p[\mathbf{A}] = \varphi_p[\mathbf{A}_{\mathrm{T}} + \nabla\alpha] = \exp\left(i\int \mathrm{d}^3x\,\alpha(\mathbf{x})\rho(\mathbf{x})\right)\varphi_p[\mathbf{A}_{\mathrm{T}}]. \tag{3.81}$$

It is easy to verify using B.49b for the functional differentiation of a function of a functional, that 3.81 is indeed a solution of 3.80. We can now begin to define some unitary gauge fixing transformations. In the original work of Lenz *et al.* (1994) a unitary gauge fixing transformation yielding the Coulomb gauge representation was given as

$$U \equiv \exp\left(-i\int \mathrm{d}^3x\,\hat{\alpha}(\mathbf{x})\rho(\mathbf{x})\right) \tag{3.82}$$

where $\hat{\alpha}$ is defined analogously to α by $\nabla\hat{\alpha} = \hat{\mathbf{A}}_{\mathrm{L}}$. In the present context we see clearly that

U eliminates the dependence of the physical state on $\mathbf{A}_{\mathrm{L}}$;

$$(U\varphi_p)[\mathbf{A}] = \varphi_p[\mathbf{A}_{\mathrm{T}}]\,. \tag{3.83}$$

Since the transverse vector potential is gauge-invariant we can use it as a coordinate with respect to which any other vector potential can be specified. We therefore write the longitudinal vector potential as the gradient of a functional of the transverse vector potential as in 2.45;

$$\mathbf{A}_{\mathrm{L}} = \nabla\chi_g(\mathbf{x},[\mathbf{A}_{\mathrm{T}}]) \tag{3.84}$$

where we could for example put

$$\chi_g(\mathbf{x},[\mathbf{A}_{\mathrm{T}}]) = \int \mathrm{d}^3x'\mathbf{g}(\mathbf{x}',\mathbf{x})\cdot\mathbf{A}_{\mathrm{T}}(\mathbf{x}') \tag{3.85}$$

as in 2.45. We can then define a more general unitary gauge fixing transformation U_g by

$$U_g := \exp\left(-i\int \mathrm{d}^3x\left(\hat{\alpha}(\mathbf{x})-\chi_g(\mathbf{x},[\hat{\mathbf{A}}_{\mathrm{T}}])\right)\rho(\mathbf{x})\right), \tag{3.86}$$

mapping from $\mathcal{H}_p$ to an isomorphic space denoted $\mathcal{H}_g$, which is the space of states for the gauge g;

$$(U_g\varphi_p)[\mathbf{A}] = \exp\left(i\int \mathrm{d}^3x\,\chi_g(\mathbf{x},[\mathbf{A}_{\mathrm{T}}])\rho(\mathbf{x})\right)\varphi_p[\mathbf{A}_{\mathrm{T}}] = \varphi_p[\mathbf{A}_{\mathrm{T}}+\nabla\chi_g] =: \varphi_g[\mathbf{A}_{\mathrm{T}}]\in\mathcal{H}_g. \tag{3.87}$$

The vector potential operator in the gauge g is $\hat{\mathbf{A}}_g(\mathbf{x}) := \hat{\mathbf{A}}_{\mathrm{T}}(\mathbf{x})+\nabla\chi_g(\mathbf{x},[\hat{\mathbf{A}}_{\mathrm{T}}])$ with action on $\mathcal{H}_g$ given by

$$(\hat{\mathbf{A}}_g\varphi_g)[\mathbf{A}_{\mathrm{T}}] = (\mathbf{A}_{\mathrm{T}}+\nabla\chi_g)\varphi_g[\mathbf{A}_{\mathrm{T}}]. \tag{3.88}$$

Finally, we can define a Unitary transformation from a fixed gauge g to a fixed gauge g' by

$$U_{gg'} := \exp\left(-i\int \mathrm{d}^3x\left(\chi_g(\mathbf{x},[\hat{\mathbf{A}}_{\mathrm{T}}])-\chi_{g'}(\mathbf{x},[\hat{\mathbf{A}}_{\mathrm{T}}])\right)\rho(\mathbf{x})\right) \tag{3.89}$$

an example of which is the well known Power-Zienau-Woolley transformation (cf. 6.14). Such a gauge transformation is not to be confused with the residual gauge (symmetry) transformation given in 3.77.

3.3.3 *The Hamiltonian in the gauge g*

To obtain the Hamiltonian in the gauge g we need to determine the effect of the transformation in 3.86 on the various operators of the theory, namely ψ, $\psi^\dagger$, $\mathbf{A}$ and $\mathbf{\Pi}$. In doing

so we will resume denoting operators without hats. Clearly U_g leaves the vector potential $\mathbf{A}$ unchanged, while the action of $\mathbf{A}$ on $\mathcal{H}_g$ is given in 3.88. To determine the effect of U_g on the remaining operators I use the Baker-Campbell-Hausdorff formula A.17. With this useful formula the effect of U_g on the Dirac field operator ψ is found using 3.45 to be

$$U_g\psi(\mathbf{x})U_g^{-1} = \psi(\mathbf{x}) + ie\left[\alpha(\mathbf{x}) - \chi_g(\mathbf{x})\right]\psi(\mathbf{x}) - \frac{e^2}{2}\left[\alpha(\mathbf{x}) - \chi_g(\mathbf{x})\right]^2\psi(\mathbf{x}) + \ldots \tag{3.90}$$

and summing up all terms in 3.90 gives

$$U_g\psi U_g^{-1} = e^{ie(\alpha-\chi_g)}\psi =: \psi_g, \tag{3.91}$$

which is clearly just a gauge transformation. To find the transformed field canonical momentum it is convenient to express U_g in terms of the polarisation field $\mathbf{P}_g$, which can be achieved by noting that

$$\alpha(\mathbf{x}) = -\frac{1}{4\pi}\int d^3x' \frac{\nabla'\cdot\mathbf{A}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} = -\int d^3x' \mathbf{g}_{\mathrm{L}}(\mathbf{x}',\mathbf{x})\cdot\mathbf{A}(\mathbf{x}'). \tag{3.92}$$

Together with 3.85 this gives

$$U_g = \exp\left(i\int d^3x \int d^3x'\,\rho(\mathbf{x}')\mathbf{g}(\mathbf{x},\mathbf{x}')\cdot\mathbf{A}(\mathbf{x})\right) = \exp\left(-i\int d^3x\,\mathbf{P}_g(\mathbf{x})\cdot\mathbf{A}(\mathbf{x})\right). \tag{3.93}$$

Using this expression along with A.17 and 3.74 one obtains

$$U_g\mathbf{\Pi}U_g^{-1} = \mathbf{\Pi} + \mathbf{P}_g. \tag{3.94}$$

Thus, in the new representation $\mathbf{\Pi}$ represents the (negative of) the gauge dependent displacement operator $\mathbf{D}_g \equiv \mathbf{E} + \mathbf{P}_g$. Using 2.37 it's easy to work out how the constraint G and the residual gauge transformation Ω transform;

$$U_g G U_g^{-1} = \nabla\cdot\mathbf{\Pi}, \qquad U_g\Omega[\lambda]U_g^{-1} = \exp\left(i\int \mathrm{d}^3x\,(\mathbf{\Pi}\cdot\nabla)\lambda(\mathbf{x})\right), \tag{3.95}$$

which are both independent of the gauge g. The constraint G implies that the longitudinal canonical momentum $\mathbf{\Pi}_{\mathrm{L}}$ vanishes on $\mathcal{H}_g$. On the one hand this means $\mathbf{P}_{\mathrm{L}}$ alone represents (the negative of) the longitudinal electric field, and on the other that the Hamiltonian density on $\mathcal{H}_g$ can be written in terms of the transverse operators $\mathbf{A}_{\mathrm{T}}$ and $\mathbf{\Pi}_{\mathrm{T}}$ only;

$$\mathscr{H} = -i\psi_g^\dagger\boldsymbol{\alpha}\cdot(\nabla - ie\mathbf{A}_g)\psi_g + \psi_g^\dagger(\beta m + e\phi_e)\psi_g + \frac{1}{2}{\mathbf{P}_{\mathrm{L}}}^2 + \frac{1}{2}\left[(\mathbf{\Pi}_{\mathrm{T}} + \mathbf{P}_{\mathrm{T}}^g)^2 + (\nabla\times\mathbf{A}_{\mathrm{T}})^2\right] \tag{3.96}$$

where $\mathbf{A}_g$ is the vector potential in the gauge g (given in 3.88), and ψ_g is the Dirac field operator in the gauge g (given in 3.91). In writing 3.96 I have neglected the cross term

$2\mathbf{P}_{\mathrm{L}} \cdot \mathbf{P}_{\mathrm{T}}^{g}$ obtained by expanding $\mathbf{P}_{g}^{2}$. This is because for suitably well-behaved transverse and longitudinal vector fields $\mathbf{W}_{\mathrm{T}}$ and $\mathbf{V}_{\mathrm{L}}$ one can show that

$$\int d^3x \mathbf{W}_{\mathrm{T}}(\mathbf{x}) \cdot \mathbf{V}_{\mathrm{L}}(\mathbf{x}) = 0. \tag{3.97}$$

Equation 3.96 gives a Hamiltonian in an arbitrary gauge, which is fully relativistic in the material degrees of freedom. It can also be written (cf. 2.61)

$$\begin{aligned}
&\mathscr{H} = \mathscr{H}_M + \mathscr{V}_{\mathrm{self}} + \mathscr{H}_{\mathrm{TF}} = \mathscr{H}_M + \mathscr{H}_{\mathrm{EM}}, \\
&\mathscr{H}_M := -i\psi_g^\dagger \boldsymbol{\alpha} \cdot (\nabla - ie\mathbf{A}_g)\psi_g + \psi_g^\dagger(\beta m + e\phi_e)\psi_g, \\
&\mathscr{H}_{\mathrm{TF}} := \frac{1}{2}\left[(\boldsymbol{\Pi}_{\mathrm{T}} + \mathbf{P}_{\mathrm{T}}^{g})^2 + (\nabla \times \mathbf{A}_{\mathrm{T}})^2\right] = \frac{1}{2}\left[\mathbf{E}_{\mathrm{T}}^2 + \mathbf{B}^2\right], \\
&\mathscr{H}_{\mathrm{EM}} := \frac{1}{2}\left[(\boldsymbol{\Pi} + \mathbf{P}_g)^2 + (\nabla \times \mathbf{A}_{\mathrm{T}})^2\right] = \frac{1}{2}\left[\mathbf{E}^2 + \mathbf{B}^2\right],
\end{aligned} \tag{3.98}$$

with $V_{\mathrm{self}} = \int d^3x \mathscr{V}_{\mathrm{self}}$ given in 2.58. This gives a partition of $\mathscr{H}$ in which the total energy density is seen to be the sum of individually *gauge-invariant* material and electromagnetic energy densities. As in 2.61, the electromagnetic energy density is itself a sum of transverse and longitudinal components.

The commutator of the transverse operators follows from 3.74 and is given by

$$[\mathrm{A}_{\mathrm{T}}^{i}(\mathbf{x}), \Pi_{\mathrm{T}}^{j}(\mathbf{x}')] = \delta_{ij}^{T}(\mathbf{x} - \mathbf{x}'). \tag{3.99}$$

Note also that denoting the Fourier transforms of $\mathbf{A}_{\mathrm{T}}$ and $\boldsymbol{\Pi}_{\mathrm{T}}$ with tildes we can define photon creation and annihilation operators in the usual way;

$$a_\lambda(\mathbf{k}) = \sqrt{\frac{1}{2\omega}}\left(\omega\tilde{A}_{\mathrm{T},\lambda}(\mathbf{k}) + i\tilde{\Pi}_{\mathrm{T},\lambda}(\mathbf{k})\right) \tag{3.100}$$

where $\lambda = 1,2$ denotes one of two polarization directions orthogonal to $\mathbf{k}$. The bosonic commutator

$$[a_\lambda(\mathbf{k}), a_{\lambda'}^\dagger(\mathbf{k}')] = \delta_{\lambda\lambda'}(\mathbf{k} - \mathbf{k}') \tag{3.101}$$

follows from 3.99.

3.3.4 The Dirac equation in the gauge g

It is an instructive exercise to calculate in the arbitrary gauge g, the equation of motion for the Dirac field operator ψ, which should be the Dirac equation in the presence of a Maxwell field. The calculation demonstrates how the scalar potential, like the longitudinal vector potential is re-expressed through the functional χ_g. The top line of the Hamiltonian density in 3.96 gives rise to the following Weyl gauge ($A_0 \equiv 0$) Dirac equation with an external

potential ϕ_e;

$$i\partial_t \psi_g = [-i\boldsymbol{\alpha}\cdot(\nabla - ie\mathbf{A}_g) + \beta m + e\phi_e]\,\psi_g \qquad \Leftrightarrow \qquad i(\gamma^\mu D_\mu - m)\psi = 0 \tag{3.102}$$

where $D_\mu := (\partial_t + ie\phi_e, \partial_i - ieA^i_g)$. The complete Dirac equation contains a scalar potential term coming from the second line in 3.96. Explicitly, one obtains with a little work

$$[\psi_g(\mathbf{x}), H] = \left[\frac{e}{4\pi}\int \mathrm{d}^3x'\,\frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} - e\int \mathrm{d}^3x'\,\mathbf{g}_{\mathrm{T}}(\mathbf{x},\mathbf{x}')\cdot\left(\boldsymbol{\Pi}_{\mathrm{T}} + \mathbf{P}^{\mathrm{T}}_g\right)\right]\psi_g(\mathbf{x}). \tag{3.103}$$

The first term in brackets is equal to eV with V denoting the static Coulomb potential of charges; this term arises from the $\mathscr{V}_{\mathrm{self}}$ term in 3.98. The second term arises from the transverse term $\mathscr{H}_{\mathrm{TF}}$ in 3.98, and evidently involves the transverse electric field $\mathbf{E}_{\mathrm{T}} = -(\boldsymbol{\Pi}_{\mathrm{T}} + \mathbf{P}^{\mathrm{T}}_g)$. Furthermore, it is straightforward to verify that

$$\dot{\mathbf{A}}_{\mathrm{T}}(\mathbf{x}) = -i[\mathbf{A}_{\mathrm{T}}(\mathbf{x}), H] = \boldsymbol{\Pi}_{\mathrm{T}}(\mathbf{x}) + \mathbf{P}^{\mathrm{T}}_g(\mathbf{x}) = -\mathbf{E}_{\mathrm{T}}(\mathbf{x}) \tag{3.104}$$

implying that 3.103 can be written in the form

$$i\dot{\psi}_g = [\boldsymbol{\alpha}\cdot(-i\nabla - e\mathbf{A}_g) + \beta m + e(\phi_e + \phi_g)]\,\psi_g \qquad \Leftrightarrow \qquad (i\gamma^\mu D_\mu - m)\psi_g = 0 \tag{3.105}$$

where $D_\mu := (\partial_t + ie[\phi_g + \phi_e], \partial_i - ieA^i_g)$ and where I have defined the scalar potential anew by

$$\phi_g := V - \frac{\partial \chi_g}{\partial t}. \tag{3.106}$$

This is the scalar (Coulomb) potential V of the Coulomb gauge transformed by the gauge function χ_g as it should be. Moreover, the Dirac equation 3.105 is clearly invariant under a gauge transformation, that is, under the three simultaneous transformations

$$\begin{aligned}
&\psi_g \to \psi_{g'} = U_{gg'}\psi_g U^{-1}_{gg'} = e^{-ie(\chi_g - \chi_{g'})}\psi_g = e^{ie(\alpha - \chi_{g'})}\psi,\\
&\phi_g \to \phi_{g'} = \phi_g + \frac{\partial(\chi_g - \chi_{g'})}{\partial t} = V - \frac{\partial \chi_{g'}}{\partial t},\\
&\mathbf{A}_g \to \mathbf{A}_{g'} = \mathbf{A}_g - \nabla(\chi_g - \chi_{g'}) = \mathbf{A}_{\mathrm{T}} + \nabla\chi_{g'}.
\end{aligned} \tag{3.107}$$

3.4 Summary and discussion

In this chapter I have given a formulation of QED in an arbitrary non-covariant gauge. It would seem that the comments made in 2.4 apply to the results of this chapter too. The decomposition of the Dirac-Maxwell system into quantum subsystems is non-unique and gauge dependent.

Having now derived both relativistic and nonrelativistic quantum-electrodynamic theories, I am still yet to discuss any real physics. In the next part I attempt to determine what

we can say about the physical content of quantum electrodynamics, starting with Maxwell's equations and the Lorentz force law, and ending with quantum mechanical photons and atoms.

PART II

The classical and quantum theories of radiation

CHAPTER 4

Classical radiation theory

In this chapter I attempt to understand the dynamics of the composite charge-electromagnetic system, using Maxwell's equations and the Lorentz force law. The motivation for doing this is to precisely pin down, at least for the system of a free classical charge, how material and electromagnetic subsystems are to be defined, and in particular, what is to be regarded as radiation. Even in the classical setting this task is fraught with difficulty. The theory predicts that a point charge exhibits a self force due to its own electromagnetic fields, and this self force gives rise to highly unphysical effects. Despite several attempts historically to develop a consistent classical theory of point charges, it seems that the only solution is to give up on the idea of a point charge altogether, and consider even a single charge as an *extended charge distribution*.

On a practical level the situation is perhaps not all that bad. The problems only arise when one attempts to solve the coupled system consisting of both Maxwell's equations *and* the Lorentz force law. On the other hand, solving Maxwell's equations for *given* source distributions yields extremely fruitful results. Likewise solving the Lorentz force law for a point charge within given electromagnetic fields, (which themselves may be due to some *other* given sources) is also possible. In this sense, it seems the electromagnetic effects of charges on *other* charges make relatively good sense. It is understanding the effect of a charge on itself, which is problematic. On the face of it this problem seems quite relevant to the present discussion regarding material and electromagnetic subsystems. The question being, how to separate out the bare charge from its own electromagnetic fields, which act back on it?

The first thing I do in this section is look at Maxwell's equations alone (4.1). After that I review one of their physical implications; a result known as *Poynting's theorem* (4.2). Finally I consider the full set of coupled equations including the Lorentz force law (4.4).

4.1 Maxwell's equations

$$\dot{\mathbf{B}} = -\nabla \times \mathbf{E}, \tag{4.1a}$$

$$\dot{\mathbf{E}} = \nabla \times \mathbf{B} - \mathbf{J}, \tag{4.1b}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{4.1c}$$

$$\nabla \cdot \mathbf{E} = \rho. \tag{4.1d}$$

The first two equations describe dynamics, while the second two are merely constraints. With a little rearranging, the dynamical equations can be written

$$\Box \mathbf{E} = -\nabla \rho - \dot{\mathbf{J}}, \qquad \Box \mathbf{B} = \nabla \times \mathbf{J}, \tag{4.2}$$

which are inhomogeneous wave equations with source terms that are functions of the charge and current densities and their derivatives. Methods of finding general solutions to these equations invariably involve the Green's function G for the wave operator $\Box$, which is defined by

$$\Box \mathrm{G}(t-t';\mathbf{x}-\mathbf{x}') = \delta(t-t')\delta(\mathbf{x}-\mathbf{x}'). \tag{4.3}$$

This equation has the solution

$$\mathrm{G} = \mathrm{G}^+ + \mathrm{G}^-, \qquad \mathrm{G}^\pm := \pm \frac{\delta(t'-t_\mp)}{4\pi R} \tag{4.4}$$

where

$$R := |\mathbf{x}-\mathbf{x}'|, \qquad t_- := t_r := t-R, \qquad t_+ := t_a := t+R. \tag{4.5}$$

The times t_r and t_a are called the *retarded* and the *advanced* times respectively, and the corresponding Green's functions G^+ and G^- are called the retarded and advanced Green's functions. One also frequently encounters the Fourier transform denoted G, which satisfies

$$\mathrm{G}(t,\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d^3k\, G(t,\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}, \qquad G(t,\mathbf{k}) := \frac{\sin(\omega t)}{\omega} \tag{4.6}$$

where $\omega := |\mathbf{k}|$. In terms of G, the inhomogeneous wave equation

$$\Box \psi(t,\mathbf{x}) = s(t,\mathbf{x}) \tag{4.7}$$

admits the general solution

$$\psi = \psi^+ + \psi^-, \qquad \psi^\pm := \int dt' \int d^3x'\, \mathrm{G}^\pm(t-t',\mathbf{x}-\mathbf{x}') s(t,\mathbf{x}'). \tag{4.8}$$

Jackson (1998) gives a clear interpretation of the solution 4.8 in the general context. Suppose that in the remote past there is an incoming wave ψ_0, and then the source s is activated. In this case the solution of the wave equation at time t depends only on the retarded Green's function G^+;

$$\psi(t) = \psi_0(t) + \psi^+(t). \tag{4.9}$$

The other situation is that in which their is a known outgoing wave ψ^0 in the remote future, in which case $\psi(t) = \psi^0(t) + \psi^-(t)$. I will deal only with the former situation. Applying these ideas directly to the wave equations 4.2 one obtains the retarded solutions

$$\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_r, \qquad \mathbf{B} = \mathbf{B}_0 + \mathbf{B}_r \tag{4.10}$$

where $\mathbf{E}_0$ and $\mathbf{B}_0$ are the initial homogeneous fields propagated up to time t and $\mathbf{E}_r$ and $\mathbf{B}_r$ are retarded source fields, given by

$$\mathbf{E}_r(t,\mathbf{x}) := -\int d^3x' \, \frac{[\nabla'\rho + \dot{\mathbf{J}}]_r}{4\pi R}, \qquad \mathbf{B}_r(t,\mathbf{x}) := -\int d^3x' \, \frac{[\nabla' \times \mathbf{J}]_r}{4\pi R}. \tag{4.11}$$

The notation $[\cdot]_r$ means that the quantity inside the brackets is to be evaluated at the retarded time t_r. These solutions show that the electric and magnetic fields produced by charged sources propagate outwards causally. The same is true of the scalar and vector potentials in the Lorentz gauge for which the four-potential satisfies $\partial_\mu A^\mu = 0$. In this gauge the potentials admit the simple solutions

$$\phi_r := \int d^3x' \, \frac{[\rho]_r}{4\pi R}, \qquad \mathbf{A}_r := \int d^3x' \, \frac{[\mathbf{J}]_r}{4\pi R} \tag{4.12}$$

from which it is often easier to obtain results. It is worth pointing out that the transverse electric field and transverse vector potential are not retarded. The transverse vector potential satisfies the wave equation for which the source term is the nonlocal transverse current $\mathbf{J}_\mathrm{T}$ defined by

$$J_{\mathrm{T},i}(t,\mathbf{x}) := \int d^3x' \, \delta^\mathrm{T}_{ij}(\mathbf{R}) J_j(t,\mathbf{x}') \equiv \frac{2}{3} J_i(t,\mathbf{x}) - \int d^3x' \, \frac{1}{4\pi R} \left(\delta_{ij} - 3\hat{R}_i\hat{R}_j\right) J_j(t,\mathbf{x}'). \tag{4.13}$$

The transverse current at $(t,\mathbf{x})$, receives contributions from all other points $\mathbf{x}'$ at the *same* time t. Since $\mathbf{E}_\mathrm{T} = -\dot{\mathbf{A}}_\mathrm{T}$ the transverse electric field like the transverse vector potential can't be a retarded field either. One can deduce this immediately from the fact that $\mathbf{E}_\mathrm{L} = -\nabla V$ is instantaneous, while the total field $\mathbf{E} = \mathbf{E}_\mathrm{T} + \mathbf{E}_\mathrm{L}$ is retarded.

For a point charge $-e$ with position $\mathbf{r}(t)$ it is useful to define the quantities $\mathbf{R} := \mathbf{x} - \mathbf{r}$ and $\mathbf{v} := \hat{\mathbf{R}} - \dot{\mathbf{r}}$, where I have used a hat to specify the unit vector in the direction of $\mathbf{R}$. Using 2.40 the expressions in 4.11 can then be written (Jackson (1998), Griffiths (1999),

Spohn (2007))

$$\mathbf{E}_r = \left[\frac{R}{4\pi(\mathbf{R}\cdot\mathbf{v})^3}\{(1-\dot{\mathbf{r}})\mathbf{v}+\mathbf{R}\times(\mathbf{v}\times\dot{\mathbf{v}})\}\right]_r, \qquad \mathbf{B}_r = [\mathbf{R}\times\mathbf{E}_r]_r \tag{4.14}$$

with the retarded time t_r now defined as the unique solution of the equation

$$t_r = t - |\mathbf{x}-\mathbf{r}(t_r)|. \tag{4.15}$$

The expression for the electric field in 4.14 consists of two components, which are added together inside the curly braces. The first term involves the position and velocity of the charge only, and falls off away from the charge with a $1/R^2$ dependence. In fact, if the velocity and acceleration of the charge are both zero, the position dependent component of this term gives the only contribution to the electric field, which is nothing but the electrostatic (longitudinal) field of the single charge, corrected such that retardation is present;

$$\mathbf{E}_{\text{static}} = \left[\frac{-e\hat{\mathbf{R}}}{4\pi R^2}\right]_r. \tag{4.16}$$

The first term, dependent on the position and velocity of the charge, can be thought of as the electric field which is tied to the charge as it moves. There is of course a corresponding magnetic field tied to the particle, which is simply obtained by taking the cross product of $\mathbf{R}$ with the corresponding electric field tied to the particle.

The second contribution to the electric field in 4.14 depends on the acceleration of the charge and falls of with a $1/R$ dependence. It is this term which survives at large distances away from the charge. Along with its magnetic counterpart this term gives the only contribution to the power radiated by the charge which survives as $R\to\infty$.[27] The acceleration dependent contributions therefore constitute the electric and magnetic *radiation* fields of the charge, and are given explicitly by

$$\mathbf{E}_{\text{rad}} = \left[\frac{R}{4\pi(\mathbf{R}\cdot\mathbf{v})^3}\mathbf{R}\times(\mathbf{v}\times\dot{\mathbf{v}})\right]_r, \qquad \mathbf{B}_{\text{rad}} = [\mathbf{R}\times\mathbf{E}_{\text{rad}}]_r. \tag{4.17}$$

There a number of other ways to obtain solutions to Maxwell's equations as well as the method used above. One can, for example, express the Green's function G associated with the wave operator $\Box$ in covariant form; $\Box G(x-x') = \delta^{(4)}(x-x')$, and find the solution to the dynamical inhomogenous Maxwell equation for the components A_μ of the four-potential directly (Jackson (1998)). This yields the solutions 4.12 directly. One can also use *geometric algebra* (also variously known as *Clifford algebra*, *Kähler-Atiyah algebra* and other permutations of these names), which I do not touch upon in this thesis. The interested reader is referred to Hestenes & Sobczyk (1984), Jancewicz (1988), Hestenes (1998), Doran (2007) and Arthur (2012). Geometric algebra allows one to write all of Maxwell's equations as

[27] I will postpone giving the precise definition of the radiated power until the next section.

a single differential equation involving F. Moreover the geometric differential operator appearing in this equation is invertible, which allows one to use the method of Green's functions to solve for the field tensor F directly. The method of solution I have opted for in this chapter is the more conventional.

So it seems one can fairly successfully work out how the electric and magnetic fields produced by a moving point charge behave. Implicitly within this sort of exposition one assumes that the material subsystem is defined in terms of the motional degrees of freedom $\mathbf{r}$ and $\dot{\mathbf{r}}$, or more generally ρ and $\mathbf{J}$. The main subject of the following section, will be the behavior of the energies of the material and electromagnetic subsystems, having made this same assumption.

4.2 Poynting's theorem

Noether's theorem reveals a deep connection between symmetries and conservation laws. Indeed, the paradigmatic example is afforded by the theory of electromagnetism, in which local conservation of charge results from global gauge symmetry. There are numerous other conserved quantities of interest. The energy represented by the Hamiltonian is conserved, due to the system's invariance under temporal translations. The total angular momentum is conserved, because the system is invariant under rotations. The total linear momentum is conserved, because the system is invariant under spatial translations. One can verify that all of these quantities are conserved by checking that their Dirac brackets with the Hamiltonian vanish.

A description of Noether's theorem can be found in numerous quantum field theory and mathematical physics textbooks (a few that I know of are Bjorken & Drell (1965), Peskin & Schroeder (1995), Weinberg (1995), Ryder (1996), Hassani (1999), Ticciati (2008), Mandl & Shaw (2010), Fecko (2011)), so I will discuss it only briefly.

Given a Lagrangian density $\mathscr{L}$ dependent on a set of fields $\{\phi_k \in FE^{1,3}\}$ and their derivatives, we expect $\mathscr{L}$ to be invariant under space-time translations and Lorentz transformations.[28] The combined group of such transformations is called the *Poincaré group*.[29]

[28] Anti-symmetry of $\varepsilon^{\mu\nu}$ follows from the properties of the Lorentz transformation.

[29] The Poincaré group is therefore the group of *pseudo-orthogonal affine transformations* $OA(1,3)$ consisting of elements (Λ, a) such that $(\Lambda, a)x = \lambda x + a$ and $\Lambda \in O(1,3)$. It can be thought of as a subgroup of $GL(5,\mathbb{R})$ with

$$\begin{pmatrix} x' \\ 1 \end{pmatrix} = \begin{pmatrix} \Lambda & a \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ 1 \end{pmatrix} = \begin{pmatrix} \Lambda x + a \\ 1 \end{pmatrix}. \tag{4.18}$$

The Lie algebra $oa(1,3)$ has as generators the generators of the Lorentz group $\ell^{\alpha\beta}$ given in 3.15, and the generators of translations P^α, which can be represented by 5×5 matrices and are such that

$$[P^\alpha, P^\beta] = 0, \qquad [\ell^{\alpha\beta}, P^\gamma] = i(P^\beta \eta^{\alpha\gamma} - P^\alpha \eta^{\beta\gamma}). \tag{4.19}$$

A general infinitesimal Poincaré transformation can be written

$$x'^{\mu} = x^{\mu} + \varepsilon^{\mu\nu} x_{\nu} + \varepsilon^{\mu} \tag{4.20}$$

where $\varepsilon^{\mu\nu} = -\varepsilon^{\nu\mu}$ is the first term in the Taylor expansion of a Lorentz transformation and ε^{μ} is an infinitesimal translation. The above transformation leads to concurrent transformations in the fields $\phi'_k = \phi_k + \delta\phi_k$ and the Lagrangian density $\mathscr{L}' = \mathscr{L} + \delta\mathscr{L}$. Requiring that $\mathscr{L}' = \mathscr{L}$ then yields various conservation laws for fields that satisfy the Euler-Lagrange equations. For example, under pure translations ($\varepsilon^{\mu\nu} = 0$) we obtain

$$\partial_{\alpha} T^{\alpha\beta} = 0 \tag{4.21}$$

where

$$T^{\alpha\beta} := \frac{\partial \mathscr{L}}{\partial(\partial_{\mu}\phi_k)} \partial^{\beta}\phi_k - \eta^{\alpha\beta}\mathscr{L} \tag{4.22}$$

are the components of *the canonical energy-momentum density tensor* T. Since the fields vanish at infinity 4.21 implies the continuity equation

$$0 = \int d^3x \, \partial_{\alpha} T^{\alpha\beta} = \partial_0 \int d^3x T^{0\beta}. \tag{4.23}$$

In the case of free electromagnetism using 2.14 we have

$$T^{\alpha\beta} = \frac{1}{4}\eta^{\alpha\beta} F_{\mu\nu}F^{\mu\nu} - \eta^{\alpha\mu} F_{\mu\nu}\partial^{\beta}A^{\nu}, \tag{4.24}$$

which in three-vector language can be written

$$T^{00} = \mathscr{E}^F + \nabla\cdot(A_0\mathbf{E}), \qquad T^{0i} = S^i + \nabla\cdot(A^i\mathbf{E}), \qquad T^{i0} = S^i + (\nabla\times A_0\mathbf{B})^i - \partial_t(A^0E^i) \tag{4.25}$$

where $\mathbf{S}$ and $\mathscr{E}^F$ are the *Poynting vector* and the *electromagnetic energy density* respectively, and are defined as follows

$$\mathbf{S} := \mathbf{E}\times\mathbf{B}, \qquad \mathscr{E}^F := \frac{1}{2}\left[\mathbf{E}^2 + \mathbf{B}^2\right]. \tag{4.26}$$

The tensor T, while adequate for the expression of the conservation of energy and momentum of the free field (see Jackson (1998)), is overly complicated by the additional terms involving the A_{μ} in 4.25. Moreover, it isn't symmetric, which means it can't possibly be used to describe the conservation of angular momentum (Jackson (1998)). A simple *symmetric* tensor Θ satisfying 4.21 can be constructed out of T as follows (Jackson (1998))

$$\Theta^{\alpha\beta} = T^{\alpha\beta} - \partial_{\mu}(F^{\mu\alpha}A^{\beta}) = \eta^{\alpha\mu}F_{\mu\nu}F^{\nu\beta} + \eta^{\alpha\beta}F_{\mu\nu}F^{\mu\nu}, \tag{4.27}$$

which due to its symmetry, is fully specified by the components

$$\Theta^{00} = \mathscr{E}^F, \qquad \Theta^{0i} = S^i, \qquad \Theta^{ij} = \frac{1}{2}\delta^{ij}\mathscr{E}^F - (E^iE^j + B^iB^j) =: T^{ij} \tag{4.28}$$

in which $\mathbf{T}$ is known as the *Maxwell stress-tensor*. The tensor Θ can also be obtained by considering the invariance of the Lagrangian density under rotations, which ultimately yields the (local) conservation of angular momentum of the free field in the form $\partial_\alpha M^{\alpha\beta\gamma} = 0$ where (Healy (1982), Rohrlich (2007))

$$M^{\alpha\beta\gamma} = \theta^{\alpha\beta}x^\gamma - \theta^{\alpha\gamma}x^\beta. \tag{4.29}$$

Combining the quantities in 4.26 one obtains the *electromagnetic four-momentum density*

$$\mathscr{P}^F_\alpha := (\mathscr{E}^F, -\mathbf{S}) = \theta_{0\alpha} = \theta_{\alpha 0}, \tag{4.30}$$

and the time component of the equation $\partial^0\Theta_{0\alpha} = 0$ yields a continuity equation expressing the local conservation of energy;

$$\partial^\alpha \mathscr{P}^F_\alpha = \partial_t\mathscr{E}^F + \nabla\cdot\mathbf{S} = 0. \tag{4.31}$$

This result is known as *Poynting's theorem* for the free field. Equation 4.23 now yields conservation of energy and momentum of the free field

$$\int d^3x\,\partial^0\Theta_{0\alpha} = \partial_t\int d^3x\,\mathscr{P}^F_\alpha = \partial_t P^F_\alpha = 0. \tag{4.32}$$

where

$$P^F_\alpha := \int d^3x\,\mathscr{P}^F_\alpha = (E^F, -\mathbf{P}^F) \tag{4.33}$$

is the four-momentum of the field.[30]

In the presence of sources the four-divergence of $\Theta^{\alpha\beta}$ no longer vanishes. Using the inhomogeneous Maxwell equations one easily finds that (Jackson (1998))

$$\partial_\alpha\theta^{\alpha\beta} = -F^{\beta\mu}j_\mu =: -f^\beta = -(\mathbf{J}\cdot\mathbf{E}, \rho\mathbf{E} + \mathbf{S}) \tag{4.34}$$

where $j_\mu = (\rho, -\mathbf{J})$. The energy of a *free* particle is $E^P := m\gamma^{-1}$ and according to the Lorentz force law, if the particle is charged the energy obeys the equation of motion[31]

$$\partial_t E^P = \int_V d^3x\,\mathbf{J}\cdot\mathbf{E} \equiv \int_V d^3x\,\mathscr{E}^P \tag{4.35}$$

[30] The designations *energy* and *momentum* for E^F and $\mathbf{P}^F$ respectively, may only be valid with respect to a specific frame of reference (see the comments at the end of this section).

[31] The results of this section stay the same if the nonrelativistic approximation $E^P \approx \frac{1}{2}m\dot{\mathbf{r}}^2$ is used instead.

within some volume V containing the charge. The quantity $\mathscr{E}^P = \mathbf{J}\cdot\mathbf{E}$ is evidently the *energy density of the charge system*. Defining the *momentum density of the charge system* $\mathbf{P}$ such that its time derivative gives the Lorentz force density;

$$\partial_t \mathbf{P} := \rho\mathbf{E} + \mathbf{J}\times\mathbf{B}, \tag{4.36}$$

the four-vector f^α is seen to be the time derivative of the *four-momentum density of the charge system*;

$$f_\alpha = \partial_t(\mathscr{E}^P, -\mathbf{P}) = \partial_t \mathscr{P}^P_\alpha, \qquad \mathscr{P}^P_\alpha := (\mathscr{E}^P, -\mathbf{P}). \tag{4.37}$$

Poynting's theorem with sources present, is given by the time component of 4.34;

$$\partial^\alpha \mathscr{P}^F_\alpha + \partial_t \mathscr{E}^P = \partial_t\left(\mathscr{E}^P + \mathscr{E}^F\right) + \nabla\cdot\mathbf{S} = 0, \tag{4.38}$$

while the space component of 4.34 reads (Jackson (1998))

$$\partial_t(S_i + P_i) = \nabla_j \Theta_{ij}. \tag{4.39}$$

Finally the conservation of the energy and momentum of the composite system can be expressed simply as

$$\int d^3x\,(\partial^\alpha\Theta_{\alpha\beta} + f_\beta) = \frac{d}{dt}\int d^3x\left[\mathscr{P}^F_\beta + \mathscr{P}^P_\beta\right] \equiv \frac{d}{dt}\int d^3x\,\mathscr{P}_\beta = 0. \tag{4.40}$$

The Poynting vector $\mathbf{S}$ has the dimensions of energy per unit time per unit area, meaning that it is a *power* density. Its integral over V gives the total momentum carried by the fields within V. Poynting's theorem 4.38 tells us that the total rate P at which energy leaves the volume V, is equal to the flux across the surface Ω, which encloses V;

$$P := \oint_\Omega d\Omega\,\mathbf{S}\cdot\hat{\mathbf{n}} \tag{4.41}$$

where $\hat{\mathbf{n}}$ is the unit normal field pointing outward from Ω. Considering a single charge at $\mathbf{r}$, and letting Ω denote the sphere with radius R centered at $\mathbf{r}$, the total power *radiated* by the charge can be defined as the component of P surviving infinitely far away;

$$P_{\text{rad}} := \lim_{R\to\infty} P. \tag{4.42}$$

Only the radiation fields $\mathbf{E}_{\text{rad}}$ and $\mathbf{B}_{\text{rad}}$ contribute to P_{rad}, which is why they are called the radiation fields. Using the expressions in 4.17 for a single charge $-e$, with some work, one obtains the Liénard formula

$$P_{\text{rad}} = \frac{e^2\gamma^6}{6\pi}\left(\ddot{\mathbf{r}}^2 - [\dot{\mathbf{r}}\times\ddot{\mathbf{r}}]^2\right) \tag{4.43}$$

for the total power radiated by the charge. These results illustrate in a concrete way, how using the motional degrees of freedom to define the material subsystem, and the electric and magnetic fields to define the electromagnetic subsystem, yields both elegant and physically meaningful results. In actual fact I will use the results of this section, much later on in chapter 9.

4.3 On the nature of covariance

I wish now to discuss the important issue of covariance with regard to the results above. The field four-momentum defined in 4.33 is not covariant when sources are present, due to the integration over three-space (Rohrlich (2007)).[32] However, one can define a covariant four-momentum using $\theta_{\alpha\beta}$ by integrating over a *spacelike hyperplane*. Such a hyperplane is defined by an equation

$$n_\mu x^\mu - \tau = 0, \tag{4.44}$$

in which τ denotes proper time, and n is a unit timelike four-vector normal to the hyperplane (Jackson (1998), Rohrlich (2007)). Supposing that the coordinates $\{x^\mu\}$ are associated with an inertial frame $\mathcal{O}$, then setting $n^\mu \equiv (1,0,0,0)$, equation 4.44 describes an inertial observer $\mathcal{O}$ at the instant $\tau = t := x^0$. The covariant field four-momentum is defined as

$$P^F_\beta = \int d\sigma^\alpha \, \theta_{\alpha\beta} \tag{4.45}$$

where $d\sigma^\alpha = n^\alpha d^3\sigma$ and $d^3\sigma$ is an invariant infinitesimal element of three-dimensional area. In the frame $\mathcal{O}$, $d^3\sigma \equiv d^3x$, so definition 4.45 reduces to 4.33 (Rohrlich (2007)). It is important to note that 4.45 only coincides with 4.33 *in the inertial frame* $\mathcal{O}$. If the inertial frame $\mathcal{O}'$ moves with respect to $\mathcal{O}$ with velocity $\mathbf{v}$, then putting $n^\mu = v^\mu = (\gamma, \gamma\mathbf{v})$, 4.44 defines a hyperplane at the instant $t' = \tau$ (in $\mathcal{O}'$) as seen by the observer $\mathcal{O}$ (Rohrlich (2007)). If we assume that expression 4.33 holds in $\mathcal{O}'$ then in $\mathcal{O}$, 4.45 reads (Jackson (1998))

$$P^F_\beta = (E^F, -\mathbf{P}^F), \qquad E^F = \gamma \int d^3\sigma \, [\mathscr{E}_F - \mathbf{v}\cdot\mathbf{S}], \qquad \mathbf{P}^F = \gamma \int d^3\sigma \, [\mathbf{S} + \mathbf{v}\cdot\mathbf{T}] \tag{4.46}$$

where $\mathbf{T}$ is defined in 4.28 and $d^3\sigma = d^3x'$. Since by assumption the frame $\mathcal{O}'$ is the rest frame of the volume under consideration, d^3x' determines a proper volume element. Any interval $|\Delta\mathbf{x}'| := |\mathbf{x}'_2 - \mathbf{x}'_1|$ denotes a "proper length", which takes the same value independent of whether or not $\mathbf{x}'_1$ and $\mathbf{x}'_2$ are taken as the spatial coordinates of simultaneous events in $\mathcal{O}'$. We can therefore choose $t'_1 \neq t'_2$ as the times at which the endpoints of the interval determing the volume element d^3x' are measured (in $\mathcal{O}'$). In particular, we may choose t'_1 and t'_2 such

[32] It turns out that in the absence of sources the four-momentum 4.33 is covariant (Rohrlich (2007)).

that in $\mathcal{O}$ the corresponding events *are* simultaneous; $t_1 = t_2$. The Lorentz transformation between frames then implies the simple contraction formula $d^3x' = \gamma d^3x$, which can be substituted into 4.46 to obtain an expression written purely in terms of quantities measured in $\mathcal{O}$.

The four-momentum 4.46 is clearly different to 4.33 and because of this it has been argued that the expression 4.33 can only be valid in a particular inertial frame $\mathcal{O}'$ (Rohrlich (2007)). Perhaps a natural choice for $\mathcal{O}'$ is the rest frame of sources in which the only field is the static longitudinal electric field. Then 4.46 yields in the frame $\mathcal{O}$ (Butler (1969))

$$P^F_\alpha = \int d^3x\, \mathscr{P}^F_\alpha, \qquad \mathscr{P}^F_\alpha := \frac{\gamma}{2}[\mathbf{E}^2 - \mathbf{B}^2](\gamma, \gamma\mathbf{v}), \tag{4.47}$$

which has been advocated as the correct energy-momentum four-vector in the past (Butler (1969)).

Although 4.33 does not define a covariant four-vector Poynting's theorem is covariant, because it follows from Maxwell's equations, which are covariant. If one calls 4.33 the energy-momentum four-vector then the energy and momentum of the field is different for each inertial observer, and moreover, if two observers are related by a Lorentz transformation, their four-momenta are not related by that Lorentz transformation. Of course, this trait is shared by the electric and magnetic fields themselves, neither of which form the components of a four-vector within conventional treatments. Like the energy density and Poynting vector in 4.26, their components make up the components of a *tensor* F, which *is* covariant. Requiring that the field energy and momentum make up a covariant four-vector forces one to either sacrifice the generality of 4.30 and use something like 4.45 instead, or to append the theory with essentially ad hoc, additional concepts, such as *Poincaré stresses* (see Schwinger (1983), Rohrlich (1997), Jackson (1998), Rohrlich (2007), Yaghjian (2010) and references therein).

4.4 The Lorentz force law

Problems arise in classical electromagnetism, when one tries to combine Maxwell's equations with the Lorentz force law, for a point charge distribution $\rho = -e\delta(\mathbf{x} - \mathbf{r})$. The Coulomb self energy diverges at the position of the charge, as do the solutions to Maxwell's equations, but this is precisely the position at which the electromagnetic fields are supposed to be evaluated within the Lorentz force law. Consequently, to obtain finite results one must regularise the so-called *radiation reaction fields*, or *self fields*, at short distances from the charge. Working out precisely how to do this seems to embody a substantial area of research. In the nonrelativistic quantum theory one usually uses ultra-violet momentum cut-offs to control the divergences, it being assumed that physical predictions will come out finite in a proper relativistic treatment, in which the high frequency modes are dealt with properly. The self force generated by a single charge can be interpreted as rescaling its observable mass. In fact it was suggested early on that perhaps *all* mass is actually

electromagnetic in origin.

I consider the case of a single extended charge distribution with effective dimension d, and give a slightly modified derivation of the electromagnetic mass due to Jackson (1998). For simplicity one neglects the magnetic contributions, which vanish anyway if one assumes the charge is instantaneously at rest. The Lorentz force law for the charge then reads

$$\dot{\mathbf{p}}_{\text{mech}} = \int_{V_\rho} d^3x \rho \mathbf{E}. \tag{4.48}$$

Separating the total electric field as $\mathbf{E} = \mathbf{E}_{\text{self}} + \mathbf{E}_{\text{ext}}$, and assuming the total momentum $\mathbf{p} = \mathbf{p}_{\text{mech}} + \mathbf{p}_{\text{self}}$ obeys Newton's second law $\dot{\mathbf{p}} = \mathbf{F}_{\text{ext}}$, one obtains

$$\dot{\mathbf{p}}_{\text{self}} = -\int_{V_\rho} d^3x \rho \mathbf{E}_{\text{self}}. \tag{4.49}$$

Next one assumes a spherically symmetric charge distribution of size d, and taking $\mathbf{E}_{\text{self}} = \mathbf{E}_r$ as given in 4.11, performs a Taylor expansion of the charge and current densities about $t' = t$. Neglecting terms nonlinear in $\dot{\mathbf{r}}$, one obtains the following expression

$$\dot{\mathbf{p}}_{\text{self}} = \frac{4}{3}\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} U_n \partial_t^n \ddot{\mathbf{r}}, \qquad U_n := \frac{1}{2}\int_{V_\rho} d^3x \int d^3x' \rho(\mathbf{x})\rho(\mathbf{x}')\mathbf{R}^{n-1}. \tag{4.50}$$

The first term in the sequence U_n is proportional to the Coulomb self energy; $U_0 \equiv 4\pi V_{\text{self}}$. Assuming the charge is uniformly distributed throughout a sphere of radius d, one obtains $U_0 = \frac{e^2}{2d}$ and $U_1 = \frac{e^2}{2}$. Newton's second law then reads

$$m_{\text{obs}}\ddot{\mathbf{r}} - \frac{2e}{3}\dddot{\mathbf{r}} + O(\partial_t^{\geq 4}\mathbf{r}) = \mathbf{F}_{\text{ext}} \tag{4.51}$$

where m_{obs} is the observable mass of the charge, which is the sum of the bare mass m and a renormalisation term

$$m_{\text{obs}} := m + \delta m, \qquad \delta m := \frac{4U_0}{3} = \frac{2e^2}{3d}. \tag{4.52}$$

For a point charge $d \to 0$, and $\delta m \to \infty$. Using $\rho = -e\delta(\mathbf{x} - \mathbf{r})$, one has explicitly

$$\delta m := \frac{4U_0}{3} = \frac{4e^2}{3\pi}\int_0^\infty d\omega. \tag{4.53}$$

At the same time the higher order terms in 4.51 vanish as $d \to 0$, which means it coincides with the so-called Abraham-Lorentz equation

$$m_{\text{obs}}(\ddot{\mathbf{r}} - \tau\dddot{\mathbf{r}}) = \mathbf{F}_{\text{ext}}, \qquad \tau := \frac{2e^2}{3m_{\text{obs}}}. \tag{4.54}$$

This notorious equation admits peculiar unphysical solutions, the so-called *runaway solutions*. If $\mathbf{F}_{\text{ext}} = \mathbf{0}$ then $\ddot{\mathbf{r}} = \ddot{\mathbf{r}}(0)e^{t/\tau}$, so that the charge's acceleration grows exponentially.

Moreover the charge can be seen to respond to changes in $\mathbf{F}_{\text{ext}}$ acausally, an effect known as *preacceleration*. The infinite mass and runaway solutions are merely manifestations of the problems associated with the point charge model.

There are however, some silver linings. The "bare mass" m appears to be an artifact of the theory, which can be chosen arbitrarily. Thus, the *observable* mass of the point charge m_{obs}, may yet come out finite. For extended charge distributions the mass renormalisation is finite, and furthermore the acceleration of the charge is bounded (Jackson (1998), Spohn (2007), Rohrlich (2007), Yaghjian (2010)). An extended charge model can be used in the quantum theory as well (Moniz & Sharp (1974)). There the results come in the form of expectation values of the appropriate operators, and the quantity d is effectively replaced by the electron's reduced Compton wavelength ($\lambda_C = \frac{\hbar}{mc}$ in units not such that $c = \hbar = 1$). The quantum treatment is remarkably successful in that there are no acausal effects and no runaway solutions. This remains true even in the presence of an external force $\boldsymbol{F}_{\text{ext}}(\omega)$, provided the frequencies are such that $\omega < \frac{c}{\lambda_C}$. In all of these models it appears that the electromagnetic mass contribution is the same as the longitudinal electric field energy, but that this mass is actually a property of the particle.

4.5 Summary and discussion

We have finished our brief survey of classical electrodynamics. We have seen that accelerating charges effect other charges by producing electric and magnetic fields, which propagate causally. Unfortunately, the action of a point charge on itself incurs an infinite mass, and peculiar runaway solutions of the Abraham-Lorentz equation. Furthermore, an accelerating charge is predicted to lose energy through radiation, which seems to contradict the observed stability of atoms and molecules. These problems associated with the classical theory are at least partly alleviated by the quantum treatment to be discussed in the coming chapters (see for example Milonni (1994)). The quantum theory however, relies heavily on the canonical formalism, which may itself entail certain problems. Specifically, the fact that canonical degrees of freedom are gauge dependent and physically ambiguous means that one must take great care when interpreting results.

CHAPTER 5

The S-matrix and perturbation theory

Having reviewed classical electromagnetism now is the time to move on to the quantum theory. The aim of this chapter is to review in a general way, the tools used to analyse problems in QED, and discern what implications they might have with regard to determining the most appropriate subsystem decomposition of the composite atom-field system. In many places my treatment will be idealised to such an extent that it will not hold for the system of interest. Certain relations will hold only under quite restrictive assumptions such as the assumption of no bound states, or the assumption of no level-shifts in the continuum. Despite the fact that the atom-field Hamiltonian 2.71 has bound states embedded within a continuous spectrum, it will be useful to review the conventional methods used to treat interacting theories and try to glean insights as to the nature of physical subsystems.

According to 2.71 the bare vacuum state $|0,0\rangle$ consisting of no photons and the atom in its ground state is the ground state of the free Hamiltonian H_0, but not the ground state of the *total* Hamiltonian H. In fact there is an infinite number of photons in the ground state (Compagno *et al.* (1995)). In the dressed atom model one interprets these photons as the virtual photons, which are continually emitted and reabsorbed by the atom. They are said to be virtual, because they appear in processes that do not conserve the free energy H_0. One interprets them as corresponding to intermediate states, in overall processes, that *do* conserve the free energy. These are the so-called real processes. Thus,

> free energy conservation becomes a crucial factor in determining the reality of physical processes. It also seems to be crucial in ensuring the gauge invariance of probability amplitudes.

It behooves us therefore, to ask under what conditions the theory necessarily describes free energy conserving processes, and to what extent the bare atom-photon degrees of free-

dom give meaningful results without these conditions. The formalism within which processes always conserve the free energy is the gauge-invariant S-matrix formalism, which is the sole tool used to make predictions within quantum field theory. Philosophically, there seems to be two possible points of view regarding the bare atom-photon degrees of freedom:

> 1. They are nothing but mathematical devices allowing us to understand atom-field interactions as *processes* conserving free energy, the associated probability amplitudes being found using the S-matrix.
>
> 2. They have real physical meaning, and predictions pertaining to them made outside of the S-matrix formalism, should at least in principle, be experimentally verifiable.

Viewpoint 1 is somewhat restrictive, because the S-matrix formalism is non-dynamical in the sense that it provides probability amplitudes associated with processes taking place between times $t_i \to -\infty$ and $t_f \to \infty$. On the other hand viewpoint 2 forces us to take as physically real, processes which do not conserve the free energy. Virtual photons belonging to the cloud surrounding the atom may therefore be measured. Moreover, we will be confronted with the problem that the bare atom-photon degrees of freedom are physically distinct in each gauge.

It does not seem permissible to me, to choose some middle ground between these two points of view by taking as meaningful those processes which conserve free energy over finite interaction times, while ignoring all others. One cannot simply pick and choose at will, which predictions to keep and which predictions to throw away. Neither does it seem we can impose free energy conservation as a fundamental law, for in general the free energy is not conserved $[H_0, V] \neq 0$, so that the imposition of its conservation as a fundamental law would actually contradict the theory.

In this chapter I consider the S-matrix from various points of view (5.1). This will be illuminating in that it will allow us to understand precisely why the S-matrix is gauge-invariant, despite it seemingly giving probability amplitudes for transitions between gauge-dependent bare states. It will also allow us to decide how physical subsystems are usually viewed from the quantum field-theoretic perspective. In 5.2 I will briefly turn my attention to time-independent perturbation theory. In doing so I will introduce briefly, the *resolvent* operator, which I will use extensively in chapter 7.

5.1 The S-matrix

In section 5.1.1 I will be using nothing but time-independent quantum theory. In sections 5.1.2 and 5.1.3, I consider the S-matrix using time-dependent approaches.

5.1.1 The S-matrix from the time-independent formalism

Suppose we are given free and interaction Hamiltonians H_0 and V, such that H_0 and $H = H_0 + V$ both have continuous spectra. We know the eigenvalues and eigenstates of H_0, and so we look for eigenstates of H, which tend to those of H_0 as $V \to 0$. These eigenstates will be denoted $|n^{\pm}\rangle$, where $|n^{+}\rangle$ is called an *in-state*, and $|n^{-}\rangle$ is called an *out-state*. The S-matrix is used to obtain probability amplitudes $\langle f^{-}|i^{+}\rangle$, in terms of the corresponding free states. The in/out-states satisfy the Schrödinger equation with respect to the composite system Hamiltonian;

$$H|n^{\pm}\rangle = \omega_n|n^{\pm}\rangle. \tag{5.1}$$

Similarly, the free eigenstates $|n_0\rangle$, satisfy

$$H_0|n_0\rangle = \omega_n|n_0\rangle. \tag{5.2}$$

where for simplicity, to begin with I have assumed that there are no level-shifts, so the spectra of H_0 and H are the same. The free eigenstates are assumed to form an orthonormal basis in the system's Hilbert space, and it is assumed moreover that they are in one-to-one correspondence with the in and out-states. It is easy to show that the in/out-states are normalised as (Roman (1965))

$$\langle n^{+}|m^{+}\rangle = \langle n^{-}|m^{-}\rangle = \langle n_0|m_0\rangle. \tag{5.3}$$

One now makes the ansatz

$$|n^{\pm}\rangle = |n_0\rangle + G^{0\pm}(\omega_n)V|n^{\pm}\rangle \tag{5.4}$$

where

$$G^{0\pm}(\omega_n) := \frac{1}{\omega_n - H_0 \pm i\eta}. \tag{5.5}$$

It is supposed to be implicitly understood here, that the limit $\eta \to 0^{+}$ will be taken at the end of the calculation, the denominator contribution $i\eta$ merely ensures that $G^{0\pm}(\omega_n)$ is not singular at ω_n. Equation 5.4 is called the *Lippman-Schwinger equation*, and it is easily verified that the $|n^{\pm}\rangle$ defined by it satisfy 5.1. Using the completeness relation over the free eigenstates, 5.4 can be written in the alternative form

$$|n^{\pm}\rangle = |n_0\rangle + \sum_m \frac{1}{\omega_{nm} \pm i\eta} T^{\pm}_{nm}|n_0\rangle \tag{5.6}$$

where $\omega_{nm} := \omega_n - \omega_m$ and

$$T^{\pm}_{nm} := \langle n_0|V|m^{\pm}\rangle. \tag{5.7}$$

It would be convenient to have an expression for the in and out-states purely in terms of the free states, as well as expressions 5.4 and 5.6, in which the in and out-states appear on both sides. This can be achieved by first multiplying 5.4 by V to obtain an expression for $V|n^{\pm}\rangle$, and then substituting the result back into 5.4 on the right-hand-side. Rearranging the resulting expression yields the result

$$(\omega_n - H \pm i\eta)|n^{\pm}\rangle = i\eta|n_0\rangle \tag{5.8}$$

from which it follows that

$$|n^{\pm}\rangle = \frac{i\eta}{\omega_n - H \pm i\eta}|n_0\rangle = |n_0\rangle + G^{\pm}(\omega_n)V|n_0\rangle. \tag{5.9}$$

where

$$G^{\pm}(\omega_n) := \frac{1}{\omega_n - H \pm i\eta}. \tag{5.10}$$

Thus, we can write the Lippman-Schwinger equation in terms of the *in/out-states* together with the *free Hamiltonian* as in 5.4, or, in terms of the *free states* together with the *total Hamiltonian* as in 5.9. By making use of 5.4, the operator $G^{\pm}(\omega_n)$ can be expanded iteratively in terms of its free counterpart as

$$G^{\pm}(\omega_n)V = G^{0\pm}(\omega_n)\sum_{m=0}^{\infty}\left[VG^{0\pm}(\omega_n)\right]^m, \tag{5.11}$$

which is known as the *Born expansion*.

We are now in a position to formally define the S-matrix. The S-matrix links the *free* initial and final states $|i_0\rangle$ and $|f_0\rangle$, with the in and out-states $|i^+\rangle$ and $|f^-\rangle$ as follows

$$\langle f_0|S|i_0\rangle := \langle f^-|i^+\rangle. \tag{5.12}$$

Using 5.6 we have

$$\langle f^-|i^+\rangle = \delta_{fi} + \frac{1}{\omega_{if} + i\eta}T^+_{fi} + \frac{1}{\omega_{fi} + i\eta}T^+_{fi} = \delta_{fi} - \frac{2i\eta}{\eta^2 + \omega^2_{fi}}T^+_{fi}, \tag{5.13}$$

and using

$$\lim_{\eta\to 0^+}\frac{\eta}{\eta^2 + x} = \pi\delta(x) \tag{5.14}$$

we can write the S-matrix as

$$S_{fi} = \delta_{fi} - 2\pi i \delta(\omega_{fi}) T_{fi} \tag{5.15}$$

where $T_{fi} := T^{+}_{fi}$. The amplitude $\langle f^{-}|i^{+}\rangle$ is completely determined through knowledge of the T-matrix element T_{fi}, which using the Born expansion can be expanded as follows

$$T_{fi} = T^{(1)}_{fi} + T^{(2)}_{fi} + T^{(3)}_{fi} + \ldots \equiv V_{fi} + \sum_{n} \frac{V_{fn}V_{ni}}{\omega_{in} + i\eta} + \sum_{n,m} \frac{V_{fn}V_{nm}V_{mi}}{(\omega_{in} + i\eta)(\omega_{im} + i\eta)} + \ldots . \tag{5.16}$$

Thus, we have a means by which to determine $\langle f^{-}|i^{+}\rangle$ up to arbitrary order in powers of the interaction V.

5.1.2 Green's functions for the Schrödinger equation

In this section I review a time-dependent approach to the S-matrix facilitated by Green's functions, or *propagators*, which shed further light onto the assumptions underlying the S-matrix formalism. It is in terms of propagators that the S-matrix is usually formulated within relativistic QED.

Consider the evolution operator

$$U(t,t_0) = e^{-iH(t-t_0)} = e^{-iH\tau} = U(\tau), \qquad \tau := t - t_0, \tag{5.17}$$

which satisfies the Schrödinger equation

$$(i\partial_t - H)U(t,t_0) = 0, \qquad U(t,t) \equiv I. \tag{5.18}$$

Define now the operators

$$\mathrm{G}^{\pm}(\tau) := \mp i\theta(\pm\tau)U(\tau) \tag{5.19}$$

where θ is the Heaviside-step function, which is defined by

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0, \end{cases} \tag{5.20}$$

and which satisfies

$$\theta(x) + \theta(-x) = 1 \tag{5.21a}$$

$$\partial_x \theta(x) = \delta(x). \tag{5.21b}$$

It follows from 5.21a and the definitions of the $\mathrm{G}^{\pm}$ that

$$-iU(\tau) = \mathrm{G}^{+}(\tau) - \mathrm{G}^{-}(\tau). \tag{5.22}$$

Similarly using 5.21b it is easy to show that

$$(i\partial_t - H)\mathrm{G}^{\pm}(\tau) = \delta(\tau)U(\tau). \tag{5.23}$$

Due to the presence of the delta function we can ignore $U(\tau)$ in 5.23, which is effectively equal to $U(0) = I$. This means we can identify $G^+(\tau)$ and $G^-(t)$ as the retarded and advanced Green's functions for the Schrödinger equation. We can construct retarded and advanced solutions of the Schrödinger equation as

$$\begin{aligned} |\psi^{\pm}(t)\rangle &= |\phi(t)\rangle + \int dt_0\, \mathrm{G}^{\pm}(\tau)V|\phi(t_0)\rangle \\ &= |\phi(t)\rangle + \int dt_0\, \mathrm{G}^{0\pm}(\tau)V|\psi^{\pm}(t_0)\rangle \end{aligned} \tag{5.24}$$

where $G^{0\pm}$ are the *free* retarded and advanced Green's functions, associated with the free Schrödinger operator $(i\partial_t - H_0)$, and $|\phi(t)\rangle$ is a bare state satisfying $(i\partial_t - H_0)|\phi(t)\rangle = 0$. It is easily verified that the $|\psi^{\pm}(t)\rangle$ satisfy the Schrödinger equation $(i\partial_t - H)|\psi^{\pm}(t)\rangle = 0$, by either applying $i\partial_t - H$ to the top line in 5.24, or by applying $i\partial_t - H_0$ to the second line.

If we now make the same no level-shifts assumption as in 5.1.1, then the energy states $|n^{\pm}\rangle$ and the bare states $|n_0\rangle$ have the same oscillatory time dependence;

$$|n^{\pm}(t)\rangle = e^{-i\omega_n t}|n^{\pm}\rangle, \qquad |n_0(t)\rangle = e^{-i\omega_n t}|n_0\rangle. \tag{5.25}$$

Setting $|\psi^{\pm}(t)\rangle \equiv |n^{\pm}(t)\rangle$ and $|\phi(t)\rangle \equiv |n_0(t)\rangle$ in 5.24, and making the substitution $\tau = t - t_0$ one obtains

$$|n^{\pm}\rangle = |n_0\rangle + \int d\tau\, e^{i\omega_n\tau}\mathrm{G}^{\pm}(\tau)V|n_0\rangle = |n_0\rangle + \int d\tau\, e^{i\omega_n\tau}\mathrm{G}^{0\pm}(\tau)V|n^{\pm}\rangle. \tag{5.26}$$

To evaluate the integrals one must ensure they converge, which will be the case if an infinitesimal term $-\eta,\ \eta > 0$ is inserted into the exponent and the limit $\eta \to 0^+$ is taken at the end. This addition ensures adiabaticity of the switching on and off of the interaction. We have for example

$$\begin{aligned} &\int d\tau\, \mathrm{G}^{+}(\tau)e^{i\omega_n\tau} = -i\int d\tau\, \theta(\tau)U(\tau)e^{i\omega_n\tau} = -i\lim_{\tau\to\infty}\int_0^{\tau} d\tau'\, e^{i(\omega - H)\tau'} \\ \longrightarrow\ &-i\lim_{\eta\to 0^+}\lim_{\tau\to\infty}\int_0^{\tau} d\tau'\, e^{i(\omega - H + i\eta)\tau'} = \lim_{\eta\to 0^+}\frac{1}{\omega_n - H + i\eta} =: G_n^{+}. \end{aligned} \tag{5.27}$$

Thus, the expressions in 5.26 reduce to the Lipmann-Schwinger equations

$$|n^{\pm}\rangle = |n_0\rangle + G_n^{\pm}V|n_0\rangle = |n_0\rangle + G^{0\pm}(\omega_n)V|n^{\pm}\rangle. \tag{5.28}$$

We see then, that the $|n^{\pm}\rangle$ are nothing but retarded and advanced energy eigenstates.

The S-matrix with level-shifts

In general the free energy eigenvalues don't coincide with the eigenvalues of the total Hamiltonian; $\omega_n - \omega_n^0 = \Delta\omega_n$. One therefore defines the *level-shift operator* R by

$$R := \sum_n \Delta\omega_n |n_0\rangle\langle n_0|, \qquad \Delta\omega_n := \omega_n - \omega_n^0 \tag{5.29}$$

where clearly R is diagonal in the free eigenbasis, with $\langle n_0|R|n_0\rangle \equiv \Delta\omega_n$. This operator allows the level-shifts to be included in the free Hamiltonian through the definition

$$\mathscr{H}_0 := H_0 + R, \tag{5.30}$$

which clearly has the same spectrum as H, but the same eigenstates as H_0;

$$\mathscr{H}_0|n_0\rangle = \omega_n|n_0\rangle. \tag{5.31}$$

Defining in addition the new interaction Hamiltonian $\mathscr{V} = V - R$, one can write the total Hamiltonian as $H = \mathscr{H}_0 + \mathscr{V}$. In the case that $R \neq 0$ the results of section 5.1.1 remain essentially valid. One simply has to replace H_0 and V with their shifted counterparts $\mathscr{H}_0$ and $\mathcal{V}$ respectively. However, as a result of the shifts the in/out-states will no longer be normalised, so they must be renormalised as follows (Roman (1965))

$$|n_R^\pm\rangle := \frac{1}{\sqrt{Z_n}}|n^\pm\rangle, \qquad Z_n := \langle n^\pm|n^\pm\rangle = \langle n_0|n^\pm\rangle. \tag{5.32}$$

The S-matrix is then defined by

$$S_{fi} := \langle f_R^-|i_R^+\rangle = \frac{1}{\sqrt{Z_i Z_f}}\langle f^-|i^+\rangle. \tag{5.33}$$

The results of this section appear to require us to know the level-shifts to begin with. I'll end this section by remarking that the T-matrix to be derived in 5.1.3 can in fact be used to find the level-shift of the i'th free state. The change in energy is due to free energy conserving scattering processes in which the initial and final states are identical. These processes are made up of energy non-conserving intermediate processes in which virtual quanta are emitted and reabsorbed.

5.1.3 The S-matrix via time-dependent perturbation theory

One of the most physically illuminating methods of deriving the S-matrix uses *time-dependent perturbation theory* formulated using the *interaction picture*. The interaction picture is defined by changing basis using the evolution operator associated with the free Hamiltonian

H_0;

$$|\tilde{\psi}(t)\rangle = U_0^{-1}(t,0)|\psi(t)\rangle, \qquad \tilde{\mathcal{O}}(t) := U_0^{-1}(t,0)\mathcal{O}U_0(t,0), \qquad U_0(t,t_0) := e^{-iH_0(t-t_0)} \tag{5.34}$$

where $|\psi(t)\rangle$ and $\mathcal{O}$ respectively denote a state and an operator in the Schrödinger picture. Using the Schrödinger equation, it is easy to show that the interaction picture state $|\tilde{\psi}\rangle$ obeys the equation of motion

$$|\dot{\tilde{\psi}}\rangle = \tilde{V}(t)|\tilde{\psi}\rangle, \tag{5.35}$$

which implies that the evolution operator $\tilde{U}$ is related to the Schrödinger picture evolution operator U by

$$\tilde{U}(t,t_0) = U_0(t_0,t_2)U(t_2,t_1)U_0(t_1,t_0). \tag{5.36}$$

It is easily shown additionally that $\tilde{U}$ like U, has the following basic properties

$$\tilde{U}(0,0) = I, \qquad \tilde{U}(t,t')\tilde{U}(t',t_0) = \tilde{U}(t,t_0), \qquad \tilde{U}^{-1}(t,t_0) = \tilde{U}(t_0,t). \tag{5.37}$$

Dyson (1949) sought to determine the dynamics of the system by solving the basic dynamical equation of the interaction picture;

$$|\tilde{\psi}(t)\rangle = \tilde{U}(t,t_0)|\tilde{\psi}(t_0)\rangle. \tag{5.38}$$

His first step was to substitute 5.38 into 5.35 and integrate to obtain

$$\tilde{U}(t,t_0) = I - i\int_{t_0}^{t} dt' V(t')\tilde{U}(t',t_0). \tag{5.39}$$

Iteration of this expression gives the *Dyson series*;

$$\tilde{U}(t,t_0) = \sum_{n=0}^{\infty} \tilde{U}_n(t,t_0) \tag{5.40}$$

where

$$\begin{aligned}\tilde{U}_n(t,t_0) &= (-i)^n \int_{t_0}^{t} dt' \ldots \int_{t_0}^{t^{(n-1)}} dt^{(n)}\, V(t')\ldots V\left(t^{(n)}\right) \\ &= \frac{(-i)^n}{n!}\int_{t_0}^{t} dt' \ldots \int_{t_0}^{t} dt^{(n)}\, \mathcal{T}\left[V(t')\ldots V\left(t^{(n)}\right)\right]\end{aligned} \tag{5.41}$$

in which $\mathcal{T}$ denotes Dyson's time-ordering operator defined by

$$\mathcal{T}[A(t)B(t')] = \begin{cases} A(t)B(t') & \text{if } t > t' \\ B(t')A(t) & \text{if } t < t'. \end{cases} \tag{5.42}$$

Armed with these ideas I'm ready to give a second definition of the S-matrix;

$$S := \tilde{U}(\infty, -\infty) = \tilde{U}(\infty, 0)\tilde{U}(0, -\infty). \tag{5.43}$$

The use of the interaction picture is necessary to obtain a well defined matrix as the initial and final times approach infinity. This however, is still not guaranteed even within the interaction picture. In order to ensure that the S-matrix 5.43 is well defined one adopts an *adiabatic switching* mechanism whereby the interaction V is replaced by the interaction term $e^{-\eta|t|}V$, $\eta > 0$ and the limit $\eta \to 0^+$ is taken at the end (Roman (1965), Cohen-Tannoudji *et al.* (1997), Lawrie (2002)). Alternatively one can use a different, more formal limiting procedure whereby one *defines* operators evaluated at infinite times as follows (Roman (1965))

$$A(\infty) := \lim_{\eta \to 0^+} \eta \int_0^\infty dt' \, e^{-\eta t'} A(t'), \qquad A(-\infty) := \lim_{\eta \to 0^+} \eta \int_{-\infty}^0 dt' \, e^{\eta t'} A(t'). \tag{5.44}$$

With these definitions in place one writes the S-matrix using the so-called *Møller operators* $\Omega^\pm$ as

$$S = (\Omega^-)^\dagger \Omega^+, \qquad \Omega^- := \tilde{U}(0, \infty), \qquad \Omega^+ := \tilde{U}(0, -\infty). \tag{5.45}$$

It is straight forward to verify that the Møller operators obey the following relations (Roman (1965))

$$\Omega^\pm |n_0\rangle = \frac{-i\eta}{\mp i\eta - \omega_n^0 + H} |n_0\rangle = |n_0\rangle + \frac{1}{\omega_n^0 + H \pm i\eta} V |n_0\rangle =: |n^\pm\rangle. \tag{5.46}$$

Thus, the S-matrix can be written

$$S_{fi} = \delta_{fi} - 2\pi i \delta(\omega_{fi}^0) T_{fi} \tag{5.47}$$

as it was in the time-independent case, but with the T-matrix defined by the formal relation

$$T = V + V G^{0+} T \tag{5.48}$$

in which

$$G^{0\pm}(\omega) = \frac{1}{\omega - H_0 \pm i\eta}. \tag{5.49}$$

The T-matrix can also be viewed as an operator-valued function of the real variable ω, defined as (Cohen-Tannoudji *et al.* (1992))

$$T(\omega) = V + VG^{+}(\omega)V, \qquad G^{\pm}(\omega) = \frac{1}{\omega - H \pm i\eta}. \tag{5.50}$$

In 5.47 $T(\omega)$ is evaluated on-energy-shell i.e. at $\omega = \omega_i = \omega_f$. It is easy to see using the Born expansion 5.11 that the two definitions of the T-matrix are equivalent. The second definition 5.50 is obtained via an alternative method by which one arrives at 5.47, which involves relating the advanced and retarded Green's functions for the Schrödinger equation to the resolvent operator $G(z) := (z - H)^{-1}$ (Cohen-Tannoudji *et al.* (1992)). The route I have opted for shows most clearly how the physical states involved in scattering processes are related to the bare states associated with H_0.

In experiments one does not usually deal with probabilities directly, but rather with *transition rates* and *cross sections*. I will end this section by using the S-matrix to define a transition rate into a final state or a set of final sates. The S-matrix can be written

$$\begin{aligned} S_{fi} &= \delta_{fi} - 2\pi i \delta(\omega^0_{fi}) T_{fi} \\ &= \delta_{fi} - i \lim_{\tau\to\infty} \int_{-\tau/2}^{\tau/2} dt\, e^{i\omega^0_{fi} t} T_{fi} \\ &= \delta_{fi} - 2\pi i \lim_{\tau\to\infty} \delta^{\tau}(\omega^0_{fi}) T_{fi} \end{aligned} \tag{5.51}$$

where

$$\delta^{\tau}(\omega^0_{fi}) := \frac{1}{\pi} \frac{\sin(\omega^0_{fi}\tau/2)}{\omega^0_{fi}} \tag{5.52}$$

is a delta-function of width $4\pi/\tau$ centered at ω^0_{fi}. This delta-function is interpreted as expressing the conservation of free energy with an uncertainty $\sim 1/\tau$ due to the finite time of the interaction. The uncertainty tends to zero as $\tau \to \infty$. It is important to recognise that this uncertainty relation is not a fundamental law following directly from the quantum mechanical formalism, as the generalised uncertainty relation pertaining to conjugate linear operators is.

In light of 5.51 and 5.52 one defines the transition rate from state $|i\rangle \to |f\rangle$, $i \neq f$ by

$$w_{i\to f} := 4\pi^2 \lim_{\tau\to\infty} \frac{\delta^{\tau}(\omega^0_{fi})^2}{\tau} |T_{fi}|^2 = 2\pi\delta(\omega^0_{fi})|T_{fi}|^2 \tag{5.53}$$

where in general $T_{fi} \equiv T_{fi}(\omega^0_f, \omega^0_i)$ depends on the initial and final state energies, as well as other parameters upon which the bare states might depend. Often one is interested in the transition rate into a group of final states with energy density ρ. If we denote collectively with λ all other parameters on which the final states might depend besides energy, the transition rate to the group of final states with energy in $\mathcal{I} := [\omega + \delta\omega/2, \omega - \delta\omega/2] \ni \omega^0_i$

is

$$w_{i\to f}^{\text{group}} := \sum_f w_{i\to f} = 2\pi \int_{\mathfrak{I}} d\omega_f^0 \sum_\lambda \rho(\omega_f^0,\lambda) w_{i\to f}$$
$$= 2\pi \sum_\lambda \rho(\omega,\lambda)|T_{fi}(\omega,\omega,\lambda)|^2\Big|_{\omega=\omega_i^0}. \tag{5.54}$$

This result is called *Fermi's golden rule*, although it was first used by Dirac.

5.2 Time-independent perturbation theory

Before summarising the results of this chapter, I wish to make a brief detour. The theory of resolvents (Kato (1976), Van Hove (1955), Van Hove (1956), Hugenholtz (1957)) provides an illuminating perspective on both S-matrix theory and perturbation theory, and I will use it quite a bit later. I will give only the definition and some basic properties here with the aim of developing time-independent perturbation theories. I will go into much more detail in chapter 6.

5.2.1 The resolvent

The resolvent of a Hamiltonian H is defined as

$$G(z) := \frac{1}{z-H}, \qquad z \in \mathbb{C}. \tag{5.55}$$

To obtain the *free resolvent* $G_0(z)$ one simply replaces H with H_0 in 5.55. Applying the operator identity

$$\frac{1}{A} \equiv \frac{1}{B} + \frac{1}{B}(B-A)\frac{1}{A} \tag{5.56}$$

with $A \equiv z-H$ and $B \equiv z-H_0$ to $G(z)$ yields the relation

$$G(z) = G_0(z) + G_0(z)VG(z), \tag{5.57}$$

which closely resembles the Born expansion 5.11. Similarly one can show that

$$G(z) = G_0(z) + G(z)VG_0(z). \tag{5.58}$$

The operators $G^\pm$ given in 5.10, can be identified in terms of the resolvent as

$$G^\pm(\omega) = \lim_{\eta\to 0^+} G(\omega \pm i\eta). \tag{5.59}$$

The resolvent is also closely related to the evolution operator $U(t,t_0)$. In fact, according to 5.22 and 5.27, we have

$$U(\tau) = i\left[\mathrm{G}^+(\tau) - \mathrm{G}^-(\tau)\right] = \frac{1}{2\pi i}\int d\omega\, e^{-i\omega\tau}\left[G^-(\omega) - G^+(\omega)\right] \tag{5.60}$$

Using 5.59 this gives (Cohen-Tannoudji *et al.* (1992))

$$U(\tau) = \frac{1}{2\pi i}\int_{\gamma^+ + \gamma^-} dz\, e^{-iz\tau} G(z) \tag{5.61}$$

where γ^+ is the complex contour running horizontally from right to left immediately above the real axis, and γ^- is the contour running left to right immediately below the real axis. As I mentioned at the end of 5.1.3 it is possible to give a derivation of the S-matrix in terms of the resolvent, regarding this I refer the reader to Cohen-Tannoudji *et al.* (1992).

5.2.2 Perturbation theory

The resolvent can be used to obtain traditional perturbative devices including *Rayleigh-Schrödinger perturbation theory* (Hubac & Wilson (2010)). To this end consider the eigenproblems

$$H_0|n_0\rangle = \omega_n^0|n_0\rangle, \qquad H|n\rangle = \omega_n|n\rangle, \qquad H = H_0 + V. \tag{5.62}$$

where H_0 is assumed to have discrete spectrum. For simplicity, I assume that the $|n_0\rangle$ are non-degenerate and moreover that the true eigenstates $|n\rangle$ satisfy the normalisation condition

$$\langle n_0|n\rangle = 1. \tag{5.63}$$

If we assume naturally that $|n\rangle \neq |n_0\rangle$, then this condition implies that the eigenstates $|n\rangle$ are not themselves normalised; $\||n\rangle\| > 1$. It will be useful to consider the operators

$$P := |n_0\rangle\langle n_0|, \qquad Q := 1 - P, \qquad G_Q(\omega) = \frac{1}{\omega - QHQ} \tag{5.64}$$

where $|n_0\rangle$ denotes a particular bare state. The operator G_Q is just the resolvent of the projected Hamiltonian QHQ. Note that using 5.63 the useful relation

$$|n_0\rangle = P|n\rangle \tag{5.65}$$

immediately follows.

With the definitions above established I turn now to the task of finding an *effective*

Hamiltonian H_{eff}, satisfying the hybrid eigen-problem $H_{\text{eff}}|n_0\rangle = \omega_n|n_0\rangle$. We have

$$H(P+Q)|n\rangle = \omega_n(P+Q)|n\rangle \tag{5.66}$$

implying

$$PHP|n\rangle + PHQ|n\rangle = \omega_n P|n\rangle. \tag{5.67}$$

Since $H(P+Q)|n\rangle = \omega_n(P+Q)|n\rangle$ we have

$$QHP|n\rangle + QHQ|n\rangle = \omega_n Q|n\rangle \tag{5.68}$$

implying

$$Q|n\rangle = G_Q(\omega_n)QHP|n\rangle. \tag{5.69}$$

Using 5.65 this implies

$$H_{\text{eff}}|n_0\rangle = \omega_n|n_0\rangle \tag{5.70}$$

where

$$H_{\text{eff}} = PHP + PHQG_Q(\omega_n)QHP. \tag{5.71}$$

With respect to the state $|n_0\rangle$ this effective Hamiltonian does the same job as the shifted Hamiltonian $\mathscr{H}_0$ in 5.30.

Next I find the inverse of the operator P, that is, the operator which takes a bare state $|n_0\rangle$ and gives the corresponding true eigenstate $|n\rangle$. One defines the *wave operator* Ω by

$$|n\rangle = \Omega|n_0\rangle, \qquad P\Omega = P, \qquad \Omega P = \Omega, \qquad \Omega^2 = \Omega. \tag{5.72}$$

We have

$$\Omega H_{\text{eff}}|n_0\rangle = \omega_n\Omega|n_0\rangle = H|n\rangle = H\Omega|n_0\rangle \Rightarrow \Omega H_{\text{eff}} = H\Omega \tag{5.73}$$

and since $PH\Omega|n_0\rangle = \omega_n|n_0\rangle$, it follows using 5.71 that

$$\Omega = [I + QG_Q(\omega_n)QV]P \tag{5.74}$$

Applying this expression onto $|n_0\rangle$ and using 5.72 one obtains an equation closely resembling the Lippmann-Schwinger equation 5.9.

Finally I define the *level-shift operator* R, which relates the various operators found

above;

$$R = V\Omega, \qquad R(z) = V + VQG_Q(z)QV. \tag{5.75}$$

We have immediately

$$H_{\text{eff}} = PH_0P + PRP, \tag{5.76}$$

from which it follows that

$$\omega_n = \omega_n^0 + \langle n_0|R|n_0\rangle, \tag{5.77}$$

hence the name level-shift operator. With respect to the state $|n_0\rangle$, this operator does the same job as the level-shift operator in 5.29. One can derive a number of useful relations between $R(z)$ and $G(z)$. Using the definition of the resolvent 5.55, and the fact that $P+Q=I$ we have

$$(z-H)(P+Q)G(z) = I. \tag{5.78}$$

Applying P from the left gives

$$P(z-H)PG(z)P - PVQG(z)P = P \tag{5.79}$$

while applying Q from the left, then P from the right, and finally rearranging gives

$$QG(z)P = QG_Q(z)QVPG(z)P. \tag{5.80}$$

Substituting 5.80 into 5.79 and rearranging yields

$$PG(z)P = P\frac{1}{z - PH_0P - PR(z)P}P, \qquad G_n(z) = \frac{1}{z-\omega_n^0 - R_n(z)} \tag{5.81}$$

where $G_n(z) := \langle n_0|G(z)|n_0\rangle$ and $R_n(z) := \langle n_0|R(z)|n_0\rangle$.

The operators above allow us to determine the true eigenvalues and eigenstates from the free eigenvalues and eigenstates. Usually however, this can't be done exactly, but only by recourse to perturbation theory. One can obtain a perturbative expansion by applying to the resolvent G_Q, the operator identities

$$\frac{1}{A+B} \equiv \frac{1}{A} + \frac{1}{A}B\frac{1}{A-B} \tag{5.82a}$$

$$\frac{1}{A+B} \equiv \frac{1}{A} + \frac{1}{A}B\frac{1}{A'-B'} \tag{5.82b}$$

where $A-B = A'-B'$. By using different partitions of $A-B$, as is allowed according to 5.82, one can obtain a number of different perturbation theories. The most common

of which is Rayleigh-Schrödinger perturbation theory, defined by the use of 5.82a along with the partition $A = \omega_n^0 - H_0,\ B = V - \Delta\omega_n$. These choices yield the following series expansions (Hubac & Wilson (2010))

$$H_{\text{eff}} = PHP + \sum_{\alpha=0}^{\infty} PHQG_Q^0 \left[(V - \Delta\omega_n)G_Q^0\right]^\alpha QHP, \tag{5.83a}$$

$$\Omega = I + \sum_{\alpha=0}^{\infty} QG_Q^0 \left[(V - \Delta\omega_n)G_Q^0\right]^\alpha QV, \tag{5.83b}$$

$$R = V + \sum_{\alpha=0}^{\infty} VQG_Q^0 \left[(V - \Delta\omega_n)G_Q^0\right]^\alpha QV \tag{5.83c}$$

where

$$G_Q^0 := \sum_{n\neq m} \frac{1}{\omega_{nm}^0} |m_0\rangle\langle m_0| \tag{5.84}$$

is sometimes called the *Rayleigh-Schrödinger resolvent*.

To get an expansion for the level-shift $\Delta\omega_n$ I first replace V with λV, where λ is a small parameter (e.g. $\lambda = \alpha$) and expand the level-shift in a power series;

$$\Delta\omega_n = \sum_{\alpha=1}^{\infty} \lambda^\alpha \Delta\omega_n^{(\alpha)} \tag{5.85}$$

with $\Delta\omega_n^{(0)} \equiv 0$. According to 5.77, by substituting 5.85 into 5.83c, and taking the matrix element for the state $|n_0\rangle$ one will obtain a second power series expansion for $\Delta\omega_n$. Setting this second series equal to the right-hand-side of 5.85, and equating coefficients of each power in λ yields expressions for the $\Delta\omega_n^{(\alpha)}$. Up to $O(\lambda^3)$ we have

$$\begin{aligned}
\Delta\omega_n^{(1)} &= V_{nn}, \\
\Delta\omega_n^{(2)} &= \sum_{m\neq n} \left[\frac{V_{nm}V_{mn}}{\omega_{nm}^0}\right], \\
\Delta\omega_n^{(3)} &= \sum_{m\neq n} \frac{1}{\omega_{nm}^0} \left[\sum_{m\neq n} \left(\frac{V_{nm}V_{mp}V_{pn}}{\omega_{np}^0}\right) - \frac{V_{nn}V_{nm}V_{mn}}{\omega_{nm}^0}\right].
\end{aligned} \tag{5.86}$$

Similarly, one can expand the eigenstate $|n\rangle$ as

$$|n\rangle = \sum_{\alpha=1}^{\infty} \lambda^\alpha |n^{(\alpha)}\rangle \tag{5.87}$$

with $|n^{(0)}\rangle \equiv |n_0\rangle$. Substituting 5.85 into 5.83b and using $\Omega|n_0\rangle = |n\rangle$ one obtains a second power series expansion for $|n\rangle$. Setting this second series equal to the right-hand-side of 5.87, and equating coefficients of each power in λ yields expressions for the $|n^{(\alpha)}\rangle$. Up to

$O(\lambda^2)$ we have

$$|n^{(1)}\rangle = \sum_{m\neq n}\left[\frac{V_{mn}}{\omega^0_{nm}}|m_0\rangle\right]$$
$$|n^{(2)}\rangle = \sum_{m\neq n}\frac{1}{\omega^0_{nm}}\left[\sum_{p\neq n}\left(\frac{V_{mp}V_{pn}}{\omega^0_{np}}|m_0\rangle\right) - \frac{V_{nn}V_{mn}}{\omega^0_{nm}}|m_0\rangle - \frac{V_{nm}V_{mn}}{2\omega^0_{nm}}|n_0\rangle\right]. \tag{5.88}$$

The expressions quickly become complicated in the higher orders, which is why I have only given the expansion up to $O(\lambda^2)$. I will use the results 5.86 and 5.88 in chapter 6.

5.3 Summary and discussion

The S-matrix; bare versus dressed states

The Møller operators $\Omega^{\pm}$ defined in 5.45, produce the in/out-states $|i^{\pm}\rangle, |f^{\pm}\rangle$ associated with the *total* Hamiltonian H, from the bare states $|i\rangle, |f\rangle$. Taking the limiting values $t_i \to -\infty$ and $t_f \to \infty$ in definition 5.44, is the means by which this is achieved. This in turn, is equivalent to the use of an adiabatic switching condition between the initial and final times over which the interaction is assumed to occur. With this mechanism in place, bare states coincide with true eigenstates of the *total* Hamiltonian, before and after the interaction takes place. These eigenstates unlike bare states, are gauge-invariant, which allows us to understand the gauge invariance of the S-matrix. Mathematically gauge invariance of the T-matrix can be proven on-energy-shell, i.e. when the free energy is conserved over the duration of a process (Woolley (1998), Woolley (2000)). Thus, gauge invariance of the S-matrix is ensured by the presence of the delta-function $\delta(\omega_{fi})$.

So the "naive" S-matrix formalism starts with the assumption that in the remote past and remote future bare particles exist, and that they are too remote to interact. These particles are described by the bare states. The Møller operator Ω^+ has the effect of *dressing* the bare particles with clouds of virtual quanta, turning them into *physical particles*. These physical particles are described by the in/out-states associated with the *total* Hamiltonian. The physical particles interact over a finite period of time, and finally, as they move away from each other, the Møller operator $(\Omega^-)^\dagger$ *undresses* them, turning them into bare particles once again.

Alternatively one can view the in-state as a retarded energy eigenstate, which in the remote past coincides with some bare state $|i_0\rangle$. The adiabatic switching on of the interaction dresses the bare state with virtual quanta to produce the physical state $|i^+\rangle$. Similarly one can view the out-state as an advanced energy eigenstate, which in the remote future coincides with some bare state $|f_0\rangle$. The adiabatic switching off of the interaction undresses this bare state (or equivalently dresses the bare state backwards in time) to produce the physical state $|f^-\rangle$.

The action of dressing and undressing described above, is somewhat unphysical. It is

difficult to see how one can adiabatically switch on and off the interaction of a massive particle with the electromagnetic field, for example. One corrects for this idealisation via the process of renormalisation, in which the virtual quanta are included within the initial and final states. Since S is proportional to a coupling constant, the expressions 5.32 and 5.33 for the renormalised S-matrix, show that the process of renormalisation simply changes the value of this coupling constant. More generally renormalisation can be viewed as the procedure by which the effects of virtual quanta are contained within renormalised physical parameters.

So, in summary, starting with the bare states, one arrives at a description of processes involving physical states via the S-matrix formalism. Within the S-matrix formalism it is the in and out-states associated with the *total* Hamiltonian, which are assumed to give *true* descriptions of physical particles. On the other hand, the bare states do not *directly* describe physical particles. We have therefore ended up at the first of the two possible points of view I gave in the introduction.

It seems to me, that this point of view is quite blatantly at odds with the assumption that tensor product structure offers the means by which one decomposes a composite system into *physical* subsystems. It is this second point of view however, which is adopted throughout many areas of physics besides quantum field theory, including quantum information theory, open quantum systems theory, and even quantum optics. Indeed, many of the strange and counter-intuitive aspects of quantum theory, such as quantum nonlocality and entanglement, rest upon this very assumption. The physical reality of any such phenomenon, is subject to whether or not the mathematical representatives of physically meaningful degrees of freedom, can actually be decomposed into tensor product based structures.

Take the Hamiltonian H in 2.71, which clearly admits an infinitude of physically distinct tensor product based decompositions in terms of canonical degrees of freedom. According to the ideas used in scattering theory, the physically meaningful states of well defined energy for the atom, are eigenstates of H itself, and not eigenstates of the free Hamiltonian H_A. A physical state describing the atomic subsystem, does not therefore appear as a tensor factor of some larger tensor product state describing the composite system. Words to this effect appear elsewhere in the literature. For example, having determined that the canonical atomic Hamiltonian H_A^C of the Coulomb gauge is physically different to H_A^P of the Poincaré gauge, Cohen-Tannoudji *et al.* (1997) write...[33]

> *"One can then ask the question: what is the "true" ground state of an atom or a molecule? Is it that of H_A^C or H_A^P? It is in fact neither one or the other. One cannot really remove the interaction of the charges with the transverse field and observe the ground state of H_A^C or H_A^P. What we call the ground state of a system of charges is in fact the ground state of the system charges + transverse*

[33] I have altered the notation in the quote, so that it fits with my own, and I have added my own equation numbering where necessary.

field, which must be an eigenstate of H_C or H_P. These operators are really related by $S = e^{-ie\chi}$ from 6.14, so that the ground state from either point of view describes the same physical state. The eigenstates of H_A^C and of H_A^P, are different approximations of the real state, involving the neglect of this or that part of the effects of the transverse field on the system of charges."

CHAPTER 6

The bare atom versus the dressed atom

We saw in chapter 5 that the question as to precisely what, in the interacting composite system, is to be taken as defining the atomic and electromagnetic subsystems, is intimately related to the question as to what extent the "bare" atom-photon degrees of freedom have any basis in physical reality. The common hypothesis is that the bare atom is surrounded by a cloud of virtual photons within which emission and reabsorption events occur over extremely short time scales (cf. 6.4.2). In seeking to determine the reality of bare degrees of freedom, I analyse in this chapter, the quintessential quantum electrodynamic effects of the Lamb shift and spontaneous emission. In order to do this I start in 6.1 by reviewing conventional quantum optical models. Section 6.2 will be dedicated to level-shifts and the numerous physical interpretations they afford. Section 6.3 will be dedicated to both spontaneous and virtual photon emission, including an analysis of the photodetection divergences brought about by the latter. Finally in 6.4 I will review the work of Compagno *et al.* (1995) on the direct measurement of the virtual cloud.

6.1 The Coulomb and Poincaré gauges in the EDA

In quantum optics one uses the canonical operators belonging to one of two gauges, the Coulomb gauge or the Poincaré gauge. Moreover, the electric dipole approximation (EDA) based on the assumption that the atomic radius is much smaller than optical wavelengths of light, is ubiquitously employed. In this section I briefly demonstrate how these formulations can be obtained from the general Hamiltonian 2.71. This should allow us to begin to assess the specific effects of gauge freedom within the conventional approaches to quantum optics, and to determine the physical natures of the corresponding subsystem decompositions.

6.1.1 Multipolar polarisation

Consider an electron $-e$ displaced by $\mathbf{r} \in E^3$ from the origin, which is the position of a fixed nucleus $+e$ located at the origin. Now suppose one links the nucleus to the electron by joining together n dipoles end to end, with each dipole consisting of charges $-e$ and $+e$ separated by a distance r/n. The sum of these dipoles is a field whose limit as $n \to \infty$ defines the *multipolar electric polarisation field* $\mathbf{P}(\mathbf{x})$;

$$\mathbf{P}(\mathbf{x}) = -e \int_0^1 d\lambda \, \mathbf{r} \delta(\mathbf{x} - \lambda \mathbf{r}). \tag{6.1}$$

The value of $\mathbf{P}$ is $\mathbf{0}$ away from the path connecting the two charges. The divergence of this field is closely related to the charge distribution ρ. In fact using the standard representation

$$\delta(\mathbf{x}) = \frac{1}{(2\pi)^3} \int d^3k \, e^{\pm i\mathbf{k}\cdot\mathbf{x}} \tag{6.2}$$

one sees that

$$i\mathbf{k} \cdot \boldsymbol{P}(\mathbf{k}) = \frac{-e}{(2\pi)^{3/2}} \left(1 - e^{-i\mathbf{k}\cdot\mathbf{r}}\right), \tag{6.3}$$

which in real space reads $\nabla \cdot \mathbf{P} = -\rho$, as is required according to 2.35.

The electric displacement field given in 2.56 is entirely transverse; $\mathbf{D} = \mathbf{D}_{\mathrm{T}}$. Moreover, it is clear that the displacement field is equal to the electric field $\mathbf{E}$ at all points outside the atom, for if $V \subset E^3$ contains the atom, then the integral of $\mathbf{P}$ over the region E^3/V, evaluates to zero. Supposing that V is a sphere of radius a, then if $\omega \ll a^{-1}$ one can perform the *electric dipole approximation*, which constitutes setting

$$e^{i\mathbf{k}\cdot\lambda\mathbf{r}} \approx 1 \tag{6.4}$$

after having used 6.2 to represent the delta-function in 6.1. This approximation necessitates the introduction of an ultra-violet frequency cut-off $\omega_c \sim m^{-1}$, which prohibits interaction with the relativistic modes. Within the EDA the multipolar polarisation field is

$$\mathbf{P}^{\mathrm{EDA}}(\mathbf{x}) = -e\mathbf{r}\delta(\mathbf{x}), \tag{6.5}$$

so the displacement field coincides with the total electric field everywhere except at the origin, which becomes the effective “position of the atom”.

6.1.2 The minimal coupling and multipolar Hamiltonians

Having specified the multipolar polarisation in full we can immediately read off its transverse component, which is given by 2.37 with

$$g_{\mathrm{T},i}(\mathbf{x},\mathbf{x}') := -\int_0^1 d\lambda\, x'_j \delta^{\mathrm{T}}_{ij}(\mathbf{x}-\lambda\mathbf{x}'). \tag{6.6}$$

According to what was said in chapter 2, choosing $\mathbf{g}_{\mathrm{T}}$ in this way specifies a choice of gauge. The Hamiltonian 2.71 in this gauge is the familiar multipolar Hamiltonian frequently used in molecular QED (Craig & Thirunamachandran (1984), Cohen-Tannoudji *et al.* (1997)). The vector potential given in 2.72, corresponding to the gauge choice 6.6, is easily shown to satisfy $\mathbf{r}\cdot\mathbf{A}(\mathbf{r}) = 0$ (Cohen-Tannoudji *et al.* (1997)). This condition is known as the *Poincaré gauge* condition, the gauge choice 6.6 is therefore variously known as the multipolar gauge and the Poincaré gauge. It is interesting to note that the Poincaré gauge condition is nothing but the Coulomb gauge condition implemented in reciprocal space; $\nabla_{\mathbf{k}}\cdot\boldsymbol{A}(\mathbf{k}) = 0$.

In the EDA the multipolar transverse polarisation field is given by 6.5, which can be obtained from 2.37 by taking the Poincaré gauge Green's function $\mathbf{g}_{\mathrm{T}}$ to be given in the EDA by

$$g^{\mathrm{EDA}}_{\mathrm{T},i}(\mathbf{x},\mathbf{x}') = -x'_j \delta^{\mathrm{T}}_{ij}(\mathbf{x}). \tag{6.7}$$

Using this expression together with the definition of the vector potential given in 2.45, we see that in the EDA, the Poincaré gauge vector potential vanishes at the origin;

$$A^{\mathrm{EDA}}_{P,i}(\mathbf{0}) = A_{\mathrm{T},i}(\mathbf{0}) - \left[\partial_i \int d^3x' x_j \delta^{\mathrm{T}}_{kj}(\mathbf{x}') A_{\mathrm{T},k}(\mathbf{x}')\right]_{\mathbf{x}=\mathbf{0}} = 0. \tag{6.8}$$

In the EDA the transverse fields $\mathbf{A}_{\mathrm{T}}(\mathbf{r})$ and $\boldsymbol{\Pi}_{\mathrm{T}}(\mathbf{r})$ taken at the relative position $\mathbf{r}$ of the electron $-e$, are approximated by their values at the origin $\mathbf{0}$.[34] This implies that in the Poincaré gauge and EDA, the canonical momentum $\mathbf{p}$ given in 2.60 coincides with the mechanical momentum $m\dot{\mathbf{r}}$. Thus, in the Poincaré gauge, not only do we have a properly retarded transverse field canonical momentum $\boldsymbol{\Pi}_{\mathrm{T}} = -\mathbf{D}_{\mathrm{T}}$, but within the EDA, we also have a true (mechanical) particle canonical momentum. The Poincaré gauge Hamiltonian in the EDA is according to 2.71 given by

$$H^{\mathrm{EDA}}_P = H_A + H_F - \mathbf{d}\cdot\mathbf{D}_{\mathrm{T}}(\mathbf{0}) \tag{6.9}$$

where $\mathbf{d} := -e\mathbf{r}$ is the atomic dipole moment operator. As I explained after giving the Hamiltonian 2.71 in chapter 2, the dot product in 6.9 must be understood as a dot product of tensor products of operators with the identity, and the Hamiltonians H_A and H_F must

[34] This approximation constitutes a zeroth order expansion of the plane waves $e^{\pm i\mathbf{k}\cdot\mathbf{r}}$ appearing in the mode expansions 2.69, and it is certainly consistent with the definition of the EDA given in 6.4.

be taken as extended to the entire composite space using the identity operator. The atomic Hamiltonian H_A includes a polarisation self energy term, which in the Poincaré gauge and EDA gives

$$H_A = \frac{\mathbf{p}}{2m} + V(\mathbf{r}) + V_{\text{self}} + \varepsilon_{\text{self}} \tag{6.10}$$

where $\varepsilon_{\text{self}}$ is the dipole self energy. Upon discretising the field modes $\varepsilon_{\text{self}}$ can be written

$$\varepsilon_{\text{self}} = \sum_{\mathbf{k}\lambda} \frac{1}{2V} (\mathbf{e}_{\mathbf{k}\lambda} \cdot \mathbf{d})^2. \tag{6.11}$$

The explicit form of the Hamiltonian 6.9 is often referred to as the *multipolar Hamiltonian* in quantum optics and molecular QED. The Hamiltonian in the Coulomb gauge meanwhile is referred to as the *minimal coupling Hamiltonian*. This labelling can serve to obscure the fact that these two Hamiltonians actually constitute different explicit forms of the same Hamiltonian. I will use the labels Coulomb gauge and Poincare gauge to refer to the different gauges themselves, whereas I will use the labels minimal coupling and multipolar to refer to the explicit form of the Hamiltonian within these gauges.

The Coulomb gauge is specified by the choice $\mathbf{g}_{\text{T}} = \mathbf{0}$, implying $\mathbf{A} = \mathbf{A}_{\text{T}}$. The associated (minimal coupling) Hamiltonian in the EDA is

$$H_C^{\text{EDA}} = H_A + H_F + \frac{e}{m} \mathbf{p} \cdot \mathbf{A}_{\text{T}}(\mathbf{0}) \tag{6.12}$$

where H_A is the same as in 6.10 minus the dipole self energy $\varepsilon_{\text{self}}$, and instead H_F includes a self energy term;

$$H_F = \sum_{\mathbf{k}\lambda} \omega \left(a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} + \frac{1}{2} \right) + \frac{e^2}{2m} \mathbf{A}(\mathbf{0})^2. \tag{6.13}$$

The minimal coupling and multipolar Hamiltonians are related by a unitary gauge fixing transformation $S = e^{-ie\chi}$ of the type given in 3.89. This transformation is known as the *Power-Zienau-Woolley* (PZW) transformation. The generator χ is the generator of the gauge transformation relating the two gauges. Explicitly we have

$$H_P = e^{-ie\chi} H_C e^{ie\chi}, \qquad \chi := \int d^3x \, \boldsymbol{g}_{\text{T}}(\mathbf{x}, \mathbf{r}) \cdot \mathbf{A}_{\text{T}}(\mathbf{x}) \equiv \frac{1}{e} \int d^3x \, \mathbf{P}_{\text{T}}(\mathbf{x}) \cdot \mathbf{A}_{\text{T}}(\mathbf{x}) \tag{6.14}$$

where $\boldsymbol{g}_{\text{T}}$ corresponds to the Poincaré gauge, so that $\mathbf{P}$ is the multipolar polarisation field. In the EDA 6.14 simplifies to

$$H_P^{\text{EDA}} = e^{-i\chi^{\text{EDA}}} H_C^{\text{EDA}} e^{i\chi^{\text{EDA}}}, \qquad \chi^{\text{EDA}} := \mathbf{d} \cdot \mathbf{A}_{\text{T}}(\mathbf{0}). \tag{6.15}$$

The generator χ appearing in 6.14 and 6.15 produces a nonlocal unitary operator $S \neq S_A \otimes S_F$. Thus, the PZW transformation mixes up the canonical degrees of freedom of

the Coulomb gauge in passing to the Poincaré gauge. This can be viewed as the cause of the physical differences in the canonical momenta between the two gauges. It is obviously important to determine which physical predictions come out gauge-invariant, despite the use of physically distinct canonical degrees of freedom. This was the subject of chapter 5.

6.1.3 *The Maxwell fields in the Coulomb and Poincaré gauges*

Classically Maxwell's equations for given sources were solved in chapter 4. On the quantum level the Hamiltonian 2.71 yields Maxwell's equations as operator equations. Formally these equations can be solved in the same way as before. Predictions however, come in the form of expectation values, with the system allowed to possess, in general, superposition states. I review here the canonical Maxwell fields in the Coulomb and Poincaré gauges, within the EDA. For more detailed accounts the reader is referred to Power & Thirunamachandran (1999a) and Power & Thirunamachandran (1999b).

Using the Hamiltonians 6.9 and 6.12 together with the Heisenberg equation we can calculate the various Maxwell fields, of the two gauges. I will assume the EDA throughout and therefore omit the superscript $^{\text{EDA}}$. In addition the canonical field operators at the origin $\mathbf{A}_{\text{T}}(\mathbf{0})$ and $\mathbf{\Pi}_{\text{T}}(\mathbf{0})$, will be written simply $\mathbf{A}_{\text{T}}$ and $\mathbf{\Pi}_{\text{T}}$. It is instructive to use the photon creation and annihilation operators to work out the Maxwell fields in the two gauges. In the Coulomb gauge one has

$$\dot{a}_{\mathbf{k}\lambda}(t) = -i[a_{\mathbf{k}\lambda}(t), H_C] = -i\omega a_{\mathbf{k}\lambda}(t) + ig\dot{\mathbf{d}}(t)\cdot\mathbf{e}_{\mathbf{k}\lambda} \tag{6.16}$$

where $m\dot{\mathbf{d}} = -e(\mathbf{p} + e\mathbf{A}_{\text{T}})$. Formal integration then yields

$$a_{\mathbf{k}\lambda}(t) = a_{\mathbf{k}\lambda}(0)e^{-i\omega t} + ig\int_0^t dt' e^{-i\omega(t-t')}\dot{\mathbf{d}}(t')\cdot\mathbf{e}_{\mathbf{k}\lambda}. \tag{6.17}$$

In the Poincaré gauge one has in a similar manner

$$a_{\mathbf{k}\lambda}(t) = a_{\mathbf{k}\lambda}(0)e^{-i\omega t} + \omega g\int_0^t dt' e^{-i\omega(t-t')}\mathbf{d}(t')\cdot\mathbf{e}_{\mathbf{k}\lambda}. \tag{6.18}$$

The term $a_{\mathbf{k}\lambda}(0)e^{-i\omega t}$ in these expressions is the component of evolution generated by the "free" field Hamiltonian H_F given in 2.71.[35] The creation and annihilation operators clearly carry different physical significance in the two gauges, and so too, does H_F. We will see shortly that in separating the Maxwell fields out into free and source components based on the corresponding partitions in 6.17 and 6.18, the individual free and source components are generally gauge dependent, even for gauge-invariant *total* fields such as the electric field.

[35] Note that with regard to the Coulomb gauge calculation, by H_F I mean H_F as in 2.71, and not as in 6.13. Therefore, the $\frac{e^2}{2m}\mathbf{A}_{\text{T}}^2$ term does not contribute to the free evolution of $a_{\mathbf{k}\lambda}$.

The transverse vector potential and the magnetic field

Substituting 6.17 into the mode expansions 2.69 for $\mathbf{A}_\mathrm{T}$ one obtains in the Coulomb gauge

$$\mathbf{A}_\mathrm{T} = \mathbf{A}^0_\mathrm{T} + \mathbf{A}^s_\mathrm{T}, \tag{6.19}$$

where $\mathbf{A}^0_\mathrm{T}$ is the free component with evolution generated by H_F;

$$\mathbf{A}^0_\mathrm{T}(t,\mathbf{x}) = \sum_{\mathbf{k}\lambda} g\mathbf{e}_{\mathbf{k}\lambda}\left(a^\dagger_{\mathbf{k}\lambda}(0)e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} + a_{\mathbf{k}\lambda}(0)e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t}\right), \tag{6.20}$$

and $\mathbf{A}^s_\mathrm{T}$ is the source component, which with a little work is found to be

$$\mathrm{A}^s_{\mathrm{T,i}}(t,\mathbf{x}) = \begin{cases} \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\displaystyle\int_{t-x}^{t} dt'\,\mathrm{d}_j(t') & \text{if } t > x, \\ \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\displaystyle\int_{0}^{t} dt'\,\left[\mathrm{d}_j(t') - \mathrm{d}_j(0)\right] & \text{if } t < x \end{cases} \tag{6.21}$$

where as always repeated spatial indices are assumed to be summed.

To obtain the Poincaré result one substitutes 6.18 into the mode expansion 2.69 for $\mathbf{A}_\mathrm{T}$. As a result one obtains 6.19 with $\mathbf{A}^0_\mathrm{T}$ as in 6.20, but with $\mathbf{A}^s_\mathrm{T}$ given instead by

$$\mathrm{A}^s_{\mathrm{T,i}}(t,\mathbf{x}) = \begin{cases} \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\displaystyle\int_{t-x}^{t} dt'\,\mathrm{d}_j(t') & \text{if } t > x, \\ \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\displaystyle\int_{0}^{t} dt'\,\mathrm{d}_j(t') & \text{if } t < x. \end{cases} \tag{6.22}$$

Despite the gauge invariance of $\mathbf{A}_\mathrm{T}$ its source and free components are different in the two gauges due to the implicit difference in the generator H_F of the "free" evolution. The free component in the Coulomb gauge implicitly contains an extra factor compared to the Poincaré gauge result;

$$\mathbf{A}^0_{\mathrm{T},CG}(t) = \mathbf{A}^0_{\mathrm{T},PG}(t) + \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\frac{t}{4\pi x}\mathrm{d}_j(0), \quad \text{for } t < x, \tag{6.23}$$

so that the total field is seen to be gauge-invariant, as it should be. The magnetic field $\mathbf{B}$ is readily obtained using $\mathbf{B} = \nabla \times \mathbf{A}_\mathrm{T}$. The result contains a causal source component which is the same in both gauges;

$$\mathrm{B}^s_i(t,\mathbf{x}) = \begin{cases} -\varepsilon_{ijk}\partial_k\dfrac{1}{4\pi x}\dot{\mathrm{d}}_j(t) & \text{if } t > x, \\ 0 & \text{if } t < x \end{cases} \tag{6.24}$$

where ε_{ijk} denotes the Levi-Civita symbol.

The transverse and total electric fields

The transverse electric field can be found using $\mathbf{E}_{\mathrm{T}} = -\dot{\mathbf{A}}_{\mathrm{T}}$. As usual we have

$$\mathbf{E}_{\mathrm{T}} = \mathbf{E}^{0}_{\mathrm{T}} + \mathbf{E}^{s}_{\mathrm{T}}. \tag{6.25}$$

In the Coulomb gauge the source component is

$$\mathrm{E}^{s}_{\mathrm{T,i}}(t,\mathbf{x}) = \begin{cases} \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\left[\mathrm{d}_j(t-x) - \mathrm{d}_j(t)\right] & \text{if } t > x, \\ \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\left[\mathrm{d}_j(0) - \mathrm{d}_j(t)\right] & \text{if } t < x, \end{cases} \tag{6.26}$$

whereas in the Poincaré gauge one has

$$\mathrm{E}^{s}_{\mathrm{T,i}}(t,\mathbf{x}) = \begin{cases} \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\left[\mathrm{d}_j(t-x) - \mathrm{d}_j(t)\right] & \text{if } t > x, \\ \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\mathrm{d}_j(t) & \text{if } t < x. \end{cases} \tag{6.27}$$

The total electric field can be found by adding the longitudinal component to the transverse component. For $\mathbf{x} \neq \mathbf{0}$, $\mathbf{E}_{\mathrm{L}}$ is given by $\mathbf{E}_{\mathrm{L}} = -\mathbf{P}_{\mathrm{L}} = \mathbf{P}_{\mathrm{T}}$, and

$$\mathrm{P}_{\mathrm{T},i}(t,\mathbf{x}) = \delta^{\mathrm{T}}_{ij}(\mathbf{x})\mathrm{d}_j(t) = \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\frac{1}{4\pi x}\mathrm{d}_j(t). \tag{6.28}$$

Adding this term to the transverse field gives in the Coulomb gauge

$$\mathrm{E}^{s}_{i}(t,\mathbf{x}) = \begin{cases} \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\mathrm{d}_j(t-x) & \text{if } t > x, \\ \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\mathrm{d}_j(0) & \text{if } t < x, \end{cases} \tag{6.29}$$

while in the Poincaré gauge we get

$$\mathrm{E}^{s}_{i}(t,\mathbf{x}) = \mathrm{D}^{s}_{\mathrm{T},i}(t,\mathbf{x}) = \begin{cases} \left(-\delta_{ij}\partial^2 + \partial_i\partial_j\right)\dfrac{1}{4\pi x}\mathrm{d}_j(t-x) & \text{if } t > x, \\ 0 & \text{if } t < x. \end{cases} \tag{6.30}$$

So, our review of the Maxwell fields in the two gauges shows that the free and source components of fields tend to differ, even when the total fields are the same. The Coulomb gauge source fields depend on additional contributions from the initial atomic dipole moment $\mathbf{d}(0)$. This is because the Coulomb gauge field Hamiltonian H_F is defined in terms of the transverse electric field, rather than the total electric field as in the Poincaré gauge. Moreover, as I have already noted the atomic source in the Poincaré gauge is defined in terms of the true mechanical dipole momentum. This seems to show that the Poincaré gauge partitioning of the composite system into subsystems is the more physical.

It should be noted however, that only in the EDA do the mechanical and canonical

dipole momentum of the Poincaré gauge coincide. Without the EDA $\mathbf{p}$ contains additional contributions from a variant of the polarisation field (Craig & Thirunamachandran (1984)). This can be understood by noting that $\mathbf{p} = m\dot{\mathbf{r}} - e\mathbf{A}(\mathbf{r})$, but outside the EDA the total vector potential in the Poincaré gauge does not vanish. Furthermore, the electric displacement field $\mathbf{D}_{\mathrm{T}}$ only coincides with the total electric field at points outside the source. In the EDA the atomic source is effectively a point source at the origin, yet strictly speaking the atomic electron wavefunction will only vanish infinitely far from the source of the binding potential. Without the EDA, and particularly within the quantum mechanical setting the distinction between the displacement field and the total electric field may be significant.

Finally, it is worth remarking that at the origin the two fields $\mathbf{E}$ and $\mathbf{D}_{\mathrm{T}}$ differ by an infinite contribution in the form of the electric polarisation field $\mathbf{P}$. This is not trivial because the atom must respond to any field at its own position. A consequence of the difference in the two fields is that one obtains the additional infinite contribution $\varepsilon_{\mathrm{self}}$ within H_A, on top of the longitudinal self energy V_{self}. We shall see in section 6.4 that the Poincaré gauge suffers more severely than the Coulomb gauge from divergences that plague the theory of photodetection, in which the atom is assumed to absorb photons at its own position.

Vacuum fluctuations and radiation reaction

The results of this section have been based on the partition of operators into free and source components. In expressions 6.17 and 6.18 the free components with evolution generated by H_F are often termed vacuum contributions. These are the only contributions in free quantum electrodynamics. The presence of a background quantum vacuum is often inferred from the non-vanishing of the expectation values of the squares of the electric and magnetic fields, taken in the photon vacuum state. This is due to the anti-normally ordered products of creation and annihilation operators, that appear in such expressions.[36] The electric and magnetic fields can be viewed as fluctuating about their mean values of zero. The existence of the quantum vacuum, which is not present according to the classical theory, can be used to explain why atoms are stable, and even to eliminate the existence of runaway solutions to the Abraham-Lorentz equation (Milonni (1994)).

The name given to the source component of a field at the position of the source is *radiation reaction*. A feature of quantum optics that has received a great deal of attention in the past, is the apparent facility to (somewhat arbitrarily) attribute physical phenomena to both radiation reaction and the vacuum; which of the two mechanism contributes more seems to be determined by the ordering employed when writing down *commuting* atom and field operators (Milonni *et al.* (1973), Dalibard *et al.* (1982), Milonni (1994), Compagno *et al.* (1995)).

We should really expect this sort of freedom, because in the presence of sources, the

[36] Creation and annihilation operators are said to be *normally (anti-normally)* ordered when all creation (annihilation) operators are found to the left of the annihilation (creation) operators.

vacuum and source components of a field are physically different in each gauge (cf. section 6.1.3). The problem of determining the complimentary nature of vacuum and radiation reaction fields, is not separate to our problem concerning how to decompose the composite system into subsystems. The fact that we can attribute physical phenomena to one or the other of vacuum and radiation reaction fields, is consistent with the viewpoint that it is only really the gauge-invariant *total* fields, that have physical meaning. If one wishes to attribute physical effects to either the vacuum field or radiation reaction, one must choose a gauge in conjunction with which one makes such attributions. This physical interpretation would have to be modified to be given in a different gauge, in order to account for any differences in the source and free components between the two gauges.

6.2 Level shifts

Given the discussion above, this seems like a good point at which to analyse the physical significance of *level shifts*, which can be attributed to both vacuum and radiation reaction fields. The *Lamb shift* named after Lamb & Retherford (1947), which is the difference in energy of the $2s^{\frac{1}{2}}$ level above the $2p^{\frac{1}{2}}$ level in atomic hydrogen, is the best known example. Without taking the electromagnetic field into account the $2s^{\frac{1}{2}}$ and $2p^{\frac{1}{2}}$ levels are predicted to be degenerate. Thus, the Lamb shift is a purely quantum electrodynamic effect. Indeed, the agreement between the theoretically predicted Lamb shift and the measured value, is probably the single most significant factor responsible for the perceived success of quantum electrodynamics.

The importance of the Lamb shift might go some way to explaining the vast amount of attention it has received over the years, as well as the surprisingly large number of different physical interpretations of level shift phenomena conceived since the original calculations of Bethe (1947).

6.2.1 The Welton interpretation

Welton (1948) has given a heuristic interpretation of atomic level shifts, in which vacuum fluctuations are seen as the root cause. In Welton's interpretation the electron experiences oscillations $\delta\mathbf{r}$ about its position $\mathbf{r}$ within the atom. These oscillations are induced by the vacuum fluctuations of the field. Their effect is to perturb the Coulomb potential due to the atomic nucleus, which gives an effective potential

$$V(\mathbf{r}+\delta\mathbf{r}) = V(\mathbf{r}) + \delta\mathbf{r}\cdot\nabla V(\mathbf{r}) + \frac{1}{2}(\delta\mathbf{r}\cdot\nabla)^2 V(\mathbf{r}) + \ldots . \tag{6.31}$$

Since $\delta\mathbf{r}$ is the oscillation induced by the vacuum fluctuations one assumes that it obeys the same equation of motion as a *free* i.e. unbound electron coupled to the free component of

the transverse electromagnetic field. In the electric dipole approximation one has

$$m\ddot{\delta\mathbf{r}} = -e\mathbf{E}_{\mathrm{T}}^{0} \tag{6.32}$$

for a stationary nucleus at the origin. Expanding $\delta\mathbf{r}$ in plane wave Fourier modes akin to the expansions in 2.69, one obtains

$$\delta\mathbf{r} = \sum_{\mathbf{k}\lambda} \mathbf{e}_{\mathbf{k}\lambda} \left(\delta\boldsymbol{r}_{\mathbf{k}\lambda} e^{-i\omega t} + \delta\boldsymbol{r}_{\mathbf{k}\lambda}^{\dagger} e^{i\omega t} \right) \tag{6.33}$$

while for the right-hand-side of 6.32 we have

$$\mathbf{E}_{\mathrm{T}}^{0} := -i \sum_{\mathbf{k}\lambda} \omega g \mathbf{e}_{\mathbf{k}\lambda} \left(a_{\mathbf{k}\lambda}^{\dagger}(0) e^{i\omega t} - a_{\mathbf{k}\lambda}(0) e^{-i\omega t} \right). \tag{6.34}$$

From 6.32 one therefore obtains

$$m\omega^2 \delta\mathbf{r}_{\mathbf{k}\lambda} = e\omega_{\mathbf{k}\lambda}, \qquad \delta\mathbf{r}_{\mathbf{k}\lambda} = \frac{eg}{m\omega} a_{\mathbf{k}\lambda}. \tag{6.35}$$

We see then, that $\delta\mathbf{r}$ is to be taken as an operator in the field Hilbert space. The vacuum fluctuations are assumed isotropic, so one can assume that

$$\langle (\delta\mathbf{r}\cdot\nabla)^2 \rangle = \frac{1}{3} \langle \delta\mathbf{r}^2 \rangle \nabla^2. \tag{6.36}$$

To obtain an expression for the effective potential experienced by the electron one substitutes the result 6.35 into 6.36 and takes the vacuum expectation value. Converting the discrete sum into an integral, performing the sum over polarisations, and substituting the resulting expression into 6.31 gives

$$V_{\mathrm{eff}}(\mathbf{r}) := V(\mathbf{r}+\delta\mathbf{r}) \approx V(\mathbf{r}) + \frac{1}{6} \left(\frac{e^2}{2\pi^2 m^2} \int d\omega \, \frac{1}{\omega} \right) \nabla^2 V(\mathbf{r}) \tag{6.37}$$

where only the first nonzero correction in the expansion 6.31 has been retained. The electric dipole approximation warrants the use of an upper frequency cut-off $\omega_u \sim m$. Also required to regularise the integral, is a lower frequency cut-off ω_l, which is taken to depend on the details of the binding potential. Introducing these cut-offs and using $\nabla^2 V = -\rho = e\delta(\mathbf{r})$ one obtains

$$\Delta V(\mathbf{r}) := V_{\mathrm{eff}}(\mathbf{r}) - V(\mathbf{r}) = \frac{e^4}{12\pi^2 m^2} \delta(\mathbf{r}) \ln \frac{\omega_u}{\omega_l}. \tag{6.38}$$

The expectation value of this operator for the atomic state $|m_0\rangle$ gives its energy shift induced by the vacuum field. Furthermore, a natural lower cut-off ω_l is obtained if one assumes that the vacuum fluctuations are at least as large as the average difference in the energy $\overline{\omega}_m$ between the state $|m_0\rangle$ and the other atomic levels. With this, one finally obtains the

standard "Bethe log" nonrelativistic level shift of the state $|m_0\rangle$;

$$\Delta\omega_m = \frac{4\alpha^2}{3m^2}|\psi_m(0)|^2 \ln\frac{\omega_u}{\overline{\omega}_m}. \tag{6.39}$$

In atomic hydrogen this shift is nonzero for s-states only. For the $2s$ state

$$|\psi_m(0)|^2 = \frac{1}{8\pi a_0^3} \tag{6.40}$$

where $a_0 = 1/m\alpha$ denotes the Bohr radius. Thus, the Lamb shift is

$$\Delta := \Delta\omega_{2s} - \Delta\omega_{2p} = \frac{m\alpha^5}{6\pi}\ln\frac{\omega_u}{\overline{\omega}_{2s}}. \tag{6.41}$$

6.2.2 The Power-Feynman interpretation

Feynman (1961) suggested a different interpretation of level shifts, which was taken to fruition by Power (1966). In contrast to Welton's idea, in the Feynman-Power interpretation, it is the zero-point energy of the *field* which is altered by the presence of the atom, rather than the atomic levels being altered by the field. The energy shift manifests itself by altering the refractive index n of the vacuum. In a medium of N atoms each in the bare state $|m_0\rangle$, the velocity of light is $1/n(m)$. The field frequency dispersion relation is consequently altered; $\omega(m) := \omega/n(m)$. The total zero-point shift between the $2s$ and $2p$ levels can now be found as the difference

$$\Delta = E_F^{\rm zp}(2s) - E_F^{\rm zp}(2p) = \frac{1}{2}\sum_{\mathbf{k}\lambda}[\omega(2s) - \omega(2p)]. \tag{6.42}$$

One takes the refractive index $n(m)$ to be given in terms of the atomic energy levels by (Becker (1982), Compagno *et al.* (1995))

$$n(m) = 1 + \frac{4\pi}{3}N\sum_p \frac{|\mathbf{d}_{pm}|^2\omega_{pm}}{\omega_{pm}^2 - \omega^2} \approx 1 + \frac{4\pi}{3}N\sum_p \frac{|\mathbf{d}_{pm}|^2}{\omega^2}\left(\omega_{pm} + \frac{\omega_{pm}^3}{\omega^2}\right) \tag{6.43}$$

with the approximate equality valid under the assumption that it is the high frequency field modes that give the dominant contribution. Using the Thomas-Reiche-Kuhn sum rule

$$\sum_p \omega_{pm}|\mathbf{d}_{pm}|^2 = \frac{3e^2}{2m} \tag{6.44}$$

and the relation

$$\mathbf{p}_{pm} = im\omega_{pm}\mathbf{r}_{pm} \tag{6.45}$$

between matrix elements of position and canonical momentum in the free energy basis, one

obtains after some straightforward manipulation (Power (1966), Compagno *et al.* (1995))

$$\frac{\Delta}{N} = \frac{m\alpha^5}{6\pi} \ln \frac{\omega_u}{\overline{\omega}_{2s}}, \tag{6.46}$$

which is the same as the result 6.41.

We have seen then that level-shifts can be attributed to the quantum vacuum or to radiation reaction fields. They can also be viewed as shifts in the bare atomic energies or as shifts in the bare vacuum field energy. This (quite considerable) freedom in the choice of physical interpretation of level-shift phenomena is of course, exactly what one might expect, given that "atom" and "field", as well as "vacuum" and "radiation reaction" are all gauge-dependent labels. The freedom one possesses in attaching these labels (somewhat arbitrarily) to physical phenomena, could be viewed as nothing but gauge freedom.

6.2.3 Self energy and renormalisation

The most common method of deriving level shifts is to use elementary time-independent perturbation theory, which does not rely on heuristic arguments. As a necessary precursor to the level shift calculation of the bound electron, I consider here the self energy shifts of a free electron.

The longitudinal self energy

We saw in 4.4 that the longitudinal field energy associated with a point charge gives rise to a divergent Coulomb self energy V_{self}. I suggested that the only directly observable effect of this energy is to contribute to the observed mass of the electron. In the fully covariant QED formalism longitudinal and scalar photons are quantised. The longitudinal self energy can be shown to give rise to a *small* contribution to the mass of the electron, due to emission and reabsorption of longitudinal photons (Heitler (1954), Lawrie (2002)). In the non-covariant gauges the Coulomb self energy term is usually omitted from consideration.

It is important to note however, that the omission of terms from the Hamiltonian is a dangerous business if one wishes to retain the crucial property that it produces the correct equations of motion. The neglect of the Coulomb self energy on the grounds that it is unobservable may be premature. It seems that it would be more correct to say that it is not *directly* observable. If however, one observes the equations of motion, and the self energy is required to yield the correct form of these equations, then it does evidently produce some observable effects. It must therefore be understood as being present, while the infinite contribution it makes in various calculations understood as renormalising the bare mass of the electron. This situation is of course, quite familiar (cf. 4.4).

The transverse self energy

In the quantum setting there arises an infinite energy shift of the free electron due to its coupling to the *transverse* field. This energy shift is dealt with in precisely the same way as the longitudinal self energy, it is taken as renormalising the bare mass of the electron. I take the Hamiltonian 6.12 in the Coulomb gauge and EDA, but without the potential term describing the binding of the electron to the nucleus;[37]

$$H = \frac{1}{2m}\left(\mathbf{p} + e\mathbf{A}_{\mathrm{T}}\right)^2 + H_F. \tag{6.47}$$

Second order perturbation theory (5.86) yields for the bare state $|\mathbf{p}_0; 0_0\rangle$ of zero photons and electronic canonical momentum $\mathbf{p}$, a shift of (see for example Craig & Thirunamachandran (1984))

$$\left[\frac{\alpha}{m\pi} - \frac{\mathbf{p}^2}{2m}\left(\frac{4\alpha}{3\pi}\right)\right]\int_0^\infty d\omega. \tag{6.48}$$

The first term in the square brackets arises from the $\mathbf{A}_{\mathrm{T}}^2$ term of the interaction Hamiltonian. Since it is independent of the state of the electron it can't lead to any directly observable effects and its contribution can be included within the zero-point energy.[38] The remaining term can be written

$$-\frac{\mathbf{p}^2}{2m}\frac{\delta m}{m}, \qquad \delta m := \frac{4\alpha}{3\pi}\int_0^\infty d\omega. \tag{6.49}$$

Defining the observable mass as $m_{\mathrm{obs}} := m + \delta m$, one obtains correct to second order

$$H - H_F = \frac{\left(\mathbf{p} + e\mathbf{A}_{\mathrm{T}}\right)^2}{2(m_{\mathrm{obs}} - \delta m)} \approx \frac{\mathbf{p}}{2m_{\mathrm{obs}}} + \frac{e}{m_{\mathrm{obs}}}\mathbf{p}\cdot\mathbf{A}_{\mathrm{T}} + \frac{e^2}{2m_{\mathrm{obs}}}\mathbf{A}_{\mathrm{T}}^2 + \frac{\mathbf{p}^2}{2m_{\mathrm{obs}}}\frac{\delta m}{m_{\mathrm{obs}}}. \tag{6.50}$$

If one now calculates the energy shift as before, the contribution from the last term in 6.50 will cancel that of the the second term, giving a total shift of zero. Thus, we can effectively absorb the shift induced by the transverse field into the observable mass of the electron, a procedure known as *mass renormalisation*. The bare energy of the electron is subsequently $\mathbf{p}^2/2m_{\mathrm{obs}}$.

6.2.4 Level shifts via elementary perturbation theory

I start-off in the Coulomb gauge and as usual neglect V_{self}. The level shift, as in the case of the free electron, is the difference in the energy of the bare eigenstate $|m_0; 0_0\rangle$ and the

[37] As is conventional, I neglect V_{self}.

[38] In a similar fashion to the longitudinal self energy, one cannot neglect the $\mathbf{A}_{\mathrm{T}}^2$ term from the Hamiltonian and hope to obtain the same equations of motion. Thus, it seems that it is only within the calculation of the self energy that it can be neglected.

corresponding true eigenstate denoted $|m;0\rangle$. Using second order perturbation theory (5.86) with mass renormalisation already carried out, and as before neglecting the contribution of the $\mathbf{A}_{\mathrm{T}}^2$ term, one obtains (see for example Craig & Thirunamachandran (1984))

$$\Delta\omega_m = \frac{2\alpha}{3\pi m_{\mathrm{obs}}} \sum_n \int d\omega \, \frac{\omega_{nm}|\mathbf{p}_{nm}|^2}{\omega_{nm}+\omega} \tag{6.51}$$

Following Bethe (1947) I introduce the upper cut-off ω_u to carry out the integration, and replace the energy difference ω_{nm} in the resulting logarithm with the average difference $\overline{\omega}$, to give

$$\Delta\omega_m = \frac{2\alpha}{3\pi m_{\mathrm{obs}}} \sum_n \omega_{nm}|\mathbf{p}_{nm}|^2 \ln\frac{\omega_u}{\overline{\omega}}. \tag{6.52}$$

Finally, using the sum rule

$$\sum_n \omega_{nm}|\mathbf{p}_{nm}|^2 = \frac{e^2}{2}|\psi_m(0)|^2 \tag{6.53}$$

one obtains the standard Bethe log result

$$\Delta\omega_m = \frac{4\alpha^2}{3m_{\mathrm{obs}}^2}|\psi_m(0)|^2 \ln\frac{\omega_u}{\overline{\omega}_m}. \tag{6.54}$$

The same result is obtained using the Poincaré gauge provided the polarisation self energy term $\varepsilon_{\mathrm{self}}$ is retained, and as in the Coulomb gauge calculation, any contributions independent of the bare electronic state are neglected (Craig & Thirunamachandran (1984)). Of course, this invariance is just a particular case of the gauge invariance of the on-energy-shell T-matrix. From the point of view of perturbation theory, the level shifts must be identical, because H_0 is identical in both gauges, while H_{CG} and H_{PG} possess identical spectra due to their unitary equivalence.

We have seen that the Lamb shift can be viewed as a shift of the bare atomic energy as in 6.2.1, or a shift in the bare field energy as in 6.2.2. It is therefore not all that surprising that as the calculation above clearly demonstrates the Lamb shift in atomic hydrogen, can also be viewed as a shift in the energy of the composite atom-field system.

If the measured energy of the hydrogen atom is an eigenvalue of the total Hamiltonian, then we appear to be no closer to achieving our goal of identifying the atom and field subsystems. It is natural to ask whether or not there is a reasonable decomposition of the Hamiltonian 2.71 into subsystem components, which is consistent with the fact that the Lamb shift coincides with a difference in eigenvalues of the total Hamiltonian. In fact, such a decomposition appears to be afforded by 2.61, in which one primitively takes the energy of the atom to be defined in terms of precisely the same *physical observables* as in the

noninteracting theory

$$H_A^{\text{true}} := \frac{1}{2} m\dot{\mathbf{r}}^2 + V(\mathbf{r}). \tag{6.55}$$

Similarly the transverse field energy is

$$H_{\text{TF}} := \frac{1}{2} \int d^3x \left(\mathbf{E}_{\text{T}}^2 + \mathbf{B}^2 \right), \tag{6.56}$$

while the longitudinal field energy is only directly observable through the mass of the electron. It is clear that after subtracting the infinite zero-point energy of the transverse field, the vacuum $|0_0\rangle$ is an eigenstate of H_F with eigenvalue 0. The shift between the energy of any bare eigenstate $|n_0;0_0\rangle$ of H_0, and the corresponding eigenvalue of H, is therefore the same as the shift between the energy of $|n_0;0_0\rangle$ viewed as an eigenstate of $H_A \otimes I$, and the corresponding eigenvalue of H_A^{true}. Thus, the observed shifted energy eigenvalue of the $2s$ state in hydrogen, is indeed an eigenvalue of H_A^{true}.

This suggests that in going from the theory of a noninteracting bound electron, to a bound electron in the electromagnetic field, one should continue to define the atomic energy in terms of the same *physical observable* as was used in the noninteracting theory, which is the *mechanical momentum*. The same is true of the transverse field, whose energy H_F^{true} should be defined in terms of $\mathbf{E}_{\text{T}}$ regardless of whether or not $\mathbf{\Pi}_{\text{T}} = -\mathbf{E}_{\text{T}}$, which happens to be the case in the Coulomb gauge.

To my knowledge, this interpretation of the Lamb shift has not been given explicitly before, although it is certainly possible that it has been tacitly assumed when interpreting level shifts as arising from emission and absorption of virtual quanta. The Coulomb gauge calculation presented above for example, is consistent with viewpoint 1 and the S-matrix formalism - that virtual quanta are emitted and reabsorbed by the bare atom, but these virtual quanta are really just mathematical devices allowing us to determine the true atomic energy.

In the Poincaré gauge and EDA, the free atomic Hamiltonian is already defined in terms of the mechanical momentum, but H_F is defined in terms of the transverse displacement field and not the transverse electric field. Thus, the Lamb shift is a shift between the bare and true transverse field energies. In both gauges, and indeed in any gauge, we have the same unambiguous subsystem definitions. In measuring the energy of a true hydrogen atom in the true electromagnetic vacuum, one obtains an eigenvalue of H_A^{true}. The notions of bare atom, bare photons and the virtual cloud therefore become superfluous. In addition one can decisively determine what the appropriate vacuum/radiation-reaction decompositions should be for the various Maxwell fields. It's a separate issue as to whether or not such a decomposition is of any physical significance.

6.3 Photon emission; spontaneous and virtual

Spontaneous emission is the process by which an excited atom makes a transition to a lower level, and in doing so emits a photon. This is the quantum interpretation of radiation, which implicitly seems to presuppose some notion of free energy conservation. Of course, in the case of bare atoms and photons the emission event must occur over an infinite time in order that the free energy is conserved with absolute certainty.

It is not surprising then that the S-matrix formalism provides the most direct route to obtaining the *spontaneous emission rate* of an excited atom. There are however, alternatives. One of the best known of these is the Weisskopf & Wigner (1930) (WW) treatment used in quantum optics. This treatment entails a series of "approximations", which eliminate the effects of virtual quanta and effectively turn the entire calculation into that of an S-matrix element. We have seen however, that rather than approximations the assumptions underlying the S-matrix formalism appear to be necessary restrictions in order that the use of bare states is actually permissible. We are therefore lead quite naturally to the question; are these so-called approximations *bona fide* approximations, and what happens if we avoid making them?

6.3.1 The spontaneous emission rate

The S-matrix calculation of the spontaneous emission rate Γ of an excited atom, consists of the straightforward application of the Fermi golden rule given in 5.1.3, and as such is standard textbook fare (see for example Craig & Thirunamachandran (1984), Cohen-Tannoudji *et al.* (1992)). Let $|f\rangle = |g;\mathbf{k}\lambda\rangle$ be the state in which the atom is in the ground state and a single photon $\mathbf{k}\lambda$ is present, and let $|i\rangle = |e;0\rangle$ be the state in which the atom is excited and there are no photons. Summing over *all* one-photon final states constitutes the prescription

$$\sum_f \rho = \int d\omega\, \omega^2 \int d\Omega \sum_\lambda \frac{V}{(2\pi)^3}. \tag{6.57}$$

Taking the minimal coupling Hamiltonian in the EDA in 6.12, the first order T-matrix element $T^{(1)}_{fi}$ is

$$T^{(1)}_{g,\mathbf{k}\lambda;e} = \frac{eg}{m}\mathbf{p}_{eg}\cdot\mathbf{e}_{\mathbf{k}\lambda}, \qquad g := \frac{1}{\sqrt{2\omega V}}. \tag{6.58}$$

The total transition rate out of the state $|e,0\rangle$ is according to 5.54

$$\Gamma := w^{\text{group}}_{f\to i} = 2\pi \int d\omega\, \omega^2 \sum_\lambda \int d\Omega\, \frac{V}{(2\pi)^3} |T_{g,\mathbf{k}\lambda;e}|^2 \delta(\omega_{eg}-\omega) = \frac{\omega_{eg}^3 |\mathbf{d}_{eg}|^2}{3\pi} \tag{6.59}$$

where the sum over polarisations and spherical solid angle integration have been carried out, and 6.45 has been used. Note that this result must be gauge-invariant, due to the gauge invariance of the S-matrix.

6.3.2 The Weisskopf-Wigner treatment

The Weisskopf & Wigner (1930) treatment can be found in most introductory texts on quantum optics (see for example Scully & Zubairy (1997), Milonni (1994)), so I will keep my review brief. My main aim is to clearly ascertain the role of the approximations made in the treatment.

I start with the minimal coupling Hamiltonian in the EDA 6.12 again, and make two further approximations. The first is the *two-level approximation* (2LA) for the atom, in which only the ground state $|g\rangle$ and first excited state $|e\rangle$ are taken into account. The atom becomes a fictitious spin with *raising and lowering operators*

$$\sigma^+ := |e\rangle\langle g|, \qquad \sigma^- := |g\rangle\langle e|. \tag{6.60}$$

This approximation is justified on the grounds that only two states of the atom are involved in spontaneous emission, so there is no need to take the other states into account.[39] The next approximation constitutes the neglect of the $\mathbf{A}_{\mathrm{T}}^2$ term of the minimal coupling interaction Hamiltonian. This can be justified, because it is second order in the coupling e. Alternatively one could argue that being independent of the (canonical) atomic operators it can be absorbed into the free field Hamiltonian H_F, and taken as renormalising the bare field frequencies.[40] In total we have

$$\mathbf{d} = \mathbf{d}_{eg}(\sigma^+ + \sigma^-), \tag{6.61a}$$

$$-e\mathbf{p} = im\omega_{eg}\mathbf{d}_{eg}(\sigma^+ - \sigma^-), \tag{6.61b}$$

$$H_A = \sum_{n=e,g} \omega_n |n\rangle\langle n| = \omega_e \sigma^+\sigma^- + \omega_g \sigma^-\sigma^+, \tag{6.61c}$$

$$V = i\sum_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}(\sigma^+ - \sigma^-)(a^\dagger_{\mathbf{k}\lambda} + a_{\mathbf{k}\lambda}), \qquad c_{\mathbf{k}\lambda} := -g\omega_{eg}(\mathbf{d}_{eg}\cdot\mathbf{e}_{\mathbf{k}\lambda}) \tag{6.61d}$$

where for simplicity I have assumed $\mathbf{d}_{eg} \in \mathbb{R}^3$.

Next I make the *rotating-wave approximation* (RWA), which constitutes the neglect of the terms in V that give rise to free energy non-conserving processes. Within our simplified model, in which the EDA and 2LA have been made, and in which the $\mathbf{A}_{\mathrm{T}}^2$ term has been neglected, the *counter-rotating* terms $\sigma^+ a^\dagger_{\mathbf{k}\lambda}$ and $\sigma^- a_{\mathbf{k}\lambda}$ are synonymous with the virtual cloud. Since spontaneous emission is a first order real process the counter-rotating terms do

[39] The 2LA is nevertheless highly non-trivial. It fundamentally alters the algebra of atomic observables, which essentially becomes $\mathfrak{su}(2)$ (cf. B.3.2). The finite dimensionality of $\mathfrak{su}(2)$ means that it is incapable of supporting the canonical commutation relations, which the original canonical atomic operators satisfied. It happens that this fact bears no consequences with regard to the WW theory of spontaneous emission.

[40] This is a second highly non-trivial approximation, because as I noted in 6.2.3 neglecting the $\mathbf{A}_{\mathrm{T}}^2$ term results in a Hamiltonian, which is incapable of producing the correct equations of motion. Of course, deriving the correct equations of motion is something the 2LA has already eliminated any possibility of achieving.

not contribute to the spontaneous emission rate. With the addition of the RWA we have

$$V = i\sum_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}(\sigma^+ a_{\mathbf{k}\lambda} - \sigma^- a^\dagger_{\mathbf{k}\lambda}). \tag{6.62}$$

This sort of rotating-wave, linear-coupling interaction Hamiltonian is ubiquitous within the quantum optics paradigm.

To calculate the rate of spontaneous emission the WW treatment starts with the assumption that the state at time t can be written

$$|\psi(t)\rangle = b_e(t)e^{-i\omega_{eg}t}|e;0\rangle + \sum_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda}(t)e^{-i\omega_{eg}t}|g;\mathbf{k}\lambda\rangle, \qquad b_e(0) = 1, \qquad b_{\mathbf{k}\lambda}(0) = 0. \tag{6.63}$$

This too, is an approximation. First of all only one-photon states have been included, because spontaneous emission is a first order process. Furthermore, only the atomic ground state appears in tensor products with the one-photon states, because spontaneous emission is a real process in which the atom must make a transition $|e\rangle \to |g\rangle$ with the emission of a photon. The Schrödinger equation is equivalent to the coupled differential equations

$$\dot{b}_e = -\sum_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda}, \qquad \dot{b}_{\mathbf{k}\lambda} = -i(\omega - \omega_{eg})b_{\mathbf{k}\lambda} + c_{\mathbf{k}\lambda} b_e, \tag{6.64}$$

from which it follows that

$$\dot{b}_e = -\sum_{\mathbf{k}\lambda} c^2_{\mathbf{k}\lambda} \int_0^t dt'\, b_e(t')e^{-i(\omega-\omega_{eg})(t-t')}. \tag{6.65}$$

Our final approximation, *the Markovian approximation* (MA), is made here. One assumes that the amplitude is approximately memoryless, so that one can write $b_e(t') \approx b_e(t)$ in the integrand in 6.65. Moreover, for times $\tau := t - t' \gg \omega_{eg}^{-1}$ we have[41]

$$\int_0^t dt'\, e^{-i(\omega-\omega_{eg})(t-t')} \approx \int_0^\infty d\tau\, e^{-i(\omega-\omega_{eg})\tau} = -i\mathscr{P}\frac{1}{\omega-\omega_{eg}} + \pi\delta(\omega-\omega_{eg}). \tag{6.66}$$

Thus,

$$\dot{b}_e \approx \left(i\Delta\omega_e - \frac{\Gamma}{2}\right) b_e, \qquad b_e \approx e^{i\Delta\omega_e t}e^{-\Gamma t/2} \tag{6.67}$$

where

$$\Gamma := 2\pi\sum_{\mathbf{k}\lambda} c^2_{\mathbf{k}\lambda}\delta(\omega-\omega_{eg}) = \frac{\omega^3_{eg}|\mathbf{d}_{eg}|^2}{3\pi} \tag{6.68}$$

[41] Note that a limiting procedure must be invoked to evaluate the integral over τ (cf. 6.3.4).

and

$$\Delta\omega_e := \mathscr{P}\sum_{\mathbf{k}\lambda}\frac{c_{\mathbf{k}\lambda}^2}{\omega-\omega_{eg}} = \frac{\omega_{eg}^2|\mathbf{d}_{eg}|^2}{6\pi^2}\left(\mathscr{P}\int d\omega\,\frac{\omega}{\omega-\omega_{eg}}\right). \tag{6.69}$$

So we see that in the WW treatment the excited state decays with a rate Γ. The term $\Delta\omega_e$ describes a radiative level-shift of the excited atomic state, but only appears in the amplitude as a complex phase meaning it doesn't contribute to the probability $|b_e(t)|^2$. Substituting 6.67 back into 6.64 and integrating yields

$$b_{\mathbf{k}\lambda}(t) = e^{-i(\omega-\omega_{eg})t}b_{\mathbf{k}\lambda}(0) + e^{-i(\omega-\omega_{eg})t}c_{\mathbf{k}\lambda}\int_0^t d\tau\, e^{i(\omega+\omega_{eg})\tau}e^{-\Gamma\tau/2} \tag{6.70}$$

from which using $b_{\mathbf{k}\lambda}(0)=0$ we obtain

$$|b_{\mathbf{k}\lambda}(t)|^2 \approx \left|c_{\mathbf{k}\lambda}\int_0^\infty d\tau\, e^{-\Gamma\tau/2+i(\omega-\omega_{eg})\tau}\right|^2 = \frac{c_{\mathbf{k}\lambda}^2}{(\omega-\omega_{eg})^2+(\Gamma/2)^2} \tag{6.71}$$

in the (Markovian) approximation holding for $\Gamma \gg 1/t$. This result implies that the line-shape of radiation spontaneously emitted by the excited atom is approximately Lorentzian. I will revisit this topic in much more detail in chapter 7.

So we have now covered two ways of obtaining the spontaneous decay rate of an excited atomic state. The WW approach entails, as we have seen, a number of approximations. To assess the general validity of these approximations and to shed further light on to the physical nature of the contributions they eliminate, I turn my attention now to probabilities of photon detection at *finite* times.

6.3.3 Photodetection divergences and the symmetric representation

I start by considering a two-level atom linearly coupled to the field. I denote by $P_{\rm ph}^+(t)$ the probability to detect a photon for an initial state $|g,0\rangle$. I denote by $P_{\rm ph}^-(t)$ the probability to detect a photon given the initial state $|e,0\rangle$. Time-dependent second order perturbation theory yields

$$P_{\rm ph}^{\pm}(t) = \sum_{\mathbf{k}\lambda}\int_0^t dt'\int_0^t dt''\, c_{\mathbf{k}\lambda}^2 e^{-i(\omega\pm\omega_{eg})(t'-t'')} = \frac{2\Gamma}{\pi}\int_0^{\omega_u} d\omega\, f^{\pm}(\omega)\frac{\sin^2\left([\omega_{eg}\pm\omega]t/2\right)}{(\omega_{eg}\pm\omega)^2}. \tag{6.72}$$

Here the coupling constant $c_{\mathbf{k}\lambda}$ is dependent on the form of the atom-field coupling, so it is different in the Coulomb and Poincaré gauges. The $f^{\pm}(\omega)$ are dimensionless and also coupling dependent. In the Coulomb gauge $f^+(\omega)=f^-(\omega)=\omega/\omega_{eg}$, so $P_{\rm ph}^+(t)$ in 6.72 diverges logarithmically. In the Poincaré gauge $f^+(\omega)=f^-(\omega)=(\omega/\omega_{eg})^3$ so $P_{\rm ph}^+(t)$ diverges quadratically.

If in 6.72 $f^-(\omega)$ is sufficiently slowly varying, and the peak at ω_{eg} of the sinc function

dominates the integration, so that effectively one has

$$\frac{\sin^2([\omega-\omega_{eg}]t/2)}{(\omega-\omega_{eg})^2} \approx \frac{t}{2}\pi\delta(\omega-\omega_{eg}) \tag{6.73}$$

then one obtains

$$P^{-}_{\rm ph}(t) \approx 2\pi t \sum_{\mathbf{k}\lambda} c^2_{\mathbf{k}\lambda}\,\delta(\omega-\omega_{eg}) = t\Gamma. \tag{6.74}$$

This is twice that obtained by applying the MA to $P^{-}_{\rm ph}$ in 6.72 and subsequently taking the real part. Defining the rates

$$\Gamma^{\pm} := \lim_{t\to\infty} \frac{P^{\pm}_{\rm ph}(t)}{t} \tag{6.75}$$

one sees that within the above approximation $\Gamma^{+}=0$ and $\Gamma^{-}=\Gamma$, so we have effectively performed the first order S-matrix calculation for each rate.

The results for $P^{+}_{\rm ph}$ are as expected different in the Coulomb and Poincaré gauges, but perhaps more surprisingly in both cases $P^{+}_{\rm ph}$ is divergent. The probability comes out nonzero, because of the counter-rotating terms present in the minimal coupling and multipolar interaction Hamiltonians; the atom can emit a virtual photon while making an upward transition. Because $P^{+}_{\rm ph}(t)/t$ vanishes in the limit $t\to\infty$, the counter-rotating contributions are often said to be transient; they are associated with the virtual cloud of photons.

Nevertheless the results are paradoxical, not only because they are divergent, but also because they appear to imply that we can extract energy from the vacuum by simply placing a ground state atom into the field. The formalism allows for this, because the *energy* we are talking about here, is actually *free energy*, and this is by no means conserved; $[H_0,H]\neq 0$. The obvious deficiency here, is the idea that a non-conserved free energy constitutes a legitimate candidate as *observable* energy.

A pragmatic approach to tackling the divergence problem would be to construct a formulation in which $[H_0,H]=0$, that is, we could try to partially diagonalise the Hamiltonian. A method of doing this by applying a generalised PZW transformation to the minimal coupling Hamiltonian was developed by Drummond (1987) (see also Baxter (1989) and Baxter *et al.* (1990)). By constructing the generalised transformation in such a way that upon making the 2LA the counter-rotating terms in the interaction are eliminated, one eliminates the photodetection divergences.

The required transformation symmetrically mixes the minimal and multipolar couplings, and so I call the resulting representation the *symmetric representation*. It has also been called the *rotating-wave representation*, due to the similar form of the resulting interaction with that obtained by employing the RWA. I use the label symmetric to refer to the representation itself whereas I use the label rotating-wave to refer to the explicit form of the Hamiltonian obtained within the symmetric representation. In the symmetric representation

the free ground state $|g;0\rangle$ is the *true* ground state of the *total* Hamiltonian and moreover, the free energy H_0 is a symmetry of the Hamiltonian; $[H_0,V]=[H_0,H]=0$. Thus, the virtual cloud dressing the vacuum is included implicitly within the bare degrees of freedom, which consequently become (at least partially) dressed.

The generalised PZW transformation required is

$$S_{\{\alpha_k\}} := e^{-i\mathbf{d}\cdot\mathbf{A}_{\{\alpha_k\}}(\mathbf{0})} \tag{6.76}$$

where

$$\mathbf{A}_{\{\alpha_k\}}(\mathbf{0}) := \sum_{\mathbf{k}\lambda} g\alpha_k \mathbf{e}_{\mathbf{k}\lambda}\left(a^\dagger_{\mathbf{k}\lambda}+a_{\mathbf{k}\lambda}\right) \tag{6.77}$$

with the α_k's being real and dimensionless. In the case $\alpha_k\equiv 1$, $S_{\{\alpha_k\}}$ reduces to the PZW transformation 6.15 in the EDA. Applying $S_{\{\alpha_k\}}$ to the minimal coupling Hamiltonian 6.12 yields the general Hamiltonian

$$\begin{aligned}
H_{\{\alpha_k\}} &:= H_0+V_{\{\alpha_k\}} \equiv H_A+H_F+V_{\{\alpha_k\}}\\
H_{\rm A} &= \frac{\mathbf{p}^2}{2m}+V(\mathbf{r})+\varepsilon^{\{\alpha_k\}}_{\rm self},\\
H_{\rm F} &= \frac{e^2}{2m}\left|\mathbf{A}(\mathbf{0})-\mathbf{A}_{\{\alpha_k\}}(\mathbf{0})\right|^2+\sum_{\mathbf{k}\lambda}\omega\, a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda},\\
V_{\{\alpha_k\}} &= \frac{e}{m}\mathbf{p}\cdot\left(\mathbf{A}(\mathbf{0})-\mathbf{A}_{\{\alpha_k\}}(\mathbf{0})\right)+\mathbf{d}\cdot\mathbf{\Pi}_{\{\alpha_k\}}(\mathbf{0})
\end{aligned} \tag{6.78}$$

where

$$\varepsilon^{\{\alpha_k\}}_{\rm self} := \sum_{\mathbf{k}\lambda}\frac{1}{2V}\alpha_k^2(\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{d})^2 \tag{6.79}$$

and

$$\mathbf{\Pi}_{\{\alpha_k\}}(\mathbf{0}) := i\sum_{\mathbf{k}\lambda}\omega g\alpha_k\mathbf{e}_{\mathbf{k}\lambda}\left(a^\dagger_{\mathbf{k}\lambda}-a_{\mathbf{k}\lambda}\right). \tag{6.80}$$

Neglecting the (self energy) terms quadratic in e and making the 2LA, one obtains the approximate model 6.61, but with the interaction Hamiltonian

$$V_{\{\alpha_k\}} = i\sum_{\mathbf{k}\lambda} g_{\mathbf{k}\lambda}\sigma^+\left(u^+_k a^\dagger_{\mathbf{k}\lambda}+u^-_k a_{\mathbf{k}\lambda}\right)+\text{H.c.}, \qquad g_{\mathbf{k}\lambda} := -\sqrt{\frac{\omega_{eg}}{2V}}\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{d} \tag{6.81}$$

where

$$u^\pm_k := (1-\alpha_k)\sqrt{\frac{\omega_{eg}}{\omega}}\mp\alpha_k\sqrt{\frac{\omega}{\omega_{eg}}}. \tag{6.82}$$

This general interaction includes the minimal coupling ($\alpha_k\equiv 0$), multipolar ($\alpha_k\equiv 1$) and

rotating-wave interactions as special cases. The rotating-wave Hamiltonian is defined by the choice

$$\alpha_k = \frac{\omega_{eg}}{\omega_{eg}+\omega} \tag{6.83}$$

yielding

$$V_s = i\sum_{\mathbf{k}\lambda} g_{\mathbf{k}\lambda}\,\frac{2\sqrt{\omega_{eg}\omega}}{\omega_{eg}+\omega}\,\sigma^+ a_{\mathbf{k}\lambda} + \text{H.c.}, \tag{6.84}$$

which is of the same form as 6.62.

The symmetric representation affords us the opportunity to eliminate the counter-rotating contributions without any need for the RWA or MA, but is this really necessary?[42] To try to answer this question I will now attempt a more systematic analysis of these approximations.

6.3.4 A survey of quantum optical approximations

The approximations used in 6.3.2 tend, in one way or another, to eliminate the effects of virtual processes. The most used approximation is perturbation theory, which requires that the perturbation is small i.e. the *coupling is weak*. Other approximations like the RWA and the MA also rely on the weak coupling condition. Determining the validity and self consistency of different combinations of these approximations can be a complicated matter.

The RWA

Starting with a linear coupling model the RWA neglects the energy non-conserving terms in the interaction. In the Coulomb or Poincaré gauge and in the interaction picture with respect to H_0 we have;

$$\begin{aligned}\tilde{V}(t) =& i\sum_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}\left(\sigma^+ a^\dagger_{\mathbf{k}\lambda} e^{i(\omega_{eg}+\omega)t} + \sigma^+ a_{\mathbf{k}\lambda} e^{i(\omega_{eg}-\omega)t} - \text{H.c.}\right)\\ \xrightarrow{\text{RWA}}\ & i\sum_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}\left(\sigma^+ a_{\mathbf{k}\lambda} e^{i(\omega_{eg}-\omega)t} - \sigma^- a^\dagger_{\mathbf{k}\lambda} e^{-i(\omega_{eg}-\omega)t}\right).\end{aligned} \tag{6.85}$$

The neglected counter-rotating terms are those which come with the alleged rapidly oscillating off-resonant exponential factors $e^{\pm i(\omega_{eg}+\omega)t}$, which it is argued will cause the counter-rotating terms to contribute much less than the terms retained. The statement that the counter-rotating contributions necessarily oscillate more rapidly than the "rotating" contributions is however, false. It holds only for mode frequencies close to ω_{eg}. As an example take the "rotating" term $e^{i(\omega_{eg}-2\omega_{eg})t}$ in which $\omega = 2\omega_{eg}$. This term is equal to the counter-

[42] It is worth asking this question, because there may be traits of other formulations that could perhaps be viewed as attractive. For example, the field canonical momentum propagates causally in the Poincaré gauge (6.1.3), so that all interactions are properly retarded. This property of interactions is something that is necessarily sacrificed when using the symmetric representation (see chapter 9 for a full discussion of this point).

rotating term $e^{-i(\omega_{eg}+0)t}$ in which $\omega = 0$. Thus, one can only legitimately neglect particular contributions based on a mode-by-mode comparison.

The RWA is justified if all the ω are close to ω_{eg}, but assuming such a resonance condition is the same as assuming free energy conservation. Since the counter-rotating terms are neglected to *ensure* free energy conservation, the entire justification becomes circular. In fact, it is quite difficult to see the sense in which the RWA constitutes any sort of approximation at all. No such problem arises in the case of a single mode, because in the single mode case one need only compare two individual terms. We have seen that the counter-rotating terms give rise to divergent contributions, but only in the continuum limit of many modes. Regarding the implications of these divergences for the consistency of the RWA, one is reminded of the famous quote by Dirac on renormalisation;

> "*sensible mathematics involves neglecting a quantity when it is small - not neglecting it just because it is infinitely great and you do not want it!*"

Of course, the divergences associated with the counter-rotating terms are ultra-violet in nature and this kind of problem is hardly unheard of in QED. The method of Drummond, which eliminates the offending terms by partially diagonalising the Hamiltonian can be viewed as a renormalisation procedure in which the effects of virtual processes are absorbed into a redefinition of the atom-field coupling constant (compare 6.62 with 6.84).

The MA

The MA is also quite interesting. The MA, part of which constitutes taking the limit $t \to \infty$ (reminiscent of the S-matrix), can sometimes obscure the behaviour of terms at *finite times*. The MA comes in different, but essentially equivalent forms. It also has close ties with the so called *pole approximation*. Let's suppose we are given an expression

$$I := \int_0^t dt' A(t')X(t-t'). \tag{6.86}$$

where

$$X(\tau) := \int_0^\infty d\omega Y(\omega) e^{-i(\omega-\omega_0)\tau}. \tag{6.87}$$

When Y is sufficiently slowly varying and has dominant peak at ω_0, X has a narrow dominant peak at $\tau = t - t' = 0$. There are two ways to proceed. As we did in 6.3.2, one can put $A(t') \approx A(t)$ and take the limit $\tau \to \infty$ in the integral. In order that this integral converges a

factor $-\eta$ must be added to the exponent. We have

$$\begin{aligned}\int_0^t dt' X(t-t') &\approx \lim_{\eta\to 0^+}\int_0^\infty d\omega Y(\omega)\int_0^\infty d\tau e^{-i(\omega-\omega_0-i\eta)\tau}\\ &= -i\lim_{\eta\to 0^+}\int_0^\infty d\omega\frac{Y(\omega)}{\omega-\omega_0-i\eta} = \pi Y(\omega_0) - i\mathscr{P}\int_0^\infty d\omega\frac{Y(\omega)}{\omega-\omega_0}\\ &\Rightarrow I \approx A(t)\left[\pi Y(\omega_0) - i\mathscr{P}\int_0^\infty d\omega\frac{Y(\omega)}{\omega-\omega_0}\right].\end{aligned} \tag{6.88}$$

On the other hand one could put $Y(\omega)\approx Y(\omega_0)$ and extend the frequency integration to $-\infty$. This gives twice the result of the MA 6.88 in the real part;

$$X(\tau)\approx Y(\omega_0)\int_0^\infty d\omega\, e^{-i(\omega-\omega_0)\tau} = 2\pi e^{i\omega_0\tau}\delta(\tau) \;\Rightarrow\; I\approx 2\pi A(t)Y(\omega_0). \tag{6.89}$$

We saw a specific example of this approximation in 6.3.3. We can apply these ideas directly to the spontaneous emission rate calculations in 6.3.2 and 6.3.3. For the calculation in 6.3.2 we identify A as the excited state amplitude b_e. The approximation $A(t')\approx A(t)$ requires that the decay of the excited atom is negligible over the time t, so for self-consistency we require $\Gamma t \ll 1$. On the other hand the alteration of the integral limits requires $\omega_{eg}t \gg 1$. We therefore obtain the *Markovian regime*

$$\frac{1}{\Gamma} \gg t \gg \frac{1}{\omega_0}. \tag{6.90}$$

The error incurred by the MA is small in the context of the calculation of Γ within the Coulomb gauge and symmetric representation, but not in the Poincaré gauge. The Poincaré gauge also suffers much more severely from the finite-time divergence problem caused by the counter-rotating terms, whose contributions vanish within the MA whereby $t\to\infty$.

Consider for example, the expression 6.72 for $P^+_{\rm ph}$, in which the dominant peak of the sinc^2 function is outside the range of integration. When combined with the function $f^-(\omega)$ also appearing in the integral the "small" oscillations outside the peak can lead to non-negligible contributions within the interval $[0,\omega_u]$. In the Coulomb gauge such contributions generally remain small, which is why $P^+_{\rm ph}(t)$ diverges only logarithmically. In the Poincaré gauge however, $P^+_{\rm ph}$ diverges *quadratically*. We will see in chapter 8 in which I employ an open quantum systems treatment of the atom, that the counter-rotating terms can lead to non-negligible emission rates.

The conclusion we must draw from our considerations of the RWA and MA is that it isn't always clear, that *virtual* contributions can be neglected within apparently *real* emission rates, on the grounds of a legitimate approximative procedure. Therefore, the use of the symmetric representation would sometimes appear to be necessary in order to retain any hope of obtaining meaningful results when it comes to interactions over finite times.

6.4 The virtual cloud

In this section I adopt the alternative viewpoint 2 (cf. chapter 4), which allows for the possibility that under certain conditions, bare atomic and/or field degrees of freedom, are at least in principle, experimentally accessible. In other words I will assume that the virtual cloud surrounding the atom is in every sense a real physical object.

Detailed investigations of the virtual cloud have been carried out in the past (see Feinberg & Sucher (1970), Persico & Power (1986), Passante & Power (1987), Compagno *et al.* (1988b), Compagno *et al.* (1988a), Compagno *et al.* (1990), Compagno *et al.* (1991), Milonni (1994), Compagno *et al.* (1995), and references therein). The starting idea is that virtual photons are emitted and reabsorbed continually by the bare atom over very short time scales. The time scales are determined by the energy-time uncertainty relation

$$\tau \sim \frac{1}{\delta\omega}. \tag{6.91}$$

Virtual emission and reabsorption can only violate free energy conservation to within $1/\tau$, where τ is the interaction time over which the event occurs. Assuming that this is the case, and assuming for now that the virtual photons propagate at the speed of light c, the virtual cloud associated with an emission-reabsorption event of duration τ extends a distance $x \sim c\tau$.[43] The cloud is therefore localised at the atom. While it is consistent with the classification of virtual processes as transient, this idea appears to promote the energy-time uncertainty relation 6.91 to the status of a fundamental law, or failing this at least requires that it is a legitimate approximation. To illustrate how the idea works consider the emission of a photon from the bare ground state. The associated energy change is $\delta\omega = \omega_{eg} + \omega$. If $\omega_{eg} \gg \omega$ then $\delta\omega \approx \omega_{eg}$. For optical frequencies one obtains $\tau \sim 10^{-14}s$ and $x \sim 10^{-4}cm$. At the other extreme $\omega \sim \omega_u \approx 10^{16}s^{-1}$ and $x \sim 10^{-6}cm$.

More rigorous quantitative results regarding the virtual cloud are obtained by analysing the EMED around the atom, as well as the associated energy flux given by the Poynting vector. The bare and dressed expectation values of these operators exhibit various $1/x^n$ behaviours (see references given in 6.4.1 shortly). These expectation values can be found in both time-dependent quantum theory utilising bare states, and in the time-independent S-matrix formalism utilising retarded true eigenstates. In the time-dependent approach one neglects the transient contributions associated with the virtual cloud, which arise from the second order fields. In this section I will begin by briefly reviewing the details of the calculation of the expectation value of the Poynting vector taken in a bare excited atomic state containing no photons. This calculation sheds no light upon whether or not the transient contributions associated with the virtual cloud are measurable. To investigate this question Compagno *et al.* (1995) have used a simple model of finite-duration quantum measurement

[43] It is far from clear that photons propagate at all, but the EMED defined in terms of the electric and magnetic fields *does* propagate at speed c, and this is often used to obtain quantitative results regarding the virtual cloud.

due to Peres & Wootters (1985). I will review this model in 6.4.2.

6.4.1 The Poynting vector

Both the virtual cloud and spontaneous emission can be described in terms of the electric and magnetic fields in the presence of an atom. We saw in 4.2 that charges in motion produce electromagnetic energy, which is carried by the Poynting vector. Using the results of 6.1.3 perturbative expressions for the electromagnetic energy density (EMED) and the Poynting vector can be obtained within both the time-dependent and time independent formalisms, and expectation values for specific states of the atom-field system can be found. I concentrate on the Poynting vector. My review will be brief, so I refer the reader to the following for details; Power & Thirunamachandran (1983a), Power & Thirunamachandran (1983b), Power & Thirunamachandran (1983c), Power & Thirunamachandran (1992), Power & Thirunamachandran (1993), Power & Thirunamachandran (1999a), Power & Thirunamachandran (1999b), Salam (2008), Salam (2009).

According to 6.1.3, within the Poincaré gauge, within the EDA, and for an atom located at $\mathbf{0}$, we have that $-\mathbf{\Pi}_{\mathrm{T}}(\mathbf{x}) = \mathbf{D}_{\mathrm{T}}(\mathbf{x}) = \mathbf{E}(\mathbf{x})$ whenever $\mathbf{x} \neq \mathbf{0}$. Moreover, we have that $m\dot{\mathbf{r}} = \mathbf{p}$. The Poincaré gauge is therefore well suited to our present task of obtaining the Poynting vector. The radiative energy flux of an excited atom is found to be

$$P = \sum_{n<m} \frac{\omega_{mn}^4 |\mathbf{d}_{mn}|^2}{3\pi} = \sum_{n<m} \Gamma_{m\to n}\omega_{mn}, \qquad \Gamma_{m\to n} := \frac{\omega_{mn}^3 |\mathbf{d}_{mn}|^2}{3\pi}, \tag{6.92}$$

where we recognise $\Gamma_{m\to n}$ as the spontaneous emission rate for the transition $|m\rangle \to |n\rangle$. The quantity $\Gamma_{m\to n}$ quantifies the number of real photons with energy ω_{mn} irreversibly emitted per unit time, and since each photon carries an energy ω_{mn}, the rate at which energy is lost via the $|m\rangle \to |n\rangle$ transition is $\Gamma_{m\to n}\omega_{mn}$. The total rate P is simply the sum over all rates $\Gamma_{m\to n}\omega_{mn}$. One way of deriving 6.92 is to use a time-dependent approach in which the expectation value $\langle \mathbf{S}(t) \rangle$ is calculated in the bare state $|n;0\rangle$. In this approach certain transient contributions associated with the virtual cloud must be neglected. The second way to arrive at 6.92 is to use the time-independent S-matrix formalism to find retarded energy eigenstates and use these to calculate the expectation value of $\mathbf{S}$. I will consider the former approach first.

Our first task is to find the equation of motion for the Poincaré gauge bare atomic operator $\zeta_{nm} := |n\rangle\langle m|$. One can then use this to obtain an integrated equation of motion for the dipole moment $\mathbf{d}$, which is something I didn't find in 6.1.3. To find the equation of motion I use 6.9 without the self energy term $\varepsilon_{\mathrm{self}}$. This is allowed because I'm only going to go up to second order in the fields, and the first contribution from this term arises at third order. We have after integration

$$\zeta_{nm}(t) = \zeta_{nm}^{(0)}(t) + ie^{i\omega_{nm}t} \int dt' \sum_p \mathbf{D}_{\mathrm{T}}(t') \cdot \left[\mathbf{d}_{mp} e^{-i\omega_{np}t'} \zeta_{np}(t') - \mathbf{d}_{pn} e^{-i\omega_{nm}t'} \zeta_{pm}(t') \right] \tag{6.93}$$

with $\zeta^{(0)}(t) := \zeta_{nm}e^{i\omega_{nm}t}$ and $\mathbf{D}_{\mathrm{T}}(t) := \mathbf{D}_{\mathrm{T}}(t,\mathbf{0})$. Using

$$\mathbf{d}(t) = \sum_{nm} \mathbf{d}_{nm}\zeta_{nm}(t) \tag{6.94}$$

6.93 gives

$$\mathbf{d}(t) = \mathbf{d}^{(1)}(t) + i\sum_{nmp} \mathbf{d}_{nm}e^{i\omega_{nm}t}\int dt'\,\mathbf{D}_{\mathrm{T}}(t')\cdot\left[\mathbf{d}_{mp}e^{-i\omega_{np}t'}\zeta_{np}(t') - \mathbf{d}_{pn}e^{-i\omega_{nm}t'}\zeta_{pm}(t')\right] \tag{6.95}$$

where the free evolution component is denoted $\mathbf{d}^{(1)}$ for reasons that will become clear shortly;

$$\mathbf{d}^{(1)}(t) := \sum_{nm} d_{nm}|n\rangle\langle m|e^{i\omega_{nm}t}. \tag{6.96}$$

Next one expands each of the dipole moment, electric field, and magnetic field *in powers of* $e = \sqrt{4\pi\alpha}$ (or equivalently $\mathbf{d}$) as follows

$$\mathbf{d}(t) = \sum_{n=1}^{\infty}\mathbf{d}^{(n)}(t), \qquad \mathbf{D}_{\mathrm{T}}(t,\mathbf{x}) = \sum_{n=0}^{\infty}\mathbf{D}_{\mathrm{T}}^{(n)}(t,\mathbf{x}), \qquad \mathbf{B}(t,\mathbf{x}) = \sum_{n=0}^{\infty}\mathbf{B}^{(n)}(t,\mathbf{x}) \tag{6.97}$$

where the zeroth order terms of the electric and magnetic field expansions are simply the free evolution components;

$$\mathbf{D}_{\mathrm{T}}^{(0)}(t,\mathbf{x}) := \mathbf{D}_{\mathrm{T}}^{0}(t,\mathbf{x}) := -i\sum_{\mathbf{k}\lambda}\omega g\mathbf{e}_{\mathbf{k}\lambda}\left(a_{\mathbf{k}\lambda}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} - a_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t}\right), \tag{6.98a}$$

$$\mathbf{B}^{(0)}(t,\mathbf{x}) := \mathbf{B}^{0}(t,\mathbf{x}) := -i\sum_{\mathbf{k}\lambda}\omega g\hat{\mathbf{k}}\times\mathbf{e}_{\mathbf{k}\lambda}\left(a_{\mathbf{k}\lambda}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} - a_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t}\right). \tag{6.98b}$$

The free component of $\mathbf{d}(t)$ is first order in the e, which is the reason for the notation used in 6.95 and 6.96.

Substituting 6.96 in place of the total dipole moment in each of 6.30 and 6.24 gives the first order components of $\mathbf{D}_{\mathrm{T}}$ and $\mathbf{B}$ respectively. Assuming as usual that repeated cartesian indices are to be summed we have

$$\mathrm{D}_{\mathrm{T},i}^{(1)}(\mathbf{x},t) := \frac{1}{4\pi}\sum_{nm}\omega_{mn}f_{ij}(\omega_{mn}x)\mathrm{d}_{nm}^{j}|n\rangle\langle m|e^{i\omega_{nm}(x-t)}, \tag{6.99a}$$

$$\mathrm{B}_{i}^{(1)}(\mathbf{x},t) := \frac{1}{4\pi}\sum_{nm}\omega_{mn}g_{ij}(\omega_{mn}x)\mathrm{d}_{nm}^{j}|n\rangle\langle m|e^{i\omega_{nm}(x-t)} \tag{6.99b}$$

where d^j_{nm} denotes the nm^{th} matrix element of the i'th cartesian component of $\mathbf{d}$, and

$$f_{ij}(\omega x) := -(\delta_{ij}-\hat{x}_i\hat{x}_j)\frac{1}{\omega x}+(\delta_{ij}-3\hat{x}_i\hat{x}_j)\left(\frac{-i}{\omega^2x^2}+\frac{1}{\omega^3x^3}\right), \tag{6.100a}$$

$$g_{ij}(\omega x) := -\varepsilon_{ijk}\hat{x}_k\left(\frac{1}{\omega x}+\frac{i}{\omega^2x^2}\right). \tag{6.100b}$$

The functions in 6.100 satisfy the relations

$$\left(-\delta_{ij}\partial^2+\partial_i\partial_j\right)\frac{e^{i\omega x}}{x}=\omega^3 f_{ij}(\omega x)e^{i\omega x}, \tag{6.101a}$$

$$\left(i\varepsilon_{ijl}\partial_l\right)\frac{e^{i\omega x}}{x}=\omega^2 g_{ij}(\omega x)e^{i\omega x}, \tag{6.101b}$$

which were used in deriving 6.99. To find the second order term in the expansion of the dipole moment one puts $\zeta_{nm}(t')\approx\zeta^{(0)}_{nm}(t')$ and $\mathbf{D}_{\mathrm{T}}(t')\approx\mathbf{D}^{(0)}_{\mathrm{T}}(t')$ in 6.95. By substituting the resulting expression into each of 6.30 and 6.24, one obtains the second order terms in the expansions of $\mathbf{D}_{\mathrm{T}}$ and $\mathbf{B}$ respectively;

$$\begin{aligned}\mathrm{D}^{(2)}_{\mathrm{T},i}(t,\mathbf{x}) =& \frac{i}{4\pi}\sum_{\mathbf{k}\lambda}\sum_{np}\omega g\mathrm{e}^l_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}|n\rangle\langle p|\left[\alpha^{jl}_{np}(\omega_{pn}+\omega)^3 f_{ij}\left([\omega_{pn}+\omega]x\right)e^{i(\omega_{pn}+\omega)(x-t)}\right.\\ &\left.-\sum_m\left\{\frac{\mathrm{d}^j_{nm}\mathrm{d}^l_{mp}}{\omega_{mp}-\omega}\omega^3_{mn}f_{ij}(\omega_{mn}x)e^{i\omega_{mn}(x-t)}+\frac{\mathrm{d}^j_{nm}\mathrm{d}^l_{mp}}{\omega_{mn}+\omega}\omega^3_{pm}f_{ij}(\omega_{pm}x)e^{i\omega_{pm}(x-t)}\right\}\right]\\ &+\mathrm{H.c.},\end{aligned} \tag{6.102a}$$

$$\begin{aligned}\mathrm{B}^{(2)}_{i}(t,\mathbf{x}) =& \frac{i}{4\pi}\sum_{\mathbf{k}\lambda}\sum_{np}\omega g\mathrm{e}^l_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}|n\rangle\langle p|\left[\alpha^{jl}_{np}(\omega_{pn}+\omega)^3 g_{ij}\left([\omega_{pn}+\omega]x\right)e^{i(\omega_{pn}+\omega)(x-t)}\right.\\ &\left.-\sum_m\left\{\frac{\mathrm{d}^j_{nm}\mathrm{d}^l_{mp}}{\omega_{mp}-\omega}\omega^3_{mn}g_{ij}(\omega_{mn}x)e^{i\omega_{mn}(x-t)}+\frac{\mathrm{d}^j_{nm}\mathrm{d}^l_{mp}}{\omega_{mn}+\omega}\omega^3_{pm}g_{ij}(\omega_{pm}x)e^{i\omega_{pm}(x-t)}\right\}\right]\\ &+\mathrm{H.c.}\end{aligned} \tag{6.102b}$$

where

$$\alpha^{ij}_{np} := \sum_m\left[\frac{\mathrm{d}^i_{nm}\mathrm{d}^j_{mp}}{\omega_{mp}-\omega}+\frac{\mathrm{d}^j_{nm}\mathrm{d}^i_{mp}}{\omega_{mn}+\omega}\right]. \tag{6.103}$$

The top lines in 6.102a and 6.99a give time-independent contributions to the Poynting vector while the second lines give oscillatory contributions.

The total Poynting vector is the sum of free and source components;[44]

$$\begin{aligned}\mathbf{S} &= \mathbf{S}^0 + \mathbf{S}^s, \\ \mathbf{S}^0 &:= \frac{1}{2}\left(\mathbf{E}^0 \times \mathbf{B}^0 - \mathbf{B}^0 \times \mathbf{E}^0\right), \\ \mathbf{S}^s &:= \frac{1}{2}\left(\mathbf{E}^{(1)} \times \mathbf{B}^{(1)} + \mathbf{E}^0 \times \mathbf{B}^{(1)} + \mathbf{E}^{(1)} \times \mathbf{B}^0 + \mathbf{E}^0 \times \mathbf{B}^{(2)} + \mathbf{E}^{(2)} \times \mathbf{B}^0\right) + \text{H.c.}\end{aligned} \tag{6.104}$$

The expectation value of $\mathbf{S}^s$ for the initial state $|i\rangle = |m;0\rangle$ gives the radiative energy flux of the bare atom in the bare vacuum. For this initial state the source vector reduces to

$$\mathbf{S}^s = \frac{1}{2}\left(\mathbf{E}^0 \times \mathbf{B}^{(2)} + \mathbf{E}^{(2)} \times \mathbf{B}^0 + \mathbf{E}^{(1)} \times \mathbf{B}^{(1)}\right) + \text{c.c.} \tag{6.105}$$

Furthermore, the off-resonant oscillatory components of the second order fields produce only *transient* contributions to $\mathbf{S}$, whose time average over a finite interval is zero. These contributions describe electromagnetic energy which is not lost *irreversibly*, but may be reabsorbed by the atom. They are consequently associated with the virtual photon cloud surrounding the atom. The question as to whether or not they give rise to observable effects depends on the time scale over which the virtual emission-reabsorption events take place within the cloud (see 6.4.2). For now, I look to obtain the rate at which energy is irreversibly lost and so neglect these contributions.

Using 6.99, with a little work one obtains

$$\begin{aligned}\langle \mathrm{S}_i^{(1)} \rangle &= \frac{\varepsilon_{ijl}}{2}\left(\mathrm{E}_j^{(1)}\mathrm{B}_l^{(1)} - \mathrm{B}_j^{(1)}\mathrm{E}_l^{(1)}\right) \\ &= \frac{\varepsilon_{ijl}}{2(4\pi)^2}\sum_n \mathrm{d}^r_{mn}\mathrm{d}^s_{nm}\omega^6_{mn}\left[f^*_{jr}(\omega_{mn}x)g_{ls}(\omega_{mn}x) + g^*_{ls}(\omega_{mn}x)f^*_{jr}(\omega_{mn}x)\right]\end{aligned} \tag{6.106}$$

and neglecting the oscillatory terms

$$\begin{aligned}\langle \mathrm{S}_i^{(2)} \rangle &= \frac{\varepsilon_{ijl}}{2}\left(\mathrm{E}_j^{(0)}\mathrm{B}_l^{(2)} - \mathrm{B}_j^{(2)}\mathrm{E}_l^{(0)} + \mathrm{E}_j^{(2)}\mathrm{B}_l^{(0)} - \mathrm{B}_j^{(0)}\mathrm{E}_l^{(2)}\right) \\ &= \frac{\varepsilon_{ijl}}{2(4\pi)^2}\sum_n \mathrm{sgn}(\omega_{mn})\mathrm{d}^r_{mn}\mathrm{d}^s_{nm}\omega^6_{mn}\left[f^*_{jr}(\omega_{mn}x)g_{ls}(\omega_{mn}x) + g^*_{ls}(\omega_{mn}x)f^*_{jr}(\omega_{mn}x)\right]\end{aligned} \tag{6.107}$$

where sgn denotes the *signum function* defined by

$$\mathrm{sgn}(x) := \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{if } x < 0. \end{cases} \tag{6.108}$$

[44] In order that it is Hermitian, in the quantum theory $\mathbf{S}$ must be symmetrised;

$$\mathbf{S} := \frac{1}{2}\left(\mathbf{E} \times \mathbf{B} - \mathbf{B} \times \mathbf{E}\right).$$

Adding 6.106 to 6.107 one obtains to second order

$$\langle \mathrm{S}_i^s \rangle = \frac{1}{8\pi^2} \sum_{n<m} \mathrm{d}_{mn}^j \mathrm{d}_{nm}^l \omega_{mn}^4 \left(\delta_{jl} - \hat{x}_j \hat{x}_l \right) \frac{\hat{x}_i}{x^2} \tag{6.109}$$

in which it is seen that only downward transitions make a net contribution. The x^{-2} dependence of S_i^s in 6.109 is highly significant. Poynting's theorem tells us that the energy flux across the surface of a sphere with radius x is (cf. 4.41)

$$P = \int d\Omega x^2 \hat{x}_i S_i(\mathbf{x}, t), \tag{6.110}$$

and using 6.109 one obtains 6.92.

The same result can be found using the S-matrix formalism, without any need to neglect particular contributions. The method consists of calculating the expectation values using the true excited eigenstate $|n;0^+\rangle =: |n;0\rangle_{\text{true}}$, rather than the bare atomic state $|n;0\rangle$ (Power & Thirunamachandran (1993)). In the Poincaré gauge we already have a properly defined atomic energy in terms of the canonical momentum $\mathbf{p} = m\dot{\mathbf{r}}$, so as in 6.2.4, one can interpret $|n;0\rangle_{\text{true}}$ as the correction to the incorrectly defined bare field vacuum. Using the T-matrix in 5.48, in conjunction with H_P from 6.9 one easily obtains the $O(g^2)$ unnormalised state

$$\begin{aligned} |n;0\rangle_{\text{true}} = |n;0\rangle &- \sum_m \sum_{\mathbf{k}\lambda} \frac{\langle m;\mathbf{k}\lambda|V|0;n\rangle}{\omega - \omega_{nm} + i\eta} |m;\mathbf{k}\lambda\rangle \\ &+ \sum_{m,m'} \sum_{\mathbf{k}\lambda} \frac{\langle m';\mathbf{k}'\lambda',\mathbf{k}\lambda|V|m;\mathbf{k}\lambda\rangle\langle m;\mathbf{k}\lambda|V|n;0\rangle}{(\omega - \omega_{nm} + i\eta)(\omega + \omega' - \omega_{nm'} + i\eta)} |m';\mathbf{k}'\lambda',\mathbf{k}\lambda\rangle. \end{aligned} \tag{6.111}$$

Long calculations (see Power & Thirunamachandran (1993)) eventually give the result 6.109 for the expectation value $\langle \mathbf{S} \rangle$ taken in the state $|n;0\rangle_{\text{true}}$. The difference between the two approaches is captured entirely within the transient contributions neglected in the first method. It is only through an analysis of these contributions and their physical implications, that we can hope to determine the reality of the initial bare state assumed in the first method.

6.4.2 Measuring the cloud directly

Suppose first that we wish to perform measurements on a single two-level atom whose zero of energy is taken as $\omega_{eg}/2$, and whose Hamiltonian can therefore be written

$$H_A := \omega_{eg} \sigma_z, \qquad \sigma_z := \frac{1}{2} \left(|e\rangle\langle e| - |g\rangle\langle g| \right). \tag{6.112}$$

In the formalism of Peres & Wootters (1985) the measurement device, or *pointer*, is described by canonical operators P and Q, which for simplicity I will assume are confined to

one spatial dimension. The pointer Hamiltonian is taken as that of a free massive particle;

$$H_M := \frac{P^2}{2M}, \tag{6.113}$$

and the atom-pointer system is described by a Hamiltonian $H_A + H_M + H_{AM}$. A *measurement* of duration τ starting immediately after $t = 0$ is assumed to be described by the interaction

$$H_{AM}(t) := \Omega(t)\sigma_z P \tag{6.114}$$

where

$$\Omega(t) = \begin{cases} \Omega > 0 & \text{if } 0 < t \leq \tau \\ 0 & \text{otherwise.} \end{cases} \tag{6.115}$$

At $t = \tau$ an *observation* is made, which causes the familiar collapse of the state of the atom. The observable relevant to determining the measurement outcome is the position $Q(\tau)$ of the pointer when the observation is made. The relevant equations of motion are

$$\dot{P}(t) = \dot{\sigma}_z(t) = 0, \qquad \dot{Q}(t) = \frac{P(t)}{M} + \Omega(t)\sigma_z(t). \tag{6.116}$$

Using the notational convention $A := A(0)$ for any operator A, 6.116 yields

$$Q(t) = Q + \frac{tP}{M} + \Omega\sigma_z, \qquad 0 \leq t \leq \tau. \tag{6.117}$$

Assuming at $t = 0$ a normalised product state $|\varphi, \phi\rangle$ with $|\varphi\rangle := a|e\rangle + b|g\rangle$ an arbitrary atomic state, and $|\phi\rangle$ chosen such that $\langle\phi|Q|\phi\rangle = \langle\phi|P|\phi\rangle = 0$, one obtains

$$\langle Q(\tau)\rangle = \Omega\langle\sigma_z\rangle = \frac{\Omega}{2}\left(|a|^2 - |b|^2\right), \qquad |a|^2 + |b|^2 = 1 \tag{6.118a}$$

$$\Sigma_Q := \langle Q(\tau)^2\rangle - \langle Q(\tau)\rangle^2 = \Omega^2\left(\frac{1}{4} - \langle\sigma_z\rangle\right) = \frac{\Omega^2}{4}\left(1 - \left[|a|^2 - |b|^2\right]\right). \tag{6.118b}$$

The position of the pointer is perfectly correlated with the atomic populations. The expectation value in 6.118a gives the average pointer position within the interval $[-\Omega/2, \Omega/2]$, taken over a series of identical measurements starting with the initial state $|\varphi, \phi\rangle$. Individual observations yield outcomes $\pm\Omega/2$, with the outcome $-\Omega/2$ revealing that the atom has ground state energy, and the outcome $\Omega/2$ revealing that the atom is excited. One deduces that there are two peaks in the probability distribution associated with the pointer's position, one at $\Omega/2$ with relative height $|a|^2$, and one at $-\Omega/2$ with relative height $|b|^2$. In this way the measurement yields information about the atomic state at $t = 0$.

Now consider the case in which the atom interacts with a single field mode. Taking the single-mode analog of the general atom-field interaction in 6.81 one obtains the total

Hamiltonian

$$H = \frac{P^2}{2M} + \omega_{eg}\sigma_z + \omega a^\dagger a + \Omega(t)\sigma_z P + \left[ig\sigma^+\left(u^+ a^\dagger + u^- a\right) + \text{H.c.}\right]. \tag{6.119}$$

This situation is obviously more complicated than the bare atom case, because the bare atomic energy is no longer a symmetry; $\dot{\sigma}_z \neq 0$. The coupled system of equations of motion can be solved perturbatively up to $O(g^2)$ in a fairly straightforward fashion. Compagno *et al.* (1990) assume that the initial state of the atom-field system is the dressed ground state $|g;0\rangle_{\text{true}}$, which is the ground state of the composite atom-field system. The second order perturbation theory results given by 5.87 and 5.88 yield the following state normalised up to $O(g^2)$

$$|g;0\rangle_{\text{true}} = \left[1 - \frac{|gu^+|^2}{2(\omega_{eg}+\omega)^2}\right]|g;0\rangle - \frac{igu^+}{\omega_{eg}+\omega}|e;1\rangle + \frac{|g|^2 u^+ u^-}{\sqrt{2}\omega(\omega_{eg}+\omega)}|g;2\rangle. \tag{6.120}$$

Assuming the same initial state $|\phi\rangle$ for the pointer, lengthy calculations give the $O(g^2)$ result (Compagno *et al.* (1990), Compagno *et al.* (1995))

$$\langle Q(\tau)\rangle = \Omega\langle\sigma_z\rangle = \frac{\Omega}{2}\left(|a|^2 - |b|^2\right), \qquad |a|^2 = \frac{|gu^+|^2}{(\omega_{eg}+\omega)^2}, \qquad |b|^2 = 1 - |a|^2, \tag{6.121a}$$

$$\Sigma_Q = \Omega^2\left(\frac{1}{4} - \langle\sigma_z\rangle^2\right)\frac{\sin^2\left([\omega_{eg}+\omega]\tau/2\right)}{([\omega_{eg}+\omega]\tau/2)^2} = \Omega^2\frac{|gu^+|^2}{(\omega_{eg}+\omega)^2}\frac{\sin^2\left([\omega_{eg}+\omega]\tau/2\right)}{([\omega_{eg}+\omega]\tau/2)^2}. \tag{6.121b}$$

There are two limiting situations; if the measurement is "short" i.e. $(\omega_{eg}+\omega)\tau \ll 1$, then the sinc^2 function in 6.121b tends to 1, and Σ_Q consequently tends to the bare result 6.118b. The distribution of pointer frequencies is therefore the same as in the bare case with a small peak (of height $|a|^2$) centered at the outcome $\Omega/2$ corresponding to the atom excited, and a large peak at $-\Omega/2$ corresponding to the atom in the bare ground state. This affords the interpretation that measurements such that $\tau < (\omega_{eg}+\omega)^{-1}$ are capable of resolving virtual emission events according to 6.91, and the atom is therefore perceived as bare by the pointer.

The second limiting situation is that in which $(\omega_{eg}+\omega)\tau \gg 1$. Then the sinc^2 function tends to 0, which implies the existence of a single peak in the distribution of pointer positions, centered at the average value $\Omega\langle\sigma_z\rangle/2 \in [-\Omega/2, \Omega/2]$. This affords the interpretation that for sufficiently long measurements the pointer is incapable of resolving virtual emission-reabsorption events and the atom is perceived as a ground state dressed atom corresponding to the single outcome $\Omega\langle\sigma_z\rangle/2$.

It is immediately clear from 6.120 that for the atom-field system in the ground state there is in general a nonzero probability to measure the bare atom as excited. The question is whether or not this actually means anything physically. The above treatment *presupposes* that free energy constitutes a physically real observable, and based on this assumption demonstrates that the atom can be detected as bare with sufficiently short measurements.

One can therefore prepare an excited atomic state by measuring the atom, even when the system is initially in the ground state. Thus, one will have apparently created "energy" from nothing.

Compagno *et al.* (1990) suggest that the measurement process is capable of transferring, according to 6.91, an energy no larger than τ^{-1} into the atom-field system. If $\tau < (\omega_{eg} + \omega)^{-1}$ then any virtual excitations become real, which accounts for the reality of the "energy" that seemingly came from nowhere. This is also consistent with the pointer's perception of the atom as bare; a real photon is separate from the atom, which consequently must be measured as bare. Precise details regarding the mechanism by which the measurement transfers energy are somewhat scarce. To be sure, the bare pointer energy is a symmetry of the Hamiltonian and is therefore conserved. The bare atom-pointer interaction energy is however, not conserved, because $\dot{\sigma}_z \neq 0$.

Compagno *et al.* (1995) have extended their considerations to the many-mode case. To do this one takes the many-mode interaction 6.81 instead of its one-mode counterpart. After lengthy calculations the results come out as follows

$$\langle Q(\tau)\rangle = \Omega\langle\sigma_z\rangle = \frac{\Omega}{2}\left(|a|^2 - |b|^2\right), \qquad |a|^2 = \sum_{\mathbf{k}\lambda}\frac{|g_{\mathbf{k}\lambda}u_k^+|^2}{(\omega_{eg}+\omega)^2}, \qquad |b|^2 = 1 - |a|^2, \tag{6.122a}$$

$$\Sigma_Q = \Omega^2\sum_{\mathbf{k}\lambda}\frac{|g_{\mathbf{k}\lambda}u_k^+|^2}{(\omega_{eg}+\omega)^2}\frac{\sin^2\left([\omega_{eg}+\omega]\tau/2\right)}{([\omega_{eg}+\omega]\tau/2)^2}. \tag{6.122b}$$

The variance Σ_Q in 6.122b is closely related to P^+_{ph} in 6.72. In fact if one identifies the coupling $c_{\mathbf{k}\lambda}$ in 6.72 with the coupling $g_{\mathbf{k}\lambda}u_k^+$, then one sees that $\Sigma_Q = (\Omega/\tau)^2 P^+_{\text{ph}}(\tau)$. A similar analysis is afforded in this situation as in the one-mode case; one simply has to perform it term-by-term. The pointer perceives the atom as dressed only by photons with high frequency relative to the inverse measurement duration, because these photons correspond to terms in the mode sum on the right-hand-side in 6.122b that don't contribute to the nonzero value of Σ_Q. For a measurement of duration τ those virtual photons for which $\omega_{eg} + \omega \gg \tau^{-1}$ are not perceived as separate from the atom. According to 6.91 the measurement is incapable of transferring sufficient energy to "release" such virtual photons. The relatively low frequency photons for which $\omega_{eg} + \omega \ll \tau^{-1}$ are however, released, and so with respect to these modes the atom is perceived as bare.

The measurement formalism employed here is extremely idealised. The pointer is modelled somewhat arbitrarily and couples directly to the bare atom. Even so a more thorough quantitative analysis of the results above is difficult, not least because the discussion depends quite heavily on the atom-pointer coupling Ω. Setting $\Omega = 1$ for simplicity, choosing an ultraviolet cut-off, and choosing ω_{eg} in the optical range, one is left with only two free parameters; τ and $g_{\mathbf{k}\lambda}u_k^+$. The small probability $|a|^2$ corresponding to the atom excited is independent of τ, and is of the order $10^{-6} - 10^{-7}$ in both the Coulomb and Poincaré gauges, while it vanishes identically in the symmetric representation. For "very long" measurements

$\tau \sim 1s$, the variance Σ_Q is of the order 10^{-6} in the Coulomb gauge, but is still as large as 10^{-2} in the Poincaré gauge. For short measurements Σ_Q can blow up rapidly due to the $1/\tau^2$ dependence. Thus, while the average pointer position remains strongly weighted in favour of detecting the bare atom in its ground state, the deviation from this average can be very large.

In any eventuality choosing the symmetric representation means there is zero chance of finding the atom excited. The virtual cloud dressing the vacuum does not exist in this representation, because the bare ground state coincides with the true ground state. Although a virtual cloud is present whenever $u_k^+ \neq 0$ it may be quite different in nature depending on the representation chosen. Thus, there are various ambiguities to be fixed in determining the nature of a photon. First, there is perhaps an occasionally quite subtle distinction to be made between real and virtual photons, but one must also decide which type of photon dresses the atom by choosing the appropriate coupling. Of course, these two facets are not entirely separate; as I have just noted, there are no virtual photons dressing the ground state within the symmetric representation. The extremely loose numerical results above suggest that short measurements are required to probe such questions pertaining to bare states, and that over such time scales it's possible that strange things occur.

The results of Compagno and co-workers are at least intriguing. If nothing else the above exposition demonstrates just how involved the question as to the reality of bare degrees of freedom can get. It suggests that, as one might already have suspected, such questions are quite intimately intertwined with questions regarding quantum measurement.

6.5 Summary and discussion

In this chapter I have tried to focus on simple atom-field interaction models utilising standard quantum-optical models and approximations. The chapter consists of an analysis of level-shifts, real and virtual photon emission, and the virtual cloud. These analyses tend to lend support to various conclusions and interpretations not all of which are mutually compatible.

We have seen that the separation of radiative and material degrees of freedom is far from clear cut, a fact that gives rise to the notion of virtual quanta subject to the energy-time uncertainty relation (6.4). I will use the ideas of 6.4.2 in chapter 8 in which I investigate an open quantum systems description of the atom-field system as a means by which to determine the most appropriate subsystem decomposition. We saw in 6.3 that numerous approximations are required in order to avoid paradoxical divergent results brought about by counter-rotating (virtual) contributions. The symmetric representation discussed in 6.3.3 eliminates these divergences without requiring the use of approximations. It is for this reason that in chapter 8, it will be seen to give the most physically sensible results. We will see in chapter 9 however, that the use of such a representation in describing interatomic interactions necessarily incurs violations of Einstein causality.

In 6.2 I discussed radiative level-shifts. The empirical verification of these shifts seems to show that measured atomic energy levels are eigenvalues of the composite atom-field Hamiltonian. However, excited atom-field eigenstates are stationary and will not decay, something that seems to be at odds with the empirical fact that excited atoms spontaneously emit. Excited dressed states and spontaneous emission are the subject of chapters 7 and 9.

PART III

Gauge-variant and gauge-invariant predictions

CHAPTER 7

Excited states and spectral lineshapes

The only dressed state I have discussed in any detail so far has been the bare atomic ground state dressed by the bare vacuum field. Excited dressed states are difficult to identify, because the Hamiltonian H does not have, as H_A does, discrete excited states. The bare field Hamiltonian H_F has purely continuous spectrum, and the discrete atomic states of H_A *dissolve* into the continuous spectrum of H due to the coupling V. In problems involving excited states one usually assumes an initially bare excited state, and as such one inevitably runs into gauge dependence problems.

The natural lineshape is the frequency distribution of radiation spontaneously emitted by an atom in an excited state. One calculates in the limit $t \to \infty$, and for an initial bare state $|e;0\rangle$ at $t = 0$, the probability to detect a photon and the atom in its ground state. Since bare states are gauge dependent, and one specifies the initial state at $t = 0$ rather than $t = -\infty$ the lineshape prediction is gauge dependent. The difference in lineshapes between the Coulomb and Poincaré gauges was investigated in detail by Power & Zienau (1959), who found that the prediction of the Poincaré gauge was in better agreement with the experiment of Lamb (1952).

It is clear that a definition of the lineshape in terms of some set of *physical* observables and states is an implicitly *gauge-invariant* definition. One can therefore view the task at hand as that of determining the representation, if any, in which the canonical operators and bare states happen to represent the physical observables and states that give rise to the correct definition. Such a determination may be possible by comparison of the theoretical predictions with experiment. Of course, this reasoning is valid only if there exists with certainty, *some* gauge in which the canonical momenta and bare states are the right ones. Failing this one would be forced to seek an entirely different method of calculation altogether.

In this chapter I review various analyses of the behaviour of excited bare and dressed

states. I then attempt a detailed analysis of the lineshape paradox using the formal theory of radiation damping (Heitler (1954), Cohen-Tannoudji *et al.* (1992)) and the arbitrary gauge Hamiltonian 2.71. This analysis constitutes the entirety of new work presented in this chapter. It can be found in sections 7.2-7.4, and is summarised in the paper Stokes (2013). I describe the preparation of the initially excited atomic state by resonant absorption of incident radiation with a sharp line, and with a slight modification use the same result to describe the Lamb transition in atomic hydrogen in a way relevant to the early experiments of Lamb (1952) (Power & Zienau (1959)). I then use a simplified treatment whereby the atom is excited by a laser pulse treated semi-classically.

7.1 Excited states

7.1.1 Excited dressed states

For the purposes of getting a feel for excited dressed states I first analyse the two-level atom coupled to the field in the symmetric representation. The Hamiltonian H for this model has the interaction component given in 6.84, and can be written

$$H := H_0 + V, \qquad H_0 := \omega_{eg}^0 \sigma_z + \sum_k \omega_k^0 a_k^\dagger a_k, \qquad V := \sum_k g_k a_k^\dagger \sigma^- + \text{H.c.}. \tag{7.1}$$

For the purpose of what follows I have collapsed the double index $\mathbf{k}\lambda$ into a single index k, and I have explicitly labelled the bare photon frequencies and coupling strengths with this index.

Even for this simplified model it quickly becomes apparent that conventional perturbative techniques fail in determining the shift in energy of the excited bare state $|e;0\rangle$ when the continuum limit of field modes is taken. This is due to the presence of divergences in the expressions obtained at higher orders. Such divergences arise, because to any arbitrarily small neighbourhood of the bare atomic energy ω_{eg}^0, there corresponds an uncountably infinite set of nearly degenerate one-photon states $|0,\mathbf{k}\lambda\rangle$ with energy $\omega_k^0 \sim \omega_{eg}^0$.

In contrast, when the set of field modes is discrete the only degeneracies that occur are countable. To try to understand the spectrum of H in the continuum limit one can attempt to solve the problem in the discrete case and then study the behaviour of the resulting expressions in the continuum limit. The basic eigen-problem to be solved is

$$H|n\rangle = \omega_n |n\rangle, \tag{7.2}$$

so we must consider the determinant $|H - \omega_n|$. The problem is tractable if we restrict ourselves to the one-excitation subspace. If we represent $H - \omega$ as a matrix in the bare atom-field basis restricted to states with *one-excitation* and let N denote the total number of field

modes, the determinant $|H-\omega|$ can be written as an $(N+1)\times(N+1)$ array;

$$|H-\omega_n| = \begin{vmatrix} \omega_{eg}^0-\omega_n & g_1 & g_2 & \cdots & g_N \\ g_1^* & \omega_1^0-\omega_n & 0 & \cdots & 0 \\ g_2^* & 0 & \ddots & & \vdots \\ \vdots & \vdots & & & \\ g_N^* & 0 & \cdots & & \omega_N^0-\omega_n \end{vmatrix}. \tag{7.3}$$

The ij^{th} entry in 7.3 is the matrix element

$$\langle 0_0;0_1,...,0,1_i,0,...,0|(H-\omega_n)|0_0;0_1,...,0,1_j,0,...,0\rangle \tag{7.4}$$

where $|0_0\rangle := |g\rangle$ and $|1_0\rangle := |e\rangle$. Owing to the simplicity of the model, all entries are zero except for the left most column, top row and main diagonal. The determinant 7.3 can be written

$$|H-\omega_n| = \left[\prod_{k=1}^{N}(\omega_k^0-\omega_n)\right]\left[\omega_{eg}^0-\omega_n-F(\omega_n)\right], \qquad F(\omega_n) := \sum_{k=1}^{N}\frac{|g_k|^2}{\omega_k^0-\omega_n}, \tag{7.5}$$

an expression which can be used to find the ω_n by setting the second factor in square brackets equal to zero. Unfortunately an analytic solution doesn't seem possible, but before addressing this issue let's turn our attention to the eigenstates $|n\rangle$. An arbitrary eigenstate $|n\rangle$ within the one-excitation subspace can be written

$$|n\rangle = A_0^n|e;0\rangle + \sum_{k=1}^{N}A_k^n|g,1_k\rangle. \tag{7.6}$$

The $A_j^n,\ j=0,...,N$ can be found via 7.2, which can be written $(H-\omega_n)_{ij}A_j^n = 0$. This equation is equivalent to the coupled equations

$$(\omega_{eg}^0-\omega_n)A_0^n + \sum_{k=1}^{N}g_kA_k^n = 0, \tag{7.7a}$$

$$g_k^*A_0^n + (\omega_k^0-\omega_n)A_k^n = 0. \tag{7.7b}$$

At the same time the normalisation condition $\langle n|n\rangle = 1$ implies that

$$|A_0^n|^2 = \frac{1}{1+F'(\omega_n)} \tag{7.8}$$

where $F'(\omega_n) := \partial F/\partial\omega_n$, and equation 7.7b together with 7.8 yield up to an arbitrary phase

$$A_k^n = -\frac{g_k^*A_0^n}{\omega_k^0-\omega_n} = \frac{1}{\sqrt{1+F'(\omega_n)}}\sum_{k=1}^{N}\frac{g_k^*}{\omega_n-\omega_k^0}. \tag{7.9}$$

Combining our results so far we have up to an arbitrary phase

$$\omega_n = \omega_{eg}^0 - F(\omega_n), \tag{7.10a}$$

$$|n\rangle = \frac{1}{\sqrt{1+F'(\omega_n)}}\left[|e;0\rangle + \sum_{k=1}^{N} \frac{g_k^*}{\omega_n - \omega_k^0}|g;1_k\rangle\right], \tag{7.10b}$$

in which

$$F(\omega_n) := \sum_{k=1}^{N} \frac{|g_k|^2}{\omega_k^0 - \omega_n}, \qquad F'(\omega_n) = \sum_{k=1}^{N} \frac{|g_k|^2}{(\omega_k^0 - \omega_n)^2}. \tag{7.11}$$

These results can be analysed with the aid of a graphical technique (see Cohen-Tannoudji *et al.* (1992), Compagno *et al.* (1995)). Within each interval $[\omega_k^0, \omega_{k+1}^0]$ there is precisely one eigenvalue ω_n, and the intervals become increasingly dense as N increases. If the g_k are nonzero and assumed independent of N, then in the limit $N \to \infty$ the width of the intervals shrinks to zero and the spectrum of H is equivalent to the free field spectrum. The discrete atomic level at ω_{eg}^0 completely dissolves in this continuum with the overlap between $|e;0\rangle$ and any of the eigenstates $|n\rangle$ tending to zero. This means that when N tends to ∞ no trace of the discrete atomic level can be found in any of the new eigenstates.

When the coupling $|g_k|^2$ is proportional to $1/V$ where V is the volume within which the field modes are quantised, the situation is different, because N is proportional to V. Consequently the interaction strength decreases with the number of modes. This is the case in the atom-field system of interest. Indeed, Fermi's golden rule 5.54 gives the excited atomic state decay rate[45]

$$\Gamma = 2\pi|g_k|^2\rho(\omega_k^0)\Big|_{\omega_k^0=\omega_{eg}^0}, \tag{7.12}$$

and in order that Γ is finite the coupling $|g_k|^2$ must scale as $1/N$. In this case the spectrum of H still forms a continuum, yet the new eigenstates seem to retain some memory of the discrete atomic level. I will consider this situation in more detail in the next section after having made the simplifying assumption of a flat continuum.

7.1.2 The case of a flat continuum

Consider now the case of a flat continuum for which the coupling $g_k\rho(\omega_k^0) = g$ is the same for each k, coupled by an interaction V to a discrete atomic level $|e;0\rangle$ with energy ω_{eg}^0.[46] I

[45] It must of course be understood that the sum over polarisations and integral over solid angle have been carried out in 7.12, and that $|g_k|^2\rho(\omega_k^0)|_{\omega_k^0=\omega_{eg}^0}$ actually represents the effective coupling after having performed this procedure.

[46] Note that I have assumed that the energy density of modes $\omega_k^{0\,2}$ is implicitly contained in the coupling, which as in 7.12 actually refers to the effective coupling after integration has been performed using Fermi's golden rule. The flat continuum approximation assumes that this effective coupling is constant.

will assume for simplicity that V is off-diagonal in the bare basis as was the case in 7.1.1. Discretising the continuum by introducing an energy spacing δ, the decay rate of the atomic level is according to Fermi's golden rule 5.54 given by

$$\Gamma = \frac{2\pi|g|^2}{\delta}. \tag{7.13}$$

This decay rate remains finite in the continuum limit $\delta \to 0^+$, provided $|g|^2$ is proportional to δ. Thus, $g \to 0$ when $\delta \to 0^+$. As before we seek a solution to the eigenvalue problem 7.2. In fact the results of 7.1.1 remain valid if one simply replaces the varying coupling g_k with the constant coupling g. Thus,

$$\omega_n = \omega_{eg}^0 - F(\omega_n) \tag{7.14}$$

where using 7.13 (Cohen-Tannoudji *et al.* (1992)) we have

$$F(\omega_n) := \sum_{k=1}^{\infty} \frac{|g|^2}{\omega_k^0 - \omega_n} = -\sum_{k=1}^{\infty} \frac{|g|^2/\delta}{\omega_n/\delta - k} = -\frac{\Gamma/2}{\tan(\Gamma\omega_n/2|g|^2)}. \tag{7.15}$$

We therefore have a solution to the eigenvalue problem in the form

$$\omega_n - \omega_{eg}^0 = \frac{\Gamma/2}{\tan(\Gamma\omega_n/2|g|^2)}. \tag{7.16}$$

The discrete eigenvalues of H can be obtained as the horizontal components of the points of intersection of the line $y_1(\omega) = \omega - \omega_{eg}^0$ and the curve $y_2(\omega) = \Gamma/2\tan\left(\Gamma\omega/2|g|^2\right)$. There is one eigenvalue ω_n per interval $[\omega_k^0, \omega_{k+1}^0]$. For large mode frequencies the eigenvalues of H get closer and closer to the asymptotes, which represent the eigenvalues ω_k^0 of the bare field Hamiltonian H_F. In order that $\omega_n \approx \omega_k^0$ we require according to 7.14 that $\Gamma \ll \omega_k^0 - \omega_{eg}^0$. We conclude that the eigenvalues of H are different to those of H_F only over an interval of width of the order of Γ, centered on ω_{eg}^0. The probability $|A_0^n|^2 = |\langle e;0|n\rangle|^2$ associated with the discrete state $|e;0\rangle$ in the new continuum, exhibits significant variations in ω_n near ω_{eg}^0. The eigenstates $|n\rangle$ with energy within $\Gamma/2$ of ω_{eg}^0 therefore seem to retain some memory of the discrete atomic level $|e;0\rangle$. Explicitly, using 7.8 and 7.15 we have

$$|A_0^n|^2 = \frac{|g|^2}{|g|^2 + (\omega_n - \omega_{eg}^0)^2 + (\Gamma/2)^2} \tag{7.17}$$

which tends to zero in the continuum limit ($|g|^2 \to 0$ as $\delta \to 0^+$). However, Cohen-Tannoudji *et al.* (1992) obtain a simple expression for the variation of this probability with ω_n, which doesn't vanish in the limit $\delta \to 0^+$. If we let $[\omega, \omega + d\omega]$ be an energy interval much greater than δ, but much less than Γ, the total probability in 7.17 within this interval

is

$$dP = \sum_{\omega<\omega_n<\omega+d\omega} |A_0^n|^2 \approx \frac{d\omega}{\delta} |A_0^n|^2\big|_{\omega_n=\omega}, \tag{7.18}$$

which using 7.17 and 7.13 gives in the limit $\delta \to 0^+$

$$\frac{dP}{d\omega} = \frac{\Gamma/2\pi}{(\Gamma/2)^2 + (\omega - \omega_{eg}^0)^2}. \tag{7.19}$$

This is a normalised Lorentzian of width Γ centred on ω_{eg}^0, which justifies my previous statement that the ω_n are different to the eigenvalues of H_F only over an interval of width of the order of Γ, centered on ω_{eg}^0, and that in this region the new eigenstates seem to retain some memory of the discrete atomic level.

Finally I wish to consider the decay of the discrete state. To work this out I start by expanding $|e;0\rangle$ in the new eigenbasis $\{|n\rangle\}$;

$$|e;0\rangle = \sum_n c_n |n\rangle, \qquad c_n = \langle n|e;0\rangle = A_n^0 = \frac{|g|}{\left[|g|^2 + (\omega_n - \omega_{eg}^0)^2 + (\Gamma/2)^2\right]^{1/2}}. \tag{7.20}$$

The Schrödinger equation yields for the temporal evolution of $|e;0\rangle$

$$|\psi(t)\rangle = e^{-iHt}|e;0\rangle = \sum_n \frac{|g|e^{-i\omega_n t}}{\left[|g|^2 + (\omega_n - \omega_{eg}^0)^2 + (\Gamma/2)^2\right]^{1/2}} |n\rangle. \tag{7.21}$$

Thus,

$$\langle e;0|\psi(t)\rangle = \sum_n \frac{A_0^n |g| e^{-i\omega_n t}}{\left[|g|^2 + (\omega_n - \omega_{eg}^0)^2 + (\Gamma/2)^2\right]^{1/2}}, \tag{7.22}$$

which using 7.13 and 7.21 becomes in the limit $\delta \to 0^+$

$$\langle e;0|\psi(t)\rangle \to \frac{\Gamma}{2\pi} \int d\omega \, \frac{e^{-i\omega_n t}}{(\omega_n - \omega_{eg}^0)^2 + (\Gamma/2)^2}. \tag{7.23}$$

The integral in 7.23 can be evaluated via the residue method, which yields (Cohen-Tannoudji *et al.* (1992))

$$|\langle e;0|\psi(t)\rangle|^2 = e^{-\Gamma|t|}. \tag{7.24}$$

Finally then, we have obtained the well-known exponential decay of the state $|e;0\rangle$, which for the case of a flat continuum appears to be exact.

7.1.3 The pole approximation

I will now begin to consider more realistic models in which the continuum is not assumed flat and there may be many discrete levels of H_0. The true atom-field system of interest is of precisely this type. Suppose $|0,e\rangle$ denotes an excited bare state with energy ω_e^0. The quantity relevant to describing the decay of this state is the corresponding matrix element of $G(z)$, which is given according to 5.81 by

$$G_e(z) = \frac{1}{z - \omega_e^0 - R_e(z)} \tag{7.25}$$

where $R_e(z)$ is defined in 5.75. In actual fact what we will usually be interested in are the propagators $G_e^{\pm}(\omega) := G_e(\omega \pm i\eta)$ from which $G_e(z)$ can always be constructed. Clearly the propagators will be known as soon as the corresponding matrix elements $R_e^{\pm}(\omega) := R_e(\omega \pm i\eta)$ of the level-shift operator have been found. Using 5.75 and the relation

$$\lim_{\eta\to 0^+} \frac{1}{x \pm i\eta} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x) \tag{7.26}$$

with $\mathcal{P}$ denoting the Cauchy principal value, we have

$$R_e^{\pm}(\omega) = \langle e;0|VQ\frac{1}{\omega - QHQ \pm i\eta}QV|e;0\rangle = V_e + \Delta_e(\omega) \mp i\frac{\Gamma_e(\omega)}{2} \tag{7.27}$$

where $Q := 1 - |e;0\rangle\langle e;0|$, $V_e := \langle e;0|V|e;0\rangle$ and

$$\Delta_e(\omega) := \mathscr{P}\langle e;0|VQ\frac{1}{\omega - QHQ}QV|e;0\rangle, \tag{7.28a}$$

$$\Gamma_e(\omega) := 2\pi\langle e;0|VQ\delta(\omega - QHQ)QV|e;0\rangle. \tag{7.28b}$$

Equation 7.28a when substituted into 7.25 gives a shift of the bare energy ω_e^0, while equation 7.28b gives an imaginary component $\Gamma_e(\omega) \geq 0$, which vanishes for $\omega < \omega_g$, ω_g being the ground state energy of H. The occurrence of $\Gamma_e(\omega)$ indicates dissipative behaviour of the excited bare state. If the complete set of eigenstates of QHQ is denoted $\{|\alpha\rangle\}$ and the completeness relation with respect to these states is used in 7.28 one easily obtains

$$\Delta_e(\omega) = \mathscr{P}\sum_\alpha \frac{|\langle e;0|VQ|\alpha\rangle|^2}{\omega - \omega_\alpha}, \qquad \Gamma_e(\omega) = 2\pi\sum_\alpha |\langle e;0|VQ|\alpha\rangle|^2\delta(\omega - \omega_\alpha), \tag{7.29}$$

from which the useful relation

$$\Delta_e(\omega) = \frac{1}{2\pi}\mathscr{P}\int d\omega' \frac{\Gamma_e(\omega')}{\omega - \omega'} \tag{7.30}$$

follows quite generally.

It is usually not possible to calculate $\Gamma_e(\omega)$ and $\Delta_e(\omega)$ exactly, so one must resort to approximations. A common approximation is the use of perturbation theory to find the

level-shift operator R (see 7.2.1).[47] I denote the perturbative approximations of $\Delta_e(\omega)$ and $\Gamma_e(\omega)$ with a tilde; $\Gamma_e(\omega) \approx \tilde{\Gamma}_e(\omega)$, $\Delta_e(\omega) \approx \tilde{\Delta}_e(\omega)$.

Another widely used approximation is the *pole approximation*, which consists of neglecting in 7.28 the variations of $\Delta_e(\omega)$ and $\Gamma_e(\omega)$ (or possibly $\tilde{\Delta}_e(\omega)$ and $\tilde{\Gamma}_e(\omega)$) with ω. The pole approximation is justified when $\Delta_e(\omega)$ and $\Gamma_e(\omega)$ are sufficiently small and vary sufficiently slowly over the neighbourhood of $\omega_e^0 + \Delta_e(\omega_e^0)$, having a width of the order of several $\Gamma_e(\omega_e^0)$. In this case one can put $\Delta_e(\omega) \approx \Delta_e(\omega_e^0)$ and $\Gamma_e(\omega) \approx \Gamma_e(\omega_e^0)$. Loosely speaking the pole approximation approximates the varying continuum as flat and therefore leads to the results for a flat continuum found in 7.1.2.

7.1.4 Analytic properties of the resolvent

As we have seen the resolvent operator serves as a useful tool in the analysis of excited states. Clearly G in 5.55 is only singular on the real axis, because H is Hermitian. One can show that the matrix element $G_\psi(z)$ with respect to a normalised state $|\psi\rangle$, is in fact analytic everywhere except on the real axis (Cohen-Tannoudji *et al.* (1992)). A discrete eigenvalue ω_n of H, corresponds to a simple pole of $G_\psi(z)$ with residue $|\langle n|\psi\rangle|^2$. Continuous eigenvalues of H correspond to branch cuts of $G_\psi(z)$ along the real axis. To determine the nature of such cuts let us take a resolution of the identity using eigenstates of H, following Cohen-Tannoudji *et al.* (1992)

$$I = \sum_n |n\rangle\langle n| + \int d\omega \int d\lambda\, \rho(\omega,\lambda)|\omega,\lambda\rangle\langle\omega\lambda|. \tag{7.31}$$

Here the $|n\rangle$ are discrete eigenstates, while $|\omega,\lambda\rangle$ is formally used to denote an "eigenstate" corresponding to ω within the continuous spectrum. The extra λ is meant to characterise all other variables besides energy upon which the continuous eigenstates might depend, while $\rho(\omega,\lambda)$ describes the density of continuous states. Now, using 7.31 and 7.26 the part of the matrix element $G_\psi^\pm(\omega)$ dependent on the continuous spectrum of H is seen to be

$$\mp i\pi f_\psi(\omega) + \int d\omega' \frac{f_\psi(\omega')}{\omega - \omega'} \tag{7.32}$$

where

$$f_\psi(\omega) := \int d\lambda\, \rho(\omega,\lambda)|\langle\omega,\lambda|\psi\rangle|^2. \tag{7.33}$$

According to 7.32 $G_\psi^+(\omega)$ and $G_\psi^-(\omega)$ differ by an amount $2\pi i f_\psi(\omega)$, which effectively represents the length of the branch cut of $G_\psi(z)$. The matrix element $G_\psi(\omega \pm i\eta)$ has

[47] It is important to recognise that a perturbative approximation of R *doesn't* amount to a perturbative approximation of G. The expression 7.25 already implies that all orders in perturbation theory have been used to find G_e. Using a perturbative approximation of R_e to find G_e in 7.25 constitutes replacing an *exact* infinite sum by an *approximate* infinite sum (Cohen-Tannoudji *et al.* (1992)).

a different value depending on whether the real axis is approached from above or below. Using 7.25 the difference between G_e^+ and G_e^- of 7.1.3 is easily found to be

$$G_e^+(\omega) - G_e^-(\omega) = \frac{-i\Gamma_e(\omega)}{(\omega - \omega_e^0 - \Delta_e(\omega))^2 + (\Gamma_e(\omega)/2)^2}, \tag{7.34}$$

which is nonzero whenever $\Gamma_e(\omega) \neq 0$, that is, whenever $\omega > \omega_g$. Thus $G(z)$ has a cut starting at ω_g and extending to infinity. The free resolvent $G_0(z)$ has a pole at ω_g^0. The fact that we have gone from a pole to a branch cut in replacing G_0 by G shows that H unlike H_0 does not possess discrete eigenvalues. The discrete eigenvalues of H_0 have dissolved in the new continuum associated with H.

Despite this, it is clear that the function $G_e^+(z)$ has no poles in the lower-half complex plane. Similarly $G_e^-(z)$ has no poles in the upper-half complex plane. The reason for this being that the imaginary parts of the denominators are necessarily nonzero on these domains. If we make the pole approximation in 7.34 then Δ_e and Γ_e are independent of ω and one can perform an *analytic continuation* of $G_e^+(z)$ defined on the domain $\mathrm{Im}(z) > 0$, into the lower-half plane.[48] The analytic continuation of $G_e^+(z)$ has a pole at $z_0 = \omega_e^0 + \Delta_e - i\Gamma_e/2$. In this way one can characterise *unstable* states as corresponding to poles in the analytic continuation of $G^+(z)$, which are also known as *resonances*.

It is worth noting that 7.34 is close to a Lorentzian centred at $\omega_e = \omega_e^0 + \Delta_e$. For this to be the case one must perform the pole approximation, so that Δ_e and Γ_e don't vary with ω. The decay of the excited state is described directly by the amplitude $U_e(\tau) := \langle e;0|U(\tau)|e;0\rangle$. Using 5.60 we have

$$U_e(\tau) = \frac{1}{2\pi i}\int d\omega \left[G_e^-(\omega) - G_e^+(\omega)\right] e^{-i\omega\tau}. \tag{7.35}$$

If we make the pole approximation in 7.34 and substitute the resulting expression into 7.35 the integral can be evaluated via Cauchy's residue formula and we obtain

$$U_e(\tau) = e^{-\Gamma_e\tau/2} e^{-i(\omega_e^0 + \Delta_e)\tau}, \tag{7.36}$$

which is the same exponential decay as was encountered in 7.1.2 for a flat continuum, and in the WW treatment of spontaneous emission (cf. 6.3.2). The pole approximation in this context gives the same result as the Markovian approximation used in 6.3.2.

Summarising results so far, we have seen that excited bare atomic states correspond to resonances in the spectrum of the composite atom-field Hamiltonian, indicating that some memory of the old discrete states is retained within the new continuum. More precisely the probability 7.17 exhibits significant variations in energy near to the bare energy ω_{eg}^0. In the case of a flat continuum an excited discrete bare state decays exponentially with a decay rate that doesn't depend on the energy ω. This result can be extended to more general continua

[48] One could of course make an analytic continuation of $G_e^-(z)$ defined on $\mathrm{Im}(z) < 0$ into the upper-half plane.

via the use of the pole approximation, which neglects the energy variation of the decay rate and level-shift.

7.2 The natural lineshape in an arbitrary gauge

Having reviewed some aspects of excited state decay I'm now in a position to look at concrete experimental situations. I look here to determine the spectral lineshape of photons emitted in the decay of an excited atomic state via spontaneous emission. The results presented from this section onwards are summarised in the paper Stokes (2013).

7.2.1 The theory of radiation damping

Assuming the atom is in the first excited state $|e;0\rangle$ at $t=0$, I calculate the long-time squared amplitude $|b_{\mathbf{k}\lambda}(\infty)|^2$, representing the probability of finding the atom in the ground state $|g\rangle$ and a photon $|\mathbf{k}\lambda\rangle$ with frequency ω present upon measurement. The lineshape is defined as

$$S(\omega) := \rho(\omega)\frac{V}{(2\pi)^3}\int d\Omega \sum_{\lambda}|b_{\mathbf{k}\lambda}(\infty)|^2, \tag{7.37}$$

where $\rho(\omega)=\omega^2$ is the density of field modes, the sum is over polarisations belonging to a given direction, and the integration is over all directions. To derive an expression for $|b_{\mathbf{k}\lambda}(\infty)|^2$ I start with the traditional method of considering the variation of the coefficients $b_f(t) := \langle f|\psi(t)\rangle$ associated with a Hamiltonian $H=H_0+V$, in the interaction picture (Dirac (1927)). For ease of writing I hereafter omit the superscript ^{0} when writing down bare energies such as ω_n^0 and a true energy ω_n will be denoted with a tilde; $\tilde{\omega}_n$. Following Heitler (1954) I introduce the Fourier transform

$$b_f(t) := \langle f|U(t,0)|i\rangle e^{i\omega_f t} = -\frac{1}{2\pi i}\int d\omega\, G_{fi}(\omega+i\eta)e^{i(\omega_f-\omega)t}, \tag{7.38}$$

where G is the resolvent of H, and $|i\rangle$ is the initial state at $t=0$. Note that only γ^+ contributes to the contour integral in 5.61, i.e., only the propagator G^+ on the left-hand-side of 5.22 contributes when $\tau>0$. The Schrödinger equation yields the amplitude equation for $t>0$

$$i\dot{b}_f(t) = \sum_m V_{fm}b_m(t)e^{i\omega_{fm}t} \tag{7.39}$$

to which we seek a solution subject to the initial conditions $\lim_{t\to 0^+} b_n(t)=\delta_{ni}$ with $|i\rangle = |e;0\rangle$. Equivalently we require a solution to the equation

$$i\dot{b}_f(t) = \sum_m V_{fm}b_m(t)e^{i\omega_{fm}t} + i\delta_{fi}\delta(t) \tag{7.40}$$

for all $t \in \mathbb{R}$, subject to the condition that the amplitudes be normalised to zero for negative times; $\forall n,\ b_n(t) = 0$ whenever $t < 0$.[49] This corresponds to imposing a sudden jump from 0 to 1 of the amplitude b_i associated with $|i\rangle$ at time $t = 0$, which clearly contrasts with the adiabatic switching on of the interaction from $t = -\infty$ used in the S-matrix. It has been argued by Milonni *et al.* (1989) that this sudden switching condition is responsible for the lineshape paradox. They claim that only in the Poincaré gauge is the imposition of such a condition justified, which is why the Poincaré gauge result is in better agreement with experiment than the Coulomb gauge result.

Substituting the representation

$$i\delta(t) = -\frac{1}{2\pi i}\int d\omega\, e^{i(\omega_i-\omega)t} \tag{7.42}$$

and 7.38 into 7.40 one finds that

$$(\omega-\omega_n)G^+_{ni}(\omega) = \delta_{ni} + \sum_m V_{nm}G^+_{mi}(\omega), \tag{7.43}$$

which implies that[50]

$$G^+_{ni}(\omega) = \zeta(\omega-\omega_n)\left[\delta_{ni} + \sum_m V_{nm}G^+_{mi}(\omega)\right] \tag{7.44}$$

where ζ is a distribution defined by

$$\zeta(x) := \lim_{\eta\to 0^+}\frac{1}{x+i\eta} = \mathscr{P}\frac{1}{x} - i\pi\delta(x). \tag{7.45}$$

Next I define for all $n \neq i$ the matrix elements $R_{ni}(\omega)$ through the relation

$$G^+_{ni}(\omega) = R_{ni}(\omega)G^+_i(\omega)\zeta(\omega-\omega_n). \tag{7.46}$$

Substituting 7.46 into the right-hand-side of 7.44, imposing the condition $n \neq i$, and finally

[49] Explicitly equation 7.40 corresponds to a solution for $b_f(t)$ of the form

$$ib_f(t) = i\theta(t)\delta_{fi} + \int_{-\infty}^{t} dt' \sum_m V_{fm}b_m(t')e^{i\omega_m t'} \tag{7.41}$$

where θ is the Heaviside step function defined in 5.20. The presence of θ in 7.41 encodes the assumption of a sharp initial bare state; $b_i(0) = 1$.

[50] This implication follows from the fact that the expressions 7.43 and 7.44 involve *distributions* in ω. It must of course be implicitly understood that such expressions are to be integrated. This presents a problem when it comes to dividing both sides of 7.43 by $\omega - \omega_n$, because such a division produces a nonintegrable singularity on the right-hand-side. In order to avoid such an eventuality one adds an infinitesimal imaginary component $i\eta$ to the prefactor $\omega - \omega_n$ appearing on the left-hand-side. One then divides through by $\omega - \omega_n + i\eta$ instead. Viewing the matrix elements of the resolvent (the G^+_{nm}) as functions of a complex variable z, the expression obtained on the right-hand-side then has a pole in the lower-half complex plane rather than on the real axis $\mathrm{Re}(z) = \omega$. Finally taking the limit of this expression as $\eta \to 0^+$ gives rise to the term $\zeta(\omega - \omega_n)$ appearing in 7.44.

equating the resulting expression with the right-hand-side of 7.46, gives

$$R_{ni}(\omega) = V_{ni} + \sum_{m\neq i} V_{nm}R_{mi}(\omega)\zeta(\omega-\omega_m), \qquad n \neq i. \tag{7.47}$$

At the same time 7.43 with $n = i$, and 7.46 imply that

$$(\omega-\omega_i)G_i^+(\omega) = 1 + V_{ii}G_i^+(\omega) + \sum_{m\neq i} V_{im}R_{mi}(\omega)G_i^+(\omega)\zeta(\omega-\omega_m) \tag{7.48}$$

from which it follows that

$$G_i^+(\omega) = \frac{1}{\omega-\omega_i - R_i^+(\omega)} \tag{7.49}$$

where

$$R_i^+(\omega) := V_{ii} + \sum_{m\neq i} V_{im}R_{mi}(\omega)\zeta(\omega-\omega_m). \tag{7.50}$$

It is easy to verify that the $R_i^+(\omega)$ appearing above is the same $R_i^+(\omega)$ as was defined in 7.27. The decay rate $\Gamma_i(\omega)$ in 7.27 can be written

$$\Gamma_i(\omega) = -\mathrm{Im}\left[R_i^+(\omega) - V_{ii}\right] = 2\pi\sum_{m\neq i}|R_{mi}(\omega)|^2\delta(\omega-\omega_m), \tag{7.51}$$

which can be verified by substituting 7.47 and its conjugate into the right-hand-side. Only the first term V_{ni} in 7.47 contributes, because the two double-sums arising from the second term cancel between 7.47 and its conjugate. The remaining contribution is exactly $\left[(R_i^+(\omega) - V_{ii}) - \mathrm{c.c}\right]/2 = -\mathrm{Im}\left[R_i^+(\omega) - V_{ii}\right]$. Using 7.51 and 7.30 one sees that the shift component $\Delta_i(\omega)$ of $R_i^+(\omega)$ can be written

$$\Delta_i(\omega) = \mathscr{P}\sum_{m\neq i}\frac{|R_{mi}(\omega_m)|^2}{\omega-\omega_m}. \tag{7.52}$$

The expressions 7.51 and 7.52 are ideally suited to obtaining perturbative approximations through perturbative approximation of the $R_{mi}(\omega)$. In order to calculate the lineshape it would also be useful to obtain an expression for the amplitude $b_f(\infty)$ purely in terms of the $R_{mi}(\omega)$. This is readily achieved by substituting 7.46 into 7.38, which yields

$$b_f(t) = -\frac{1}{2\pi i}\int d\omega R_{fi}(\omega)G_i^+(\omega)\zeta(\omega-\omega_f)e^{i(\omega_f-\omega)t}, \qquad f \neq i. \tag{7.53}$$

Since we require $b_f(0) = 0$ for $f \neq i$ we require that

$$\frac{1}{2\pi i}\int d\omega R_{fi}(\omega)G_i^+(\omega)\zeta(\omega-\omega_f) = 0. \tag{7.54}$$

We can therefore add the left-hand-side of 7.54 to the right-hand-side of 7.53, which gives

$$b_f(t) = -\frac{1}{2\pi i}\int d\omega R_{fi}(\omega)G_i^+(\omega)\zeta(\omega-\omega_f)\left[e^{i(\omega_f-\omega)t}-1\right]. \tag{7.55}$$

The delta-function contribution from the ζ-distribution in 7.55 is zero, because the complex exponential term in square brackets vanishes at $\omega=\omega_f$. Furthermore,

$$\lim_{t\to\infty}\frac{e^{i(\omega_f-\omega)t}-1}{\omega-\omega_f} = \zeta(\omega_f-\omega), \tag{7.56}$$

so

$$b_f(\infty) = -\frac{1}{2\pi i}\mathscr{P}\int d\omega R_{fi}(\omega)G_i^+(\omega)\zeta(\omega_f-\omega). \tag{7.57}$$

Subtracting 7.54 from this expression we obtain

$$b_f(\infty) = -\frac{1}{2\pi i}\mathscr{P}\int d\omega R_{fi}(\omega)G_i^+(\omega)\left[\zeta(\omega_f-\omega)+\zeta(\omega-\omega_f)\right], \tag{7.58}$$

but $\zeta(\omega_f-\omega)+\zeta(\omega-\omega_f) = -2\pi i\delta(\omega-\omega_f)$, which implies using 7.49 that

$$b_f(\infty) = R_{fi}(\omega_f)G_i^+(\omega_f) = \frac{R_{fi}(\omega_f)}{\omega_{fi}-R_i^+(\omega_f)} \tag{7.59}$$

and this is the expression for $b_f(\infty)$ in terms of R that we sought. Finally using 7.27 the associated probability can be written

$$|b_f(\infty)|^2 = \frac{|R_{fi}(\omega_f)|^2}{(\omega_{fi}-\Delta_i(\omega_f))^2+(\Gamma_i(\omega_f)/2)^2}, \tag{7.60}$$

whenever $V_{ii}=0$. When $V_{ii}\neq 0$ we can absorb it into $\Delta_i(\omega)$, which means 7.60 is actually completely general. In the case $|f\rangle = |g;\mathbf{k}\lambda\rangle$ and $|i\rangle = |e;0\rangle$, 7.60 defines the amplitude in 7.37.

Since according to 7.51 and 7.52 $\Gamma_i(\omega_f)$ and $\Delta_i(\omega_f)$ can be written in terms of the $R_{mi}(\omega_f)$ alone, our task now reduces to that of obtaining explicit expressions for the $R_{mi}(\omega_f)$. Such expressions can only be found by using a perturbative expansion of $R(\omega)$ in powers of V. Therefore, in order to go further I make the first approximation $R_{nm}(\omega)\approx V_{nm}$. The components of the lineshape now only depend on matrix elements of the form $\langle n;\mathbf{k}\lambda|V|e;0\rangle$. Using 2.71 we have

$$\begin{aligned}\langle n;\mathbf{k}\lambda|V|e;0\rangle = {}& \frac{eg}{m}\mathbf{e}_{\mathbf{k}\lambda}\cdot[\mathbf{p}e^{-i\mathbf{k}\cdot\mathbf{r}}]_{ne} \;+\; ie\omega g\,\mathbf{e}_{\mathbf{k}\lambda}\cdot\tilde{\mathbf{g}}_{ne}(\mathbf{k},\mathbf{r}) \\ & + \frac{eg}{2m}\left[\mathbf{p}\cdot\nabla_r\left\{\mathbf{e}_{\mathbf{k}\lambda}\cdot\tilde{\mathbf{g}}(\mathbf{k},\mathbf{r})\right\}+\nabla_r\left\{\mathbf{e}_{\mathbf{k}\lambda}\cdot\tilde{\mathbf{g}}(\mathbf{k},\mathbf{r})\right\}\cdot\mathbf{p}\right]_{ne},\end{aligned} \tag{7.61}$$

where

$$g := \frac{1}{\sqrt{2\omega V}}, \qquad \tilde{\mathbf{g}}(\mathbf{k},\mathbf{r}) := \int d^3x\, \mathbf{g}(\mathbf{x},\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{x}}. \tag{7.62}$$

The matrix element in 7.61 is clearly explicitly dependent on the gauge choice g. Choosing the Coulomb gauge and making the EDA, one obtains the following approximate expressions for respectively, the numerator, level shift and decay rate in 7.60

$$\begin{aligned}
|R_{e;0,g;\mathbf{k}\lambda}(\omega_g+\omega)|^2 &\approx \frac{e^2}{m^2}\frac{1}{2\omega V}|\mathbf{p}_{eg}\cdot\mathbf{e}_{\mathbf{k}\lambda}|^2,\\
\Delta(\omega_g+\omega) &\approx \mathscr{P}\sum_n \sum_{\mathbf{k}'\lambda'} \frac{e^2}{m^2}\frac{1}{2\omega' V}\frac{|\mathbf{p}_{ne}\cdot\mathbf{e}_{\mathbf{k}'\lambda'}|^2}{\omega-\omega_{ng}-\omega'},\\
\Gamma(\omega_g+\omega) &\approx 2\pi\sum_n \sum_{\mathbf{k}'\lambda'} \frac{e^2}{m^2}\frac{1}{2\omega' V}|\mathbf{p}_{ne}\cdot\mathbf{e}_{\mathbf{k}'\lambda'}|^2\delta(\omega-\omega_{ng}-\omega').
\end{aligned} \tag{7.63}$$

where for convenience I have omitted the subscript $_i$ in writing the decay rate and shift. Similarly using the Poincaré gauge and EDA one obtains

$$\begin{aligned}
|R_{e;0,g;\mathbf{k}\lambda}(\omega_g+\omega)|^2 &\approx \frac{\omega}{2V}|\mathbf{d}_{eg}\cdot\mathbf{e}_{\mathbf{k}\lambda}|^2,\\
\Delta(\omega_g+\omega) &\approx \mathscr{P}\sum_n \sum_{\mathbf{k}'\lambda'} \frac{\omega'}{2V}\frac{|\mathbf{d}_{ne}\cdot\mathbf{e}_{\mathbf{k}'\lambda'}|^2}{\omega-\omega_{ng}-\omega'},\\
\Gamma(\omega_g+\omega) &\approx 2\pi\sum_n \sum_{\mathbf{k}'\lambda'} \frac{\omega'}{2V}|\mathbf{d}_{ne}\cdot\mathbf{e}_{\mathbf{k}'\lambda'}|^2\delta(\omega-\omega_{ng}-\omega').
\end{aligned} \tag{7.64}$$

We see that, as is implied by 7.61, the expressions in 7.63 are not the same as those in 7.64.

7.2.2 The approximations ensuring gauge invariance

I review here the various approximations, which can be used to reproduce previous results and eliminate the dependence of the lineshape on the choice of gauge. I note first that three approximations have already been used; first the limiting value $t \to \infty$ ensures the level shift and decay rate in 7.60 are evaluated at $\omega_f = \omega_g + \omega$. Second an approximation $R_{nm}(\omega) \approx V_{nm}$ is used for the matrix elements of the level-shift operator. Finally the EDA is used to give the eventual expressions in 7.63 and 7.64.

Crucial in ensuring gauge invariance is the further approximation of insisting that the emission process conserves energy i.e. that $\omega = \omega_{eg}$. In the decay rate Γ the delta function then ensures that the matrix element of V_g is evaluated on-energy-shell. It is a standard result that such matrix elements are quite generally invariant for two Hamiltonians related by a unitary transformation of the form $R = \exp(ieS)$ (Craig & Thirunamachandran (1984), Woolley (1999)). The invariance of Γ can easily be verified explicitly for the Coulomb and Poincaré gauges by using the relation 6.45. The result is nothing but the well-known first order decay rate found using Fermi's golden rule.

Turning our attention to the level shift Δ, it is easy to check that the imposition of energy conservation alone does not suffice to ensure gauge invariance. For this, one must also add to Δ the contribution $\langle e;0|V|e;0\rangle$, which produces the total shift

$$\Delta_{\text{total}} = \langle e;0|V|e;0\rangle + \sum_n \frac{|\langle n|V|e;0\rangle|^2}{\omega_e - \omega_n}. \tag{7.65}$$

This is the same on-energy-shell shift in energy of the excited state $|e;0\rangle$ as is obtained through second order perturbation theory. Note that the term V_{ii} *does* appear explicitly in 7.59, but was omitted when writing 7.60, where it was remarked that V_{ii} *can be absorbed into* Δ. Thus, the shift term in 7.65 is nothing but the actual shift appearing in the lineshape denominator once the additional contribution V_{ii} has been absorbed. Like Γ, Δ_{total} is invariant for two Hamiltonians related by a unitary transformation $R = \exp(ieS)$ (Craig & Thirunamachandran (1984)). As with Γ this invariance is easily verified for the Coulomb and Poincaré gauges. In the Coulomb gauge the additional contribution in 7.65 comes from the $e^2\mathbf{A}^2/2m$ part of the minimal coupling interaction Hamiltonian to give a total shift

$$\Delta_{\text{total}} = \sum_{\mathbf{k}\lambda} \frac{e^2}{m} \frac{1}{2\omega V} \left(\frac{|\mathbf{e}_{\mathbf{k}\lambda}|^2}{2} - \sum_n \frac{1}{m} \frac{|\mathbf{p}_{ne} \cdot \mathbf{e}_{\mathbf{k}\lambda}|^2}{\omega_{ne} + \omega} \right). \tag{7.66}$$

In the Poincaré gauge the additional contribution comes from the polarisation field term $e^2|\mathbf{r}\delta^{\mathrm{T}}|^2/2$. Hence, the total shift is

$$\Delta_{\text{total}} = \sum_n \sum_{\mathbf{k}\lambda} \frac{1}{2V} |\mathbf{d}_{ne} \cdot \mathbf{e}_{\mathbf{k}\lambda}|^2 \left(1 - \frac{\omega}{\omega_{ne} + \omega} \right). \tag{7.67}$$

Using the expansion

$$\frac{1}{\omega_{ne} + \omega} = \frac{1}{\omega} + \frac{\omega_{ne}}{\omega^2} + \frac{\omega_{ne}^2}{\omega^3} - \frac{\omega_{ne}^3}{\omega^3(\omega_{ne} + \omega)} \tag{7.68}$$

and 6.45 it is straightforward to show that 7.66 and 7.67 are identical (Craig & Thirunamachandran (1984)). Neglecting in Δ_{total}, all contributions not dependent on the state of the electron, and removing the electron self-energy contribution through mass renormalization gives the standard nonrelativistic Lamb shift 6.39 (Craig & Thirunamachandran (1984)).

The energy conservation condition $\omega = \omega_{eg}$ has been justified on the grounds that $\Gamma(\omega)$ and $\Delta(\omega)$ do not vary appreciably over the interval $w \gg \Gamma, \Delta$ centered at ω_e, and they can therefore be evaluated at ω_e to within sufficient accuracy (Cohen-Tannoudji *et al.* (1992)). This argument however, is somewhat ruined by the gauge arbitrariness of the matrix elements of $R(\omega)$. More precisely, the required slow variations of $\Gamma(\omega)$ and $\Delta(\omega)$ cannot be guaranteed irrespective of $\mathbf{g}$. At the same time it is clear that without energy conservation the denominator in 7.60 is gauge dependent. Nevertheless, for most "sensible" choices of gauge energy conservation as an approximation may certainly be valid and good. In such cases its use would be of little or no practical significance.

The numerator $|R_{fi}(\omega_f)|^2$ in 7.60 is more troublesome. It is typically neglected altogether, or otherwise evaluated on-energy-shell, yielding the gauge-invariant result $\Gamma/2\pi$. Either procedure can only be justified on the grounds that the numerator's dependence on ω is sufficiently slow so as to be undetectable when compared with the denominator. If this is not the case then it should be possible to determine with an experiment, which form of the Hamiltonian produces the most accurate lineshape prediction.

7.2.3 The lineshape after removal of the virtual field

Starting in the Coulomb gauge and EDA I define the unitary operator

$$R_{\rm s} := \exp\left[-\sum_{\mathbf{k}\lambda}\sum_{nm} ig(\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{d}_{nm})\alpha_{k,nm}|n\rangle\langle m|(a^{\dagger}_{\mathbf{k}\lambda}+a_{\mathbf{k}\lambda})\right], \tag{7.69}$$

This transformation is the extension to the case of a general multi-level atom, of 6.76. The term $\alpha_{k,nm}$ is as before, chosen so as to eliminate the energy non-conserving terms in the linear part of the interaction Hamiltonian. The appropriate choice being

$$\alpha_{k,nm} = \frac{|\omega_{nm}|}{\omega+|\omega_{nm}|}. \tag{7.70}$$

It is important to note that $R_{\rm s}$ only eliminates the energy non-conserving terms to first order in the coupling, and within the EDA. The resultant Hamiltonian $H_{\rm s} := R_{\rm s}HR_{\rm s}^{-1}$ has to first order in e, the interaction component

$$V_{\rm s} = \sum_{\mathbf{k}\lambda}\sum_{n,m}^{n>m} g_{\mathbf{k}\lambda,nm}\frac{2(\omega_{nm}\omega)^{1/2}}{\omega_{nm}+\omega}|n\rangle\langle m|a_{\mathbf{k}\lambda}+\text{H.c.} \tag{7.71}$$

where

$$g_{\mathbf{k}\lambda,nm} := -i\left(\frac{\omega_{nm}}{2V}\right)^{1/2}(\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{d}_{nm}). \tag{7.72}$$

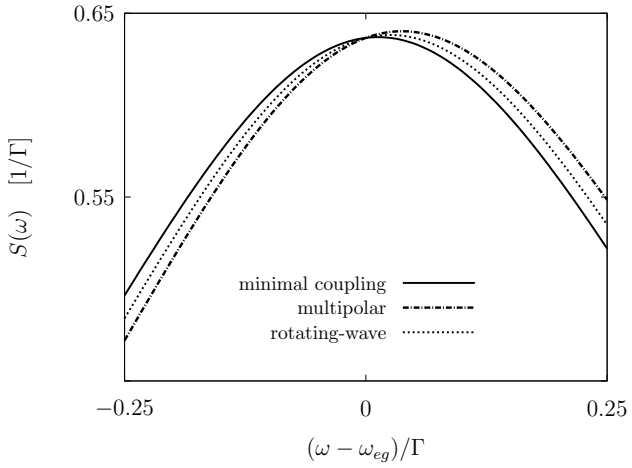
Terms of $O(e^2)$ have been omitted, because they give rise to $O(e^4)$ contributions in the lineshape; their only contribution is to the term $\langle e;0|V|e;0\rangle$ in 7.65. Yet we know this level shift is invariant under a unitary transformation $R=\exp(ieS)$, so the total level shift obtained in the new representation must be the same as for the Coulomb gauge. The same is true of the decay rate Γ, and therefore of the denominator in 7.60. The lineshape in the symmetric representation is therefore

$$S(\omega) = \frac{4\omega^3}{\omega_{eg}(\omega_{eg}+\omega)^2}\frac{\Gamma/2\pi}{(\omega-\omega_{eg}-\Delta_{\rm LS})^2+\Gamma^2/4}, \tag{7.73}$$

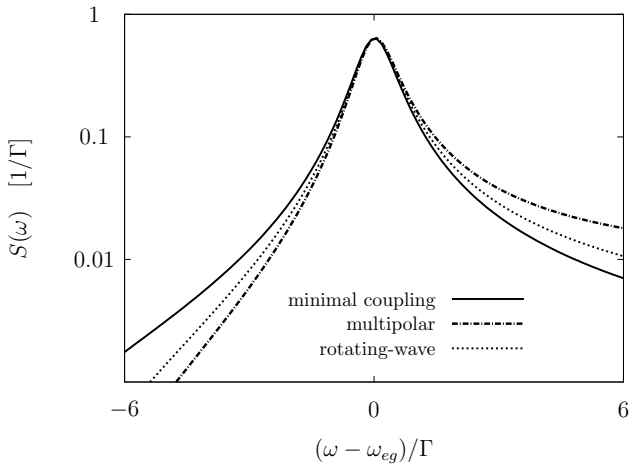
which is plotted in Figs. 7.1(a) and 7.1(b) along with the Coulomb and Poincaré gauge results. The difference in lineshapes between gauges is a result of the differing $|R_{fi}(\omega_f)|^2$ terms of 7.60, which are collected in table 7.1 for the three main cases.

H	$2\pi\lvert R_{fi}(\omega_f)\rvert^2/\Gamma$, to $O(e^2)$
H_s	$\frac{4\omega^3}{\omega_{eg}(\omega_{eg}+\omega)^2}$
H_C	$\frac{\omega}{\omega_{eg}}$
H_P	$\left(\frac{\omega}{\omega_{eg}}\right)^3$

Table 7.1: The frequency dependence of the lineshape numerator $|R_{fi}(\omega_f)|^2$ (c.f. 7.60) in different representations.



(a)



(b)

Figure 7.1: The lineshapes associated with the minimal coupling, multipolar and rotating-wave Hamiltonians. In each plot $\Gamma = \omega_{eg}/10$ and the Lamb shift Δ_{LS} has been suppressed. In 7.1(a) $S(\omega)$ is plotted on a linear axis, whereas in 7.1(b) it is plotted on a logarithmic axis. Since the rotating-wave coupling is a symmetric mixture of the minimal and multipolar couplings, the corresponding curve interpolates between the curves associated with the Coulomb and Poincaré gauges.

7.3 The atom's excitation through resonant absorption

The lineshapes obtained so far have all assumed a sharp bare state $|e;0\rangle$ at $t = 0$. It was noticed some time ago however, that the shape of spectral lines is bound to depend on the mechanism by which the atom is excited (Low (1952)). In this section I describe the process by which the atom is initially excited, as well as the emission process itself.

7.3.1 Absorption of incident radiation with a sharp line

Let's first consider the situation whereby the atom starts in its ground state in the presence of incident radiation with intensity distribution S. A primary photon with frequency ω_0 is absorbed by the atom out of S and a photon with frequency ω near ω_0 is emitted. The quantity of interest is the total rate γ at which the system leaves the initial state $|i\rangle$. This can be obtained using the theory of radiation damping used in the preceding sections (Heitler (1954)). Another method is to use the S-matrix element for the process by which the atom absorbs and re-emits a photon.

Suppose $|i\rangle = |g;\mathbf{k}\lambda\rangle$ and $|f\rangle = |m;\mathbf{k}'\lambda\rangle$. The associated T-matrix element is

$$T_{fi}(\omega_i) = V_{fi} + \sum_{n,m} V_{fn} G^{+}_{mn}(\omega_i) V_{ni}. \tag{7.74}$$

If we are interested in emission out of the state $|e;0\rangle$ it seems natural to restrict attention to the single intermediate state $|e;0\rangle$ in 7.74. This also seems necessary in order to obtain a lineshape formula. Of course such a restriction will break the gauge invariance of the matrix element. The restricted matrix element is

$$T_{m;\mathbf{k}'\lambda',g;\mathbf{k}\lambda}(\omega_e) = \langle m;\mathbf{k}'\lambda'|V|e;0\rangle G^{+}_{e}(\omega_e)\langle e;0|V|g;\mathbf{k}\lambda\rangle = -\frac{\langle m;\mathbf{k}'\lambda'|V|e;0\rangle\langle e;0|V|g;\mathbf{k}\lambda\rangle}{\tilde{\omega}_{eg} - \omega - i\Gamma/2} \tag{7.75}$$

where Γ is the gauge-invariant on-energy-shell spontaneous decay rate of the excited atomic state, and $\tilde{\omega}_{eg} = \omega_{eg} + \tilde{\Delta}_e(\omega_e)$ is the shifted transition frequency with $\tilde{\Delta}_e(\omega_e) \equiv \Delta$ given by 7.65.

I now assume for simplicity that $|m\rangle \equiv |g\rangle$ meaning that the atom returns to the ground state after it has emitted the photon $\mathbf{k}'\lambda'$. The total rate $w^{\text{group}}_{i\to f}$ at which the system leaves the state $|i\rangle$ is given by Fermi's golden rule 5.54 whereby all one-photon final states are summed over;

$$\begin{aligned} w^{\text{group}}_{i\to f} &= 2\pi \frac{|\langle e;0|V|g;\mathbf{k}\lambda\rangle|^2}{(\tilde{\omega}_{eg} - \omega)^2 + (\Gamma/2)^2} \sum_{\mathbf{k}'\lambda'} |\langle g;\mathbf{k}'\lambda'|V|e;0\rangle|^2 \delta(\omega - \omega') \\ &= \tilde{\Gamma}_e(\omega) \frac{|\langle e;0|V|g;\mathbf{k}\lambda\rangle|^2}{(\tilde{\omega}_{eg} - \omega)^2 + (\Gamma/2)^2} \end{aligned} \tag{7.76}$$

where

$$\tilde{\Gamma}_e(\omega) := 2\pi \sum_{\mathbf{k}'\lambda'} |\langle g;\mathbf{k}'\lambda'|V|e;0\rangle|^2 \delta(\omega-\omega') \tag{7.77}$$

is the first order approximation of the exact decay rate in 7.51 evaluated at the incident photon frequency ω. I'm interested in the case in which the distribution $S(\omega)$ of incident radiation is sharp i.e. different from zero only at some ω_0. The total rate of *resonance fluorescence* γ after absorption of incident radiation with a sharp line is

$$\gamma = \int d\omega\, \omega^2 S(\omega) w_{i\to f}^{\text{group}}(\omega). \tag{7.78}$$

If we assume the explicit distribution

$$\frac{S(\omega)}{V} = S\frac{\delta(\omega-\omega_0)}{\omega^3} \tag{7.79}$$

for some constant intensity S we obtain the result

$$\frac{\gamma}{V} = \frac{S\Gamma(\omega_0)}{\omega_0} \frac{|\langle g;\mathbf{k}_0\lambda|V|e;0\rangle|^2}{(\omega_0-\omega_{eg})^2+\Gamma^2/4}, \tag{7.80}$$

which is the same as the result obtained using the radiation damping formalism (Heitler (1954)). The transition rate γ is clearly dependent on the form of the interaction and therefore gauge dependent. For the Coulomb gauge, Poincaré gauge and symmetric representations in the EDA γ can be written

$$\gamma = \frac{S\Gamma|\mathbf{e}\cdot\mathbf{d}_{ge}|^2}{2} \frac{n(\omega_0,\omega_{eg})}{(\omega_0-\omega_{eg})^2+\Gamma^2/4}, \tag{7.81}$$

where the incident signal, intensity S is polarised along $\mathbf{e}$. The "numerator" n differs between the different representations, analogously to the difference in the $|R_{fi}(\omega_f)|^2$ terms listed in 7.1. This is summarised in table 7.2 for the three main cases.

H	$n(\omega_0,\omega_{eg})$
H_s	$\frac{16\omega_{eg}\omega_0^3}{(\omega_{eg}+\omega_0)^4}$
H_C	$\frac{\omega_{eg}}{\omega_0}$
H_P	$\left(\frac{\omega_0}{\omega_{eg}}\right)^3$

Table 7.2: The frequency dependence of the different resonance fluorescence rates.

7.3.2 The Lamb line in hydrogen

The $2s \to 1s$ transition in atomic hydrogen has received a great deal of attention over the years (Lamb & Retherford (1947), Lamb (1952), Power & Zienau (1959), Fried (1973), Bassani *et al.* (1977), Cohen-Tannoudji *et al.* (1997)). We know that T-matrix elements on-energy-shell are gauge-invariant, the matrix element of the two photon resonant transition $2s \to 1s$ is a particular example. This has been amply verified with semi-classical treatments when complete sets of intermediate states are used (Fried (1973), Bassani *et al.* (1977), Cohen-Tannoudji *et al.* (1997)). On the other hand lineshape formulas including radiation damping will not in general produce the same results in each gauge.

The quantity relevant to the experiments of Lamb is the fluorescence rate γ out of the metastable state $2s$ in a process of stimulated decay, due to the presence of a microwave signal with frequency ω_0 near the Lamb separation $\omega_{2s,2p}$ of the $2s \to 2p$ transition. Free energy conservation implies that a photon with frequency $\omega_{2s,2p} + \omega_{2p,1s} - \omega_0$ is emitted in the cascade $2s \to 2p \to 1s$. It is assumed that the *spontaneous* single photon decay process $2s \to 2p$ is negligible, as is the spontaneous two photon decay process $2s \to 2p \to 1s$. Moreover, the $2s$-level can be considered sharp in the presence of an incident microwave signal for all signal levels, which means the treatment of 7.3.1 should be valid. This time we have $|i\rangle = |2s;\mathbf{k}\lambda\rangle$ and $|f\rangle = |1s;\mathbf{k}'\lambda'\rangle$, and we restrict our attention to the single intermediate state $|2p;0\rangle$. The resonance condition determining the frequency dependence of the delta-function in the rate $w^{\text{group}}_{i\to f}$ must be modified, so that it now reads (Power & Zienau (1959), Cohen-Tannoudji *et al.* (1997))

$$\omega_{2s,1s} \equiv \omega_{2s,2p} + \omega_{2p,1s} = \omega + \omega' \quad \Rightarrow \quad \omega_f = \omega' = \omega_{2s,2p} + \omega_{2p,1s} - \omega. \tag{7.82}$$

The total process consists of an induced emission (due to the presence of the sharp incident microwave signal) of a microwave photon $\mathbf{k}\lambda$ with frequency close to the Lamb frequency $\omega_{2s,2s}$, followed by spontaneous emission of a *Lyman-*α, ultraviolet photon $\mathbf{k}'\lambda'$ with frequency close to the transition frequency $\omega_{2p,1s}$. Proceeding as in 7.3.1 we obtain

$$w^{\text{group}}_{i\to f} = \tilde{\Gamma}_{2p,1s}(\omega_{2s,2p} + \omega_{2p,1s} - \omega)\frac{|\langle 2p;0|V|2s,\mathbf{k}\lambda\rangle|^2}{(\tilde{\omega}_{2s,2p} - \omega)^2 + (\Gamma_{2p,1s}/2)^2}, \tag{7.83}$$

which upon using 7.79 gives

$$\frac{\gamma}{V} = \frac{S\Gamma_{2p,1s}(\omega_{2s,2p} + \omega_{2p,1s} - \omega_0)}{\omega_0}\frac{|\langle 2s;\mathbf{k}_0\lambda|V|2p;0\rangle|^2}{(\omega_0 - \omega_{2s,2p})^2 + \Gamma^2_{2p,1s}/4}. \tag{7.84}$$

With this we obtain

$$\gamma = \frac{S\Gamma_{2p,1s}|\mathbf{e}\cdot\mathbf{d}_{2s,2p}|^2}{2}\frac{n'(\omega_0,\omega_{2s,2p},\omega_{2p,1s})}{(\omega_0 - \omega_{2p,2s})^2 + \Gamma^2_{2p,1s}/4}, \tag{7.85}$$

where as before n' differs between the different representations, as is summarised in table

H	$n'(\omega_0, \omega_{2s,2p}, \omega_{2p,1s})$
H_S	$\frac{4(\omega_{2s,2p}+\omega_{2p,1s}-\omega_0)^3}{\omega_{2p,1s}(\omega_{2s,2p}+2\omega_{2p,1s}-\omega_0)^2}\,\frac{4\omega_{2s,2p}^2}{(\omega_{2s,2p}+\omega_0)^2}$
H_C	$\frac{\omega_{2s,2p}+\omega_{2p,1s}-\omega_0}{\omega_{2p,1s}}\,\frac{\omega_{2s,2p}^2}{\omega_0^2}$
H_P	$\left(\frac{\omega_{2s,2p}+\omega_{2p,1s}-\omega_0}{\omega_{2p,1s}}\right)^3$

Table 7.3: The frequency dependence of the Lamb line in different representations.

7.3. Lamb's experiments yielded a distribution of frequencies $\omega_{2s,2p}$ as a function of intensity. The relative differences in the distributions $\gamma(\omega_{2s,2p})$ associated with the different n' in table 7.3 are essentially the same as the relative differences in the lineshapes plotted in Figs. 7.1(a) and 7.1(b). The Poincaré gauge result is indistinguishable from the bare Lorentzian whereas the other curves exhibit small deviations.

A good deal of work has been put into clarifying the conditions under which predictions pertaining to the two-photon Lamb transition $2s \to 1s$ in atomic hydrogen are gauge-invariant. For two-photon scattering processes the S-matrix in second order yields the *Kramers-Heisenberg dispersion relation* (Craig & Thirunamachandran (1984)), which can be obtained by a direct second order approximation of $G_e^+(z)$ in 7.75. However, a treatment limited to second order is insufficient to describe the exponential decay of the excited atomic state, which gives rise to the decay rate in the denominator of the lineshape. Thus, in order to obtain a lineshape formula from the Kramers-Heisenberg formula one must add by hand a decay term into the denominator of the resonant contribution (Sakurai (1967)). Ignoring the non-resonant contribution and restricting one's attention to the apparently dominant $2p$ intermediate state, the Kramers-Heisenberg formula can be used to obtain the results of 7.3.1 (Power & Zienau (1959)). Of course in carrying out these steps one breaks the gauge invariance of the matrix element.

Furthermore, as soon as finite times are considered, predictions pertaining to canonical degrees of freedom will yield different results in different gauges. The experiments of Lamb were in sufficiently close agreement with the Poincaré gauge result to rule out the Coulomb gauge result. A simple explanation for this is that the physical degrees of freedom represented by the canonical operators in the Poincaré gauge are closer to the correct ones. This is essentially the explanation first offered by Power & Zienau (1959). Milonni *et al.* (1989) show that if the "sudden switching" condition of assuming a sharp bare state at $t = 0$ is avoided, the Poincaré gauge lineshape result can be found using the Coulomb gauge. The proposed method to avoid this condition is tantamount to using the canonical observables of the Poincaré gauge within the Coulomb gauge, so they essentially resolve the discrepancy in the same way as Power & Zienau (1959).

7.4 The atom's excitation by a laser pulse

In this section I choose the WW approach to lineshape derivations (cf. 6.3.2), because it is easily adapted to include a description of the atom's excitation by laser light. Although this treatment does not really allow for any frequency variation of the lineshape numerator in a self-consistent manner, it yields the same results as the resolvent method provided the Lamb shift is suppressed in the latter. Since the previous lineshapes have only depended on one transition frequency ω_{eg}, and we have seen that the quadratic parts of the interaction Hamiltonian do not contribute, I adopt a two-level model for the atom, and the purely linear atom-field interaction Hamiltonian 6.81.

7.4.1 Modelling the laser

To describe the laser I add an appropriate semi-classical interaction term to 6.84. For consistency the laser should be taken to couple to the atom in the same way as the quantised field does. Thus I define the atom-laser interaction by

$$V_l = \frac{i\Omega(t)}{2}\sigma^+\left(u_l^+ e^{i\omega_l t} + u_l^- e^{-i\omega_l t}\right) + \text{H.c.}, \tag{7.86}$$

where $\Omega(t)$ is a real but otherwise completely arbitrary time dependent coupling envelope. Assuming resonant driving $\omega_l = \omega_{eg}$, 7.86 reduces to

$$V_l = \frac{i\Omega(t)}{2}\sigma^+\left((1-2\alpha)e^{i\omega_{eg}t} + e^{-i\omega_{eg}t}\right) + \text{H.c.}, \tag{7.87}$$

where α is an arbitrary real number. Choosing $\alpha = 0$ and defining $\Omega(t) = (e/m)\langle\mathbf{p}\rangle\cdot\mathbf{A}_0(t)$, 7.87 gives a (semi-classical) minimal coupling interaction in which the electron's canonical momentum couples to a classical vector potential of the form $\mathbf{A}_0(t)\cos\omega_{eg}t$;

$$V_l = i\frac{e}{m}\langle\mathbf{p}\rangle\cdot\mathbf{A}_0(t)(\sigma^+ - \sigma^-)\cos\omega_{eg}t. \tag{7.88}$$

Choosing $\alpha = 1$ and defining $\Omega(t) = \langle\mathbf{d}\rangle\cdot\mathbf{E}_0(t)$ yields an interaction in which the electron's position (dipole moment) couples to a classical electric field of the form $\mathbf{E}_0(t)\sin\omega_{eg}t$;

$$V_l = \langle\mathbf{d}\rangle\cdot\mathbf{E}_0(t)(\sigma^+ + \sigma^-)\sin\omega_{eg}t. \tag{7.89}$$

The appropriate choice to accompany the symmetric representation is $\alpha = 1/2$.

Before continuing to derive the lineshape I wish to make a note on the rotating wave approximation, which I'll use in the following section. The RWA for the atom-laser interaction constitutes the prescription $u_l^+ = 0$, which of course holds as an identity in the symmetric representation. We have seen that if it is to be made in the atom-field interaction use of the RWA ($u^+ = 0$) may be questionable. However, for a single mode or a semi-classical interaction no sum over modes is present and the counter-rotating contributions promise to

be very small. When used together with the resonant driving assumption it is clear from 7.87 that the RWA gives an atom-laser interaction which does not depend on α.

7.4.2 Calculation of the lineshape

To derive the lineshape I assume an initial state $|g;0\rangle$. At $t=-\pi/\Omega$ a laser π-pulse irradiates the atom until $t=0$. If we assume $\Omega \gg \Gamma$ then we can ignore spontaneous emission over the duration of the pulse and set $g_{\mathbf{k}\lambda} \equiv 0$. For $t \geq 0$ the laser has ceased and we make the WW ansatz of exponential decay of the excited atomic state; $b_e = e^{-\Gamma t/2}$. With these assumptions in place I calculate the long time amplitude $b_{\mathbf{k}\lambda}(\infty)$ as in 7.2.1.

I will consider the rectangular envelope

$$\Omega(t) = \begin{cases} \Omega & \text{if } -\pi/\Omega < t < 0 \\ 0 & \text{otherwise,} \end{cases} \tag{7.90}$$

and begin with the assumption that the state at time t can be expanded as

$$|\psi(t)\rangle = b_g|g;0\rangle e^{-i\omega_g t} + b_e|e;0\rangle e^{-i\omega_e t} + \sum_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda}|g;\mathbf{k}\lambda\rangle e^{-i(\omega_g+\omega)t}. \tag{7.91}$$

Adding the general two-level atom-field interaction in 6.81 to the atom-laser interaction in 7.86 and using 7.91, the Schrödinger equation yields the set of coupled differential equations

$$\begin{aligned} \dot{b}_{g;\mathbf{k}\lambda} &= -ig^*_{\mathbf{k}\lambda} u^- e^{-i(\omega_{eg}-\omega)t} b_e, \\ \dot{b}_{g;0} &= -\frac{\Omega(t)}{2}(u_l^+ e^{-i\omega_l t} + u_l^- e^{i\omega_l t}) e^{-i\omega_{eg} t} b_e, \\ \dot{b}_{e;0} &= \frac{\Omega(t)}{2}(u_l^+ e^{i\omega_l t} + u_l^- e^{-i\omega_l t}) e^{i\omega_{eg} t} b_g - i\sum_{\mathbf{k}\lambda} g_{\mathbf{k}\lambda} u^- b_{g;\mathbf{k}\lambda} e^{i(\omega_{eg}-\omega)t}. \end{aligned} \tag{7.92}$$

Setting $g_{\mathbf{k}\lambda} = 0$ for $-\pi/\Omega < t < 0$ and implementing the RWA we obtain

$$\begin{aligned} \dot{b}_{g;0} &= -\frac{\Omega(t)}{2} u_l^- e^{-i(\omega_{eg}-\omega_l)t} b_e, \\ \dot{b}_{e;0} &= \frac{\Omega(t)}{2} u_l^- e^{i(\omega_{eg}-\omega_l)t} b_g. \end{aligned} \tag{7.93}$$

In conjunction wth the initial conditions $b_g(-\pi/\Omega) = 1$, $b_{e,0}(-\pi/\Omega) = 0$, 7.93 yields

$$b_e = -\frac{i\Omega u_l^-}{\mu} e^{i\delta(t-\pi/\Omega)/2} \sin\left[\frac{\mu}{2}\left(t+\frac{\pi}{\Omega}\right)\right], \tag{7.94}$$

where $-\pi/\Omega < t < 0$, and $\delta := \omega_{eg} - \omega_l$, and $\mu := \left[(\Omega u_l^-)^2 + \delta^2\right]^{1/2}$. Substituting this solution into 7.92, along with $b_e = e^{-\Gamma t/2}$ for $t \geq 0$, and then integrating with respect to t

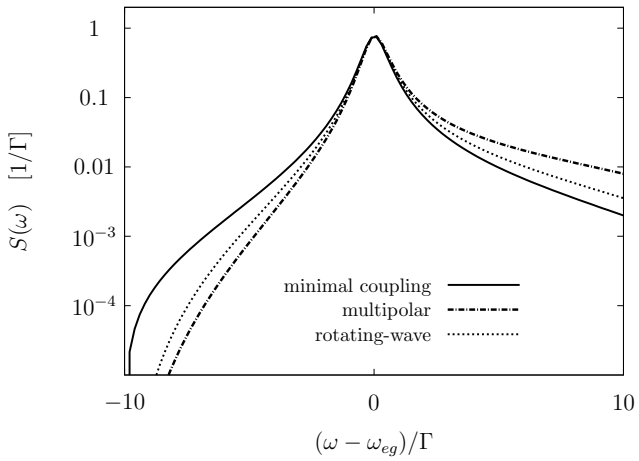
yields the result

$$b_{\mathbf{k}\lambda}(\infty) = \frac{-ig^*_{\mathbf{k}\lambda}u^-}{i\delta'+\Gamma/2} - \frac{2ig^*_{\mathbf{k}\lambda}u^-u_l^-\Omega e^{-i\pi\delta/2\Omega}}{(\Omega u_l^-)^2+4\delta'\delta_l}\left[e^{i\pi(2\delta'-\delta)/2\Omega} - \cos\left(\frac{\pi\mu}{2\Omega}\right) - \frac{i}{\mu}(2\delta'-\delta)\sin\left(\frac{\pi\mu}{2\Omega}\right)\right] \tag{7.95}$$

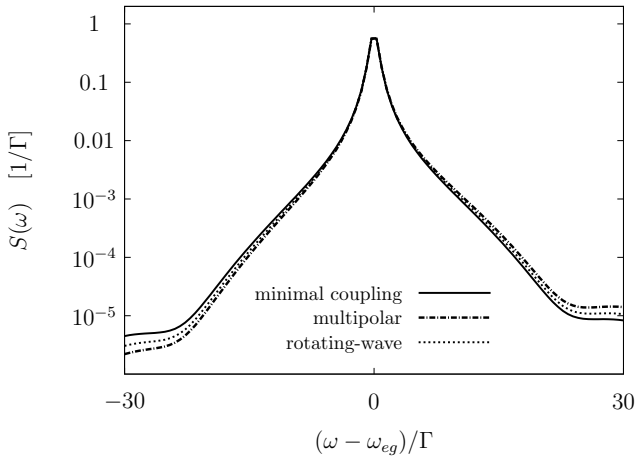
where $\delta' := \omega_{eg} - \omega$ and $\delta_l := \omega - \omega_l$. Unless the laser driving is resonant $b_{\mathbf{k}\lambda}(\infty)$ depends on the laser detuning, and therefore on the form of the atom-laser coupling through u_l^-. It happens that this dependence is actually extremely weak, so the only notable dependence on the laser comes through Ω. A great simplification is afforded by assuming a resonant pulse whereby 7.95 reduces to

$$b_{\mathbf{k}\lambda}(\infty) = -ig^*_{\mathbf{k}\lambda}u^-\left[\frac{1}{i\delta'+\Gamma/2} + \frac{2}{\Omega^2-4\delta'^2}\left(\Omega e^{i\pi\delta'/\Omega} - 2i\delta'\right)\right]. \tag{7.96}$$

The lineshape is defined in 7.37. Near resonance the Lorentzian component dominates, but in the wings the lineshape is sensitive to Ω. It is dependent on the representation chosen through the function u^-. Various lineshapes including the laser contribution are plotted in Figs. 7.2(a)-7.3(b). For an optical transition $\omega_{eg} \sim 10^{-15}\mathrm{s}^{-1}$ with decay rate $\Gamma \sim 10^8\mathrm{s}^{-1}$ the differences in lineshapes associated with different representations are extremely small, significant differences only occurring for much larger decay rates relative to ω_{eg}. It is worth noting that even for these parameters, the difference between lineshapes with and without taking into account the laser should be detectable with modern spectroscopy.

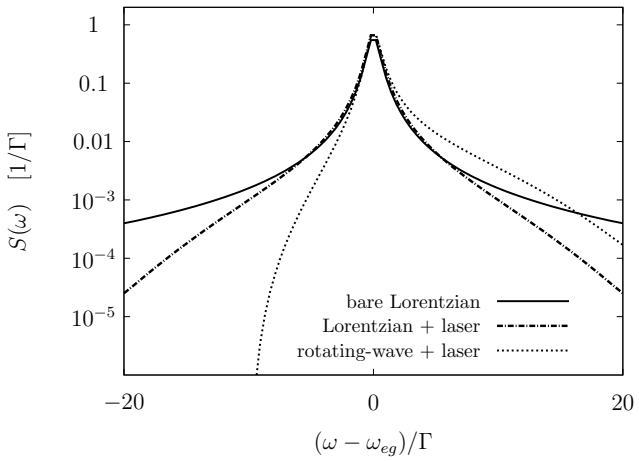


(a)

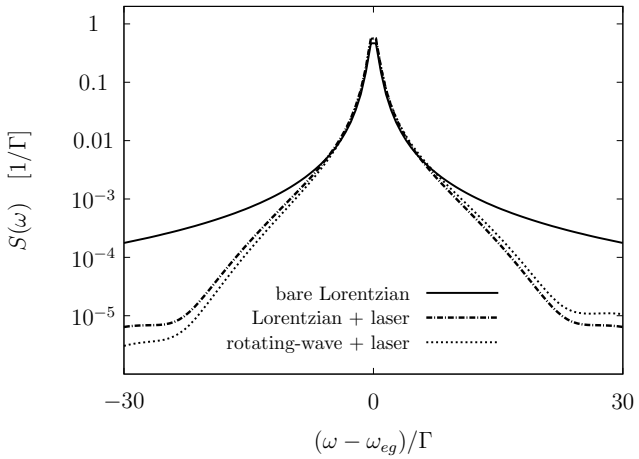


(b)

Figure 7.2: $\Omega = \omega_{eg}$ and $\delta = 0$. The lineshapes associated with the minimal coupling, multipolar and rotating-wave Hamiltonians are plotted. Each lineshape includes the laser contribution. In 7.2(a) $\Gamma = \omega_{eg}/10$ and in 7.2(b) $\Gamma = \omega_{eg}/100$.



(a)



(b)

Figure 7.3: The lineshape in the symmetric representation including the laser contribution is compared to the bare Lorentzian curve $(\Gamma/2\pi)/(\delta'^2 + \Gamma^2/4)$, and to the Lorentzian including the laser contribution. In 7.3(a) $\Gamma = \omega_{eg}/10$ and in 7.3(b) $\Gamma = \omega_{eg}/100$.

7.5 Summary and discussion

The purpose of this chapter has been to investigate excited atomic states and their decay. In particular, I have considered the spectral lineshape of radiation emitted by an excited atom. As expected the lineshape result depends on the choice of gauge due to the use of gauge dependent bare states and canonical operators. This sharpens the question as to whether or not physically meaningful time-dependent probabilities can actually be obtained in QED. It has been demonstrated yet again (see for example Cohen-Tannoudji *et al.* (1997)) that all intermediate states must be retained to maintain gauge invariance of S-matrix elements. Since all orders in perturbation theory are also required to yield the characteristic exponential de-

cay and accompanying lineshape denominators, the calculation of an exact gauge-invariant lineshape formula seems out of reach. This in turn shows how limiting a restriction the use of the exact S-matrix can be.

On the other hand if we take bare states and canonical operators as physically meaningful the question becomes what gauge do we choose to model spontaneous emission? There are various criteria we might require to be fulfilled in order to determine this, which was largely the subject of chapter 6. The Poincaré gauge incurs a causally propagating field canonical momentum, as well as a definition of the atomic energy in terms of the electronic velocity operator. These observables, at least according to classical intuition, would appear to represent the physical degrees of freedom, that are directly involved in the emission of radiative energy. On the other hand the symmetric representation incurs the elimination of virtual contributions, which in the quantum optics paradigm are interpreted as renormalising bare parameters to give the physical parameters describing *real* interactions. Finally the Coulomb gauge offers a definitive separation of longitudinal and transverse field degrees of freedom, with the longitudinal field energy and momentum included entirely within the material subsystem. This again does not seem unreasonable when we recall that, according to the classical theory, the longitudinal field energy merely renormalises the bare electronic mass. In any case a precise experiment would be required to distinguish between the lineshapes associated with the different light-matter coupling models discussed.

On top of the situations studied in this chapter one can also imagine hybrid approaches in which the bare states of one gauge are combined with the canonical observables of another (see Power & Thirunamachandran (1999b)). In fact one could take this idea further and argue on physical grounds that since the causally propagating *total* electric field is responsible for the transport of radiative energy, the *observables* that we are really interested in are those represented by the canonical field operators in the Poincaré gauge. At the same time, when it comes to identifying the correct *states*, one could argue that the initial vacuum state of the field should be defined in terms of the *transverse* electric field as it is in the Coulomb gauge, because the total longitudinal field energy just renormalises the electronic mass. Furthermore, there appears to be no good reason to suddenly abandon the idea that the atomic energy be defined in terms of the electronic velocity, as is the case in the classical setting. Thus, the initial atomic state should be taken as an excited eigenstate of the Poincaré gauge bare atomic Hamiltonian. It is clear however, that the transverse electric field energy and the Poincaré gauge atomic Hamiltonian do not commute, so the specification of an initial state, which is simultaneously an eigenstate of both operators becomes much more involved. Here again, we appear to be confronted with limitations built into subsystem decompositions based on tensor product structure.

CHAPTER 8

Radiation as a reservoir

This chapter is dedicated to a treatment of the atom-field system from an open quantum systems perspective. I derive a master equation governing the evolution of the reduced density matrix associated with the atomic system for which the field is viewed as a reservoir. The aim is to try and avoid approximations such as the RWA and MA wherever possible. The results presented in this chapter are summarised in the paper Stokes *et al.* (2012).

The main new result obtained is the general master equation 8.29. The method of derivation of this master equation is also original. It works by combining the quantum jump approach (cf. Hegerfeldt & Wilser (1992), Gardiner *et al.* (1992), Mølmer *et al.* (1993), Carmichael (1993)) with the ideas of Zurek (2003) on einselection. This method, which is presented in sections 8.1 and 8.2, was developed by myself and the coauthors A. Kurcz, A. Beige and T. P. Spiller of the paper Stokes *et al.* (2012). All authors of this paper also contributed to the interpretation of the master equation constants presented in 8.3.

The reduced atomic density matrix is by definition obtained by tracing over the field canonical Fock space $\mathcal{F}_B\left(L^2(\mathbb{R}^3,\mathbb{C}^2)\right)$, which is a tensor factor within the total atom-field Hilbert space $\mathcal{H}_A\otimes\mathcal{F}_B\left(L^2(\mathbb{R}^3,\mathbb{C}^2)\right)$. For simplicity I will be assuming a two-level model for the atom, and so identify $\mathcal{H}_A$ as simply $\mathbb{C}^2$. Since atom-field tensor product decompositions are physically non-unique and gauge-dependent, one should expect the resulting reduced atomic dynamics to exhibit the same traits. It turns out that indeed they do, but only when the RWA and MA are avoided. This again should not be too surprising, because these approximations tend to transform calculations in such a way that they become quite similar to calculations of S-matrix elements (see 6.3.2 and 6.3.4).

Many derivations of quantum optical master equations can be found in the literature (Agarwal (1974), Cohen-Tannoudji *et al.* (1992), Mandel & Wolf (1995), Gardiner & Zoller (2004), Breuer & Petruccione (2007), Walls & Milburn (2008)). One expects that with regard to spontaneous emission, the field should not retain any memory of the atomic dynam-

ics. The atomic master equation should therefore be Markovian in nature. The standard Born-Markov master equation for a two-level atom, which is found using both the RWA and MA is of this type, and it has been successfully applied to the study of a range of phenomena.

However, virtual emission events described by counter-rotating terms, are not irreversible, and are non-Markovian in nature. The approach in this chapter posits that irrespective of any distinction between real and virtual photons the physical mechanism of environment-induced decoherence is responsible for the Markovian nature of the quantum optical master equation. The model to be used yields a Markovian quantum optical master equation without requiring the use of the RWA and the MA.

8.1 The photon-absorbing environment

Following the ideas of Hegerfeldt & Wilser (1992) (see also Gardiner *et al.* (1992), Mølmer *et al.* (1993), Carmichael (1993) and Hegerfeldt (2009)), the approach I adopt takes the coupling of the field to an additional external environment, like a detector or the walls of the lab explicitly into account. This external environment thermalises very rapidly and is generally in an equilibrium state $\rho_{\rm ss}^{\rm env}$. Following the ideas of Zurek (2003) on decoherence and einselection and applying them to the field and its external environment, I assume that the environment resets the field on a coarse-grained time-scale Δt onto its vacuum state $|0\rangle$.

We begin by assuming the atom-field-environment density matrix can be written

$$\rho_A \otimes |0\rangle\langle 0| \otimes \rho_{ss}^{\rm env} \tag{8.1}$$

where $\rho_{ss}^{\rm env}$ denotes a stationary state of the environment consisting of a large number of degrees of freedom. It's assumed that any coherences between the field and its environment are rapidly destroyed by decoherence (Zurek (2003)). This is the justification for the factorisation of the field-*environment* density matrix in 8.1. The other factorisation appearing in 8.1, that of the *atom*-field density matrix, will be justified shortly.

The environment is assumed not to interact with the atom directly, but only with the field. Starting with 8.1 the interaction between the atom and the field will create a small photon population in the field modes $\{\mathbf{k}\lambda\}$;

$$\rho_A \otimes |0\rangle\langle 0| \otimes \rho_{ss}^{\rm env} \longrightarrow \sum_n \sum_{\mathbf{k}\lambda} c_{n;\mathbf{k}\lambda} |n\rangle\langle n| \otimes |\mathbf{k}\lambda\rangle\langle \mathbf{k}\lambda| \otimes \rho_{\rm ss}^{\rm env}. \tag{8.2}$$

where the $|n\rangle = |g\rangle, |e\rangle$ form an orthogonal basis in $\mathcal{H}_A$. The photon $\mathbf{k}\lambda$ is free to interact with the environment, which is assumed to have the effect

$$|\mathbf{k}\lambda\rangle\langle \mathbf{k}\lambda| \otimes \rho_{\rm ss}^{\rm env} \longrightarrow |0\rangle\langle 0| \otimes \rho_{\mathbf{k}\lambda}^{\rm env}. \tag{8.3}$$

In words, any initial excitation in the field vanishes very quickly as a result of the inter-

action between the field and the environment. Note that this does not *a priori* preclude the possibility of virtual photons being intercepted and absorbed by the environment. The time-scale over which the field-environment interaction occurs is assumed to be sufficiently small so that population of the field by more than one photon is negligible. This justifies the inclusion of one-photon states only in 8.2. Finally, the environment itself is assumed to thermalise extremely quickly;

$$\rho_{\mathbf{k}\lambda}^{\text{env}} \to \rho_{ss}^{\text{env}}. \tag{8.4}$$

The time over which the entire interaction occurs is denoted Δt, and is called the *environmental response time*. The complete atom-field-environment evolution over Δt can be summarised as

$$\rho_A \otimes |0\rangle\langle 0| \otimes \rho_{ss}^{\text{env}} \xrightarrow{\Delta t} \rho_A' \otimes |0\rangle\langle 0| \otimes \rho_{ss}^{\text{env}}. \tag{8.5}$$

In the language of Zurek (2003) the vacuum state $|0\rangle$ is an environmentally-selected, or *einselected* state of the field. Einselected states are states which remain stable in spite of the environment. In the absence of an atomic emitter but in the presence of a photon-absorbing environment, the vacuum state $|0\rangle$ is the only state of the field which does not evolve in time. The environmental interaction giving rise to 8.5 acts as a monitor, which continuously measures the field (Hegerfeldt & Wilser (1992), Gardiner *et al.* (1992), Mølmer *et al.* (1993), Carmichael (1993)). Regardless of whether or not a photon is found in such a hypothetical measurement, decoherence destroys any coherences between the field and the environment, and transfers the field into the einselected state $|0\rangle$ (Zurek (2003)).

8.2 Non-equivalent master equations

Assuming a two-level model for the atom I define the free Hamiltonian H_0 by

$$H_0 := \omega_{eg}\sigma_z + \sum_{\mathbf{k}\lambda} \omega a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} \tag{8.6}$$

and take the general interaction V given in 6.81. In the interaction picture with respect to H_0 the interaction Hamiltonian $\tilde{V}$ is given by

$$\tilde{V} = \sum_{\mathbf{k}\lambda} g_{\mathbf{k}\lambda}\,\sigma^+ \mathrm{e}^{i\omega_{eg}t}\left(u_k^+ a_{\mathbf{k}\lambda}^\dagger \mathrm{e}^{i\omega t} + u_k^- a_{\mathbf{k}\lambda}\,\mathrm{e}^{-i\omega t}\right) + \text{H.c.}, \tag{8.7}$$

while the atomic density matrix becomes

$$\tilde{\rho}_A(t) = U_0^{-1}(t,0)\rho_A(t)U_0(t,0). \tag{8.8}$$

Defining the superoperator $\mathcal{L}$ by

$$\dot{\rho}_A(t) = \mathcal{L}\left[\rho_A(t)\right] \tag{8.9}$$

and taking the time derivative of $\tilde{\rho}_A$ in 8.8, one obtains

$$\dot{\tilde{\rho}}_A(t) = i\omega_{eg}[\sigma_z, \tilde{\rho}_A] + U_0^{-1}(t,0)\mathcal{L}\left[U_0(t,0)\tilde{\rho}_A U_0^{-1}(t,0)\right] U_0(t,0). \tag{8.10}$$

I seek a description of the evolution $\rho_A \to \rho_A'$ given in 8.5, in the form of an atomic master equation akin to 8.9, or 8.10. To this end the model in 8.1 permits us to write the interaction picture density matrix at time t as

$$\tilde{\rho}(t) = \tilde{\rho}_A(t) \otimes |0\rangle\langle 0|. \tag{8.11}$$

This factorisation of the density matrix is often referred to as the *Born approximation* and is usually justified on the grounds of weak coupling (see for example Breuer & Petruccione (2007)). The emergence of this condition as the result of environmental interaction justifies the derivation of a master equation without employing the RWA and MA, while still employing 8.11. Any such master equation is automatically Markovian, but contains terms that depend on an additional parameter – the environmental response time Δt. The only approximations I will use are second order perturbation theory and the resetting of the field over the coarse-grained time-scale into its vacuum state. The first is well justified as long as the environmental response time Δt is short compared to the characteristic time-scale of the effective atomic evolution (weak-coupling). The second is justified by the decoherence model laid out in 8.1.

Over a time interval Δt, $\tilde{\rho}(t)$ in 8.11 evolves into

$$\tilde{\rho}(t+\Delta t) = \tilde{U}(t+\Delta t, t)\left[\tilde{\rho}_A(t) \otimes |0\rangle\langle 0|\right]\tilde{U}^{-1}(t+\Delta t, t). \tag{8.12}$$

This atom-field density matrix corresponds in general to an entangled state with population in most modes $(\mathbf{k}, \lambda)$ of the field. Using 8.3 and 8.4, we see that the atom-field-environment density matrix $\tilde{\rho}(t+\Delta t) \otimes \rho_{\text{ss}}^{\text{env}}$ corresponding to 8.12, transforms in the present model as

$$\tilde{\rho}(t+\Delta t) \otimes \rho_{\text{ss}}^{\text{env}} \longrightarrow \text{tr}_F\left[\tilde{U}(t+\Delta t, t)\tilde{\rho}_A(t) \otimes |0\rangle\langle 0|\tilde{U}^{-1}(t+\Delta t, t)\right] \otimes |0\rangle\langle 0| \otimes \rho_{\text{ss}}^{\text{env}}, \tag{8.13}$$

where tr_F denotes the partial trace over the field. This equation shows that the atom-field density matrix remains uncorrelated on the coarse-grained time-scale given by Δt.

The trace over the field in 8.13 ensures that the density matrix on the right hand side is always normalised. It also implies that the interaction between the field and the environment occurs on a very short time-scale avoiding nonlocal effects on the atom. Since I'm only interested in the time evolution of the atomic density matrix $\tilde{\rho}_A(t)$, evaluating the trace over

the field in 8.13 shows that $\tilde{\rho}_A(t)$ can be written

$$\tilde{\rho}_A(t+\Delta t) = \tilde{\rho}_A^0(t+\Delta t) + \tilde{\rho}_A^>(t+\Delta t), \tag{8.14}$$

where

$$\tilde{\rho}_A^0(t+\Delta t) := \langle 0|\tilde{U}(t+\Delta t,t)|0\rangle \tilde{\rho}_A(t) \langle 0|\tilde{U}^{-1}(t+\Delta t,t)|0\rangle, \tag{8.15a}$$

$$\tilde{\rho}_A^>(t+\Delta t) := \sum_{n=1}^{\infty} \sum_{\mathbf{k}\lambda} \langle n_{\mathbf{k}\lambda}|\tilde{U}(t+\Delta t,t)|0\rangle \tilde{\rho}_A(t) \langle 0|\tilde{U}^{-1}(t+\Delta t,t)|n_{\mathbf{k}\lambda}\rangle. \tag{8.15b}$$

The density matrix ρ_A^0 describes the subensemble of atoms for which a photon *wasn't* detected in the environmental "measurement" that occurred within $(t, t+\Delta t)$, whereas $\rho_A^>$ describes the subensemble for which a photon *was* detected.

The interaction picture difference quotient $\tilde{\mathcal{L}}$ is defined as

$$\tilde{\mathcal{L}}\left[\tilde{\rho}_A(t)\right] := \frac{\tilde{\rho}_A(t+\Delta t) - \tilde{\rho}_A(t)}{\Delta t}. \tag{8.16}$$

In the limit $\Delta t \to 0$ the right hand becomes the derivative of ρ_A at t, but because the superoperator $\tilde{\mathcal{L}}$ is obtained via a partial trace, by applying the limit $\Delta t \to 0$ one encounters the *quantum Zeno effect* in which the dynamics of the atom-field system become completely restricted to the zero photon subspace (Hegerfeldt & Wilser (1992)). We must therefore avoid this limit and only assume that the time increment Δt is sufficiently small compared to the time-scale over which the atomic system evolves that an effectively continuous evolution equation results. Equation 8.16 then constitutes a Markovian approximation of the true (non-Markovian) continuous dynamics.

The next step in our derivation is the explicit calculation of $\tilde{\mathcal{L}}$, which is independent of t as long as no time-dependent interactions, like laser fields, are applied. In contrast one can easily check that $\tilde{\mathcal{L}}$ depends explicitly on Δt. In the following Δt will be treated as an external parameter, which can be absorbed into the coefficients of the master equation.

8.2.1 The subensemble without photon detection

Assuming Δt is small compared to the time-scale on which the atomic density matrix $\tilde{\rho}_A(t)$ evolves we can calculate $\tilde{\rho}_A^0(t+\Delta t)$ in 8.15 using second order perturbation theory. Up to second order one has

$$\langle 0|\tilde{U}(t+\Delta t,t)|0\rangle = 1 - \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \, \langle 0|\tilde{V}(t')\tilde{V}(t'')|0\rangle. \tag{8.17}$$

Using 8.7 and introducing the time-independent constants

$$A'_{\pm} := \frac{1}{\Delta t} \int_0^{\Delta t} dt' \int_0^{t'} dt'' \sum_{\mathbf{k}\lambda} |g_{\mathbf{k}\lambda}|^2 u_k^{\pm 2} \mathrm{e}^{\mp i(\omega_{eg} \pm \omega)(t'-t'')}, \tag{8.18}$$

8.17 simplifies to

$$\langle 0|\tilde{U}(t+\Delta t,t)|0\rangle = 1 - \left(A'_{-}\sigma^{+}\sigma^{-} + A'_{+}\sigma^{-}\sigma^{+}\right)\Delta t. \tag{8.19}$$

The constants $A'_{\pm}$ in 8.18 are complex numbers and their real and imaginary parts have different physical significance. It is convenient to consider them separately by defining

$$A_{\pm} := 2\mathrm{Re}(A'_{\pm}), \tag{8.20a}$$

$$\Delta\omega_{g,e} := \mathrm{Im}(A'_{\pm}) \tag{8.20b}$$

such that $A'_{\pm} = \frac{1}{2}A_{\pm} + i\Delta\omega_{g,e}$. The $A_{\pm}$ in 8.20a are *emission rates* related to the $P^{\pm}_{\mathrm{ph}}$ in 6.72 by

$$A_{\pm} = \frac{P^{\pm}_{\mathrm{ph}}(\Delta t)}{\Delta t} = \sum_{\mathbf{k}\lambda} |g_{\mathbf{k}\lambda}|^2 u^{\pm 2}_{k} \frac{\sin^2\left([\omega_{eg} \pm \omega]\Delta t/2\right)}{(\omega_{eg} \pm \omega)^2 \Delta t}. \tag{8.21}$$

The $\Delta\omega_{g,e}$ are radiative shifts of the bare atomic energies $\omega_{g,e}$. Substituting 8.17 into 8.15 and using 8.19, one finds that

$$\begin{aligned}\tilde{\rho}^{0}_{A}(t+\Delta t) = \tilde{\rho}_{A}(t) &+ i\sum_{n=g,e}\Delta\omega_{n}[\tilde{\rho}_{A}(t), |n\rangle\langle n|]\Delta t \\ &- \frac{1}{2}\left[\left(A_{-}\sigma^{+}\sigma^{-} + A_{+}\sigma^{-}\sigma^{+}\right)\tilde{\rho}_{A}(t) - \tilde{\rho}_{A}(t)\left(A_{-}\sigma^{+}\sigma^{-} + A_{+}\sigma^{-}\sigma^{+}\right)\right]\Delta t\end{aligned} \tag{8.22}$$

up to first order in Δt.

8.2.2 The subensemble with photon detection

Evaluating $\tilde{U}(t+\Delta t,t)$ again using second order perturbation theory, the density matrix $\tilde{\rho}^{>}_{A}(t+\Delta t)$ in 8.15 for the subensemble with photon detection during $(t+\Delta t,t)$ can be found;

$$\tilde{\rho}^{>}_{A}(t+\Delta t) = \sum_{\mathbf{k}\lambda}\int_{t}^{t+\Delta t} dt' \int_{t}^{t+\Delta t} dt'' \,\langle 1_{\mathbf{k}\lambda}|\tilde{V}(t')|0\rangle\tilde{\rho}_{A}(t)\langle 0|\tilde{V}(t'')|1_{\mathbf{k}\lambda}\rangle. \tag{8.23}$$

Substituting 8.7 into this equation, $\tilde{\rho}^{>}_{A}(t+\Delta t)$ simplifies to

$$\tilde{\rho}^{>}_{A}(t+\Delta t) = \tilde{\mathcal{R}}[\tilde{\rho}_{A}(t)]\Delta t, \tag{8.24}$$

where the *reset superoperator* $\tilde{\mathcal{R}}$ is defined by

$$\tilde{\mathcal{R}}[\tilde{\rho}_{A}] := A_{+}\sigma^{+}\tilde{\rho}_{A}\sigma^{-} + A_{-}\sigma^{-}\tilde{\rho}_{A}\sigma^{+} + B_{+}\sigma^{+}\tilde{\rho}_{A}\sigma^{+} + B_{-}\sigma^{-}\tilde{\rho}_{A}\sigma^{-} \tag{8.25}$$

with

$$B_+ := \frac{1}{\Delta t}\int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' \sum_{\mathbf{k}\lambda} g_{\mathbf{k}\lambda}^2 u_k^+ u_k^- \mathrm{e}^{i\omega_{eg}(t'+t'')}\mathrm{e}^{i\omega(t'-t'')}, \tag{8.26a}$$

$$B_- := \frac{1}{\Delta t}\int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' \sum_{\mathbf{k}\lambda} (g_{\mathbf{k}\lambda}^*)^2 u_k^+ u_k^- \mathrm{e}^{-i\omega_{eg}(t'+t'')}\mathrm{e}^{i\omega(t'-t'')}. \tag{8.26b}$$

Substituting 8.22, 8.24, and 8.25 into 8.16, one obtains the superoperator $\tilde{\mathcal{L}}$ in 8.16;

$$\begin{aligned}\tilde{\mathcal{L}}[\tilde{\rho}_A] =& i\sum_{n=1}^{2}\Delta\omega_i[\tilde{\rho}_A, |n\rangle\langle n|] + \frac{1}{2}A_+\left(2\sigma^+\tilde{\rho}_A\sigma^- - \sigma^-\sigma^+\tilde{\rho}_A - \tilde{\rho}_A\sigma^-\sigma^+\right)\\ &+\frac{1}{2}A_-\left(2\sigma^-\tilde{\rho}_A\sigma^+ - \sigma^+\sigma^-\tilde{\rho}_A - \tilde{\rho}_A\sigma^+\sigma^-\right) + B_+\sigma^+\tilde{\rho}_A\sigma^+ + B_-\sigma^-\tilde{\rho}_A\sigma^-.\end{aligned} \tag{8.27}$$

8.2.3 The general Lindblad master equation

To determine the superoperator $\mathcal{L}$ in the Schrödinger picture I use 8.10, which implies

$$\mathcal{L}[\rho_A] = -i\omega_{eg}[\sigma_z, \rho_A] + U_0(t,0)\tilde{\mathcal{L}}\left[U_0^{-1}(t,0)\rho_A U_0(t,0)\right]U_0^{-1}(t,0). \tag{8.28}$$

Combining this equation with 8.27 and redefining the atomic transition frequency ω_{eg} such that the first term in 8.27 is absorbed into the free energy of the atom, we obtain the general master equation

$$\begin{aligned}\dot{\rho}_A =& -i\tilde{\omega}_{eg}[\sigma_z, \rho_A] + \frac{1}{2}A_+\left(2\sigma^+\rho_A\sigma^- - \sigma^-\sigma^+\rho_A - \rho_A\sigma^-\sigma^+\right)\\ &+\frac{1}{2}A_-\left(2\sigma^-\rho_A\sigma^+ - \sigma^+\sigma^-\rho_A - \rho_A\sigma^+\sigma^-\right) + B\sigma^+\rho_A\sigma^+ + B^*\sigma^-\rho_A\sigma^-,\end{aligned} \tag{8.29}$$

where $\tilde{\omega}_{eg}$ is the shifted atomic frequency and where B is defined as

$$B := \sum_{\mathbf{k}\lambda} g_{\mathbf{k}\lambda}^2 u_k^+ u_k^- \mathrm{e}^{-i\omega_{eg}\Delta t}\frac{\sin\left([\omega_{eg}+\omega]\Delta t/2\right)\sin\left([\omega_{eg}-\omega]\Delta t/2\right)}{(\omega_{eg}+\omega)(\omega_{eg}-\omega)}. \tag{8.30}$$

The general master equation 8.29 reduces to the standard Born-Markov master equation within the RWA and MA, in which one has $A_+ = B = 0$ and $A_- = \Gamma$ (cf. 8.21 and 6.75). In the symmetric representation $A_+ = B = 0$, and as we will see in 8.3.1 $A_- \approx \Gamma$. Thus, the symmetric representation yields the standard result without any need for the RWA and MA. One might wonder whether it is the case that $A_+ \approx 0$, $B \approx 0$ and $A_- \approx \Gamma$ regardless of the chosen atom-field coupling. This would imply that the RWA and MA are universally justified in the present context, and would make our endeavors somewhat pointless. We will see in 8.3.1 however, that this is certainly not the case.

One can show that for a wide range of experimental parameters the master equations associated with the Coulomb gauge, the Poincaré gauge and the symmetric representation

can be written in Lindblad (1976) form

$$\dot{\rho}_A = -i\tilde{\omega}_0[\sigma_z, \rho_A] + \sum_{n=1}^{2} \lambda_n \left[L_n \rho_A L_n^\dagger - \frac{1}{2}\{L_n^\dagger L_n, \rho_A\} \right], \tag{8.31}$$

where $\{,\}$ denotes the anti-commutator, and where $\forall n\ \mathrm{tr}(L_n) = 0$ and $\lambda_n \geq 0$. The Lindblad form is the most general form that a Markovian (non-unitary) dynamical equation for ρ_A can take, which is completely positive and trace-preserving. These properties are essential in order that the density matrices the master equation yields are valid physically.

To obtain the Lindblad form, notice first that 8.29 is an equation in *first standard form*

$$\dot{\rho}_A = -i\tilde{\omega}_0[\sigma_z, \rho_A] + \sum_{n,m=1}^{2} M_{nm} \left[\tilde{\sigma}_n \rho_A \tilde{\sigma}_m^\dagger - \frac{1}{2}\{\tilde{\sigma}_m^\dagger \tilde{\sigma}_n, \rho_A\} \right], \tag{8.32}$$

where the M_{nm} are matrix elements of an Hermitian operator M. A transformation of this equation into Lindblad form can be achieved via diagonalisation of M using the spectral representation

$$M = \sum_{n=1}^{2} \lambda_n |\lambda_n\rangle\langle\lambda_n|, \tag{8.33}$$

where the λ_n and $|\lambda_n\rangle$ are the eigenvalues and eigenvectors of M. One can now easily check that M is diagonalised by the unitary matrix

$$U := \sum_{n=1}^{2} |e_n\rangle\langle\lambda_n|, \qquad U^{-1}MU = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}. \tag{8.34}$$

where $|e_1\rangle = (1,0)^{\mathrm{T}}$ and $|e_2\rangle = (0,1)^{\mathrm{T}}$ are canonical vectors. Finally, defining operators L_n by

$$\begin{pmatrix} \tilde{\sigma}_1 \\ \tilde{\sigma}_2 \end{pmatrix} = U^{-1} \begin{pmatrix} L_1 \\ L_2 \end{pmatrix} \tag{8.35}$$

and substituting them into 8.32 gives a diagonal master equation in Lindblad form 8.31, provided the L_n are traceless and the λ_n are non-negative. Now, if we identify the operators $\tilde{\sigma}_{1,2}$ in 8.35 as the $\sigma^{\pm}$ in 8.29, and we identify the matrix M as

$$M = \begin{pmatrix} A_+ & B \\ B^* & A_- \end{pmatrix} \tag{8.36}$$

we obtain a master equation of the form 8.31 in which the L_n are given by 8.35 and the λ_n are the eigenvalues of M. The obtained Lindblad operators L_n are certainly traceless, so the resultant master equation is of Lindblad form provided the λ_n are positive semi-definite.

This applies when $\det(M) \geq 0$, or equivalently when

$$A_+ A_- \geq |B|^2, \tag{8.37}$$

which can only be verified through explicit calculation of the master equation constants.

8.3 Analysis of the master equation constants

As expected the master equation 8.29 is dependent on the form of atom-field coupling chosen. I analyse in this section, the master equation constants in the Coulomb and Poincaré gauges, and the symmetric representation.

8.3.1 Analysis of the rates

To determine the rates $A_\pm$ as functions of Δt and ω_u, it is convenient to write them in the form

$$A_\pm = \frac{2\Gamma}{\pi \omega_{eg}^2 \Delta t} \int_0^{\omega_u} d\omega f_\pm(\omega) \sin^2\left[\frac{1}{2}(\omega_{eg} \pm \omega)\Delta t\right] \tag{8.38}$$

with the $f_\pm(\omega)$ defined by

$$f_\pm(\omega) := \frac{\left(u_k^\pm \omega\right)^2}{(\omega_{eg} \pm \omega)^2}. \tag{8.39}$$

In the limit $\Delta t \to \infty$, one obtains $A_+ = 0$ and $A_- = \Gamma$ as expected (cf. 5.1.3).

Table 8.1 summarises the $u_k^\pm$ and $f_\pm(\omega)$ for the Coulomb gauge, Poincaré gauge and symmetric representation cases. In case of the rotating-wave and the minimal coupling Hamiltonian, $f_-(\omega)$ tends to zero when ω tends to infinity. Thus, when performing the integration in 8.38, we are likely to obtain a rate A_- which depends only weakly on the cut-off frequency ω_u. This is confirmed in figure 8.3, which shows that in both cases A_- is essentially the same as the spontaneous decay rate Γ for a wide range of environmental response times and cut-off frequencies. The same is not true in the Poincaré gauge, within which $f_-(\omega)$ grows rapidly as ω increases. As a result A_- diverges badly with ω_u as is illustrated in 8.3.

The other rate appearing in the master equation has been labelled A_+. This is the rate associated with virtual photon emission from the bare ground state. As such $A_+ \equiv 0$ in the symmetric representation. In the Coulomb gauge and the Poincaré gauges A_+ is relatively straightforward to calculate, because $f_+(\omega)$ has no singularity for finite values of ω. It is clear that in the Coulomb gauge A_+ diverges logarithmically, while in the Poincaré gauge it diverges quadratically. Explicit results are obtained by replacing the $\sin^2$ function in 8.38 by its average value $1/2$. This approximation is certainly well justified when $\Delta t \gg 1/\omega_{eg}$,

and gives

$$A_+ = \frac{\Gamma}{\pi\omega_{eg}\Delta t}\left[\frac{1}{x}+\ln x\right]_1^{\omega_u/\omega_{eg}+1} \tag{8.40}$$

in the Coulomb gauge, and

$$A_+ = \frac{\Gamma}{\pi\omega_{eg}\Delta t}\left[\frac{1}{x}-3x+\frac{1}{2}x^2+3\ln x\right]_1^{\omega_u/\omega_{eg}+1} \tag{8.41}$$

in the Poincaré gauge. Both rates depend strongly on the environmental response time Δt as well as the cut-off frequency ω_u. This is illustrated in figure 8.4 which shows A_+ as a function of ω_u for fixed Δt. The rates $A_\pm$ diverge badly in the Poincaré gauge, which entails a cubic coupling ω^3 in the numerators of the functions in table 8.1. These results show that for sufficiently large cut-offs the Poincaré gauge coupling can no longer be classed as weak, consequently the entire treatment will break down.

H	u_k^-	u_k^+	$f_-(\omega)$	$f_+(\omega)$
H_s	$\frac{2\sqrt{\omega_{eg}\omega}}{\omega_{eg}+\omega}$	0	$\frac{4\omega_{eg}\omega^3}{(\omega_{eg}^2-\omega^2)^2}$	0
H_C	$\sqrt{\frac{\omega_{eg}}{\omega}}$	$\sqrt{\frac{\omega_{eg}}{\omega}}$	$\frac{\omega_{eg}\omega}{(\omega_{eg}-\omega)^2}$	$\frac{\omega_{eg}\omega}{(\omega_{eg}+\omega)^2}$
H_P	$\sqrt{\frac{\omega}{\omega_{eg}}}$	$-\sqrt{\frac{\omega}{\omega_{eg}}}$	$\frac{\omega^3}{\omega_{eg}(\omega_{eg}-\omega)^2}$	$\frac{\omega^3}{\omega_{eg}(\omega_{eg}+\omega)^2}$

Table 8.1: The coefficients $u_k^\pm$ in 6.82 and the coefficients $f_\pm(\omega)$ in 8.39, in the Coulomb gauge, the Poincaré gauge and the symmetric representation.

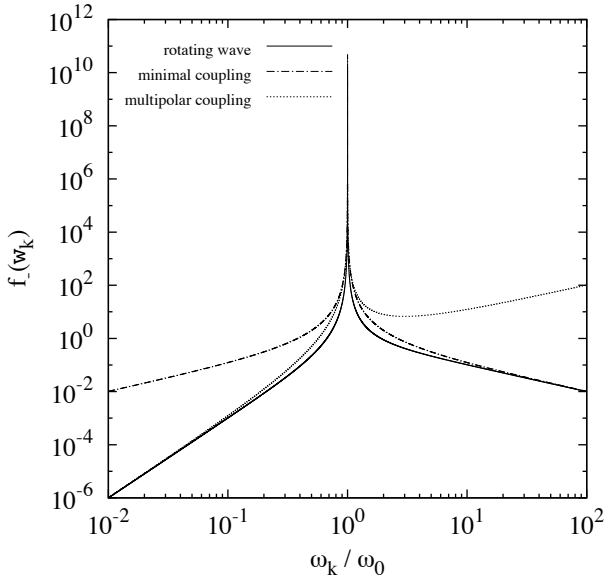


Figure 8.1: Logarithmic plot of the function $f_{-}(\omega)$ in 8.39, in the Coulomb gauge, the Poincaré gauge and the symmetric representation.

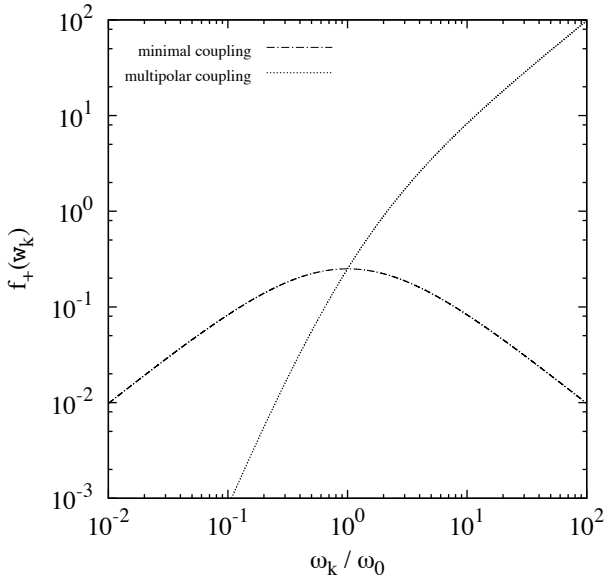


Figure 8.2: Logarithmic plot of the function $f_{+}(\omega)$ in 8.39, in the Coulomb and Poincaré gauges. (In the symmetric representation $f_{+} \equiv 0$.)

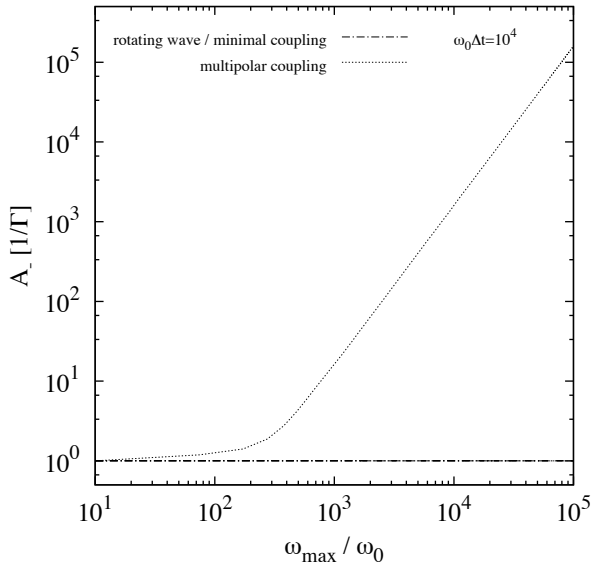


Figure 8.3: Logarithmic plot of the rate A_- in 8.38, in the Coulomb gauge, the Poincaré gauge and the symmetric representation as functions of the upper cut-off frequency ω_u, with $\omega_{eg}\Delta t = 10^4$.

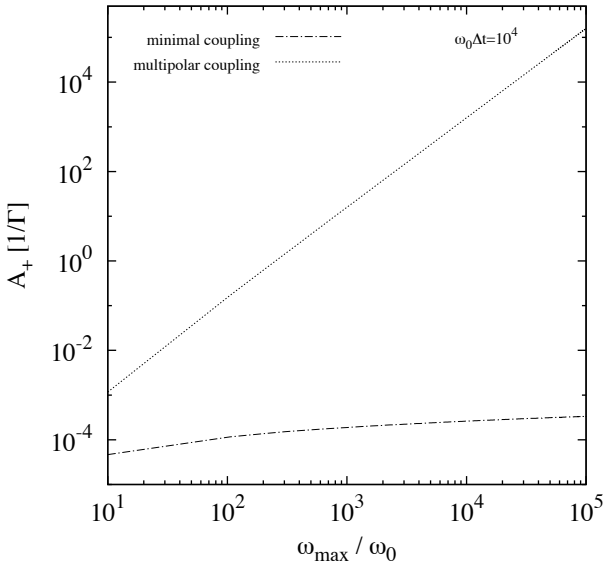


Figure 8.4: Logarithmic plot of the rates A_+ in 8.38, in the Coulomb gauge and the Poincaré gauge as functions of the upper cut-off frequency ω_u, with $\omega_{eg}\Delta t = 10^4$. The results are in very good agreement with the analytical results in 8.40 –8.41.

8.3.2 Verifying the Lindblad form

The Lindblad-form condition 8.37 clearly holds in the symmetric representation. To check whether it holds in the Coulomb and Poincaré gauges the constant B must be calculated as

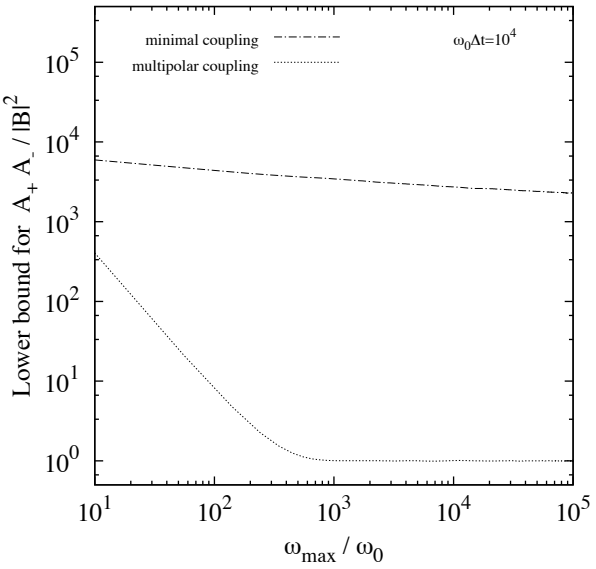


Figure 8.5: Logarithmic plot of lower bounds for $(A_+A_-)/|B|^2$ in the Coulomb and Poincaré gauges obtained via numerical integration of the expressions in 8.38 and 8.30. The plots confirm that 8.37 holds for the experimental parameters of interest and that the corresponding master equations are therefore of Lindblad form.

a function of Δt and ω_u. Assuming for simplicity that the atomic dipole moment is real, one easily finds that

$$B = -\frac{2\Gamma}{\pi\omega_{eg}^2\Delta t}\mathrm{e}^{-i\omega_{eg}\Delta t}\int_0^{\omega_u} d\omega\,\frac{\omega^2 u_k^+ u_k^-}{\omega_{eg}^2-\omega^2}\sin\left[\frac{1}{2}(\omega_{eg}+\omega)\Delta t\right]\sin\left[\frac{1}{2}(\omega_{eg}-\omega)\Delta t\right]. \quad (8.42)$$

Using trigonometric relations and approximating the integral over $\cos(\omega\Delta t)$ as zero, this expression simplifies to

$$B = \frac{\Gamma}{\pi\omega_{eg}^2\Delta t}\mathrm{e}^{-i\omega_{eg}\Delta t}\cos(\omega_{eg}\Delta t)\int_0^{\omega_u} d\omega\,\frac{\omega^2 u_k^+ u_k^-}{\omega_{eg}^2-\omega^2}. \quad (8.43)$$

Concrete expressions for the $u_k^\pm$ can be found in table 8.1. Replacing $|\cos(\omega_{eg}\Delta t)|$ by its maximum of one, we obtain an upper bound for $|B|$. Figure 8.5 uses this bound and verifies that the condition 8.37 holds in both the Coulomb and Poincaré gauges, for a wide range of experimental parameters. This shows that the master equations associated with these gauges are generally of Lindblad form.

8.4 The stationary state photon emission rates

In this section I calculate the stationary state photon emission rate I_{ss} for the three coupling models considered in 8.3.1. The probability density $I(t)$ for the emission of a photon at time t is given by the trace over the density matrix $\tilde{\mathcal{R}}[\tilde{\rho}_A]$ in 8.25. Denoting the matrix elements

of the atomic density matrix as follows

$$\rho_A = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}, \tag{8.44}$$

one obtains

$$I(t) = A_- \rho_{22}(t) + A_+ \rho_{11}(t). \tag{8.45}$$

According to 8.29, the matrix elements evolve according to

$$\begin{aligned} \dot{\rho}_{11} &= -A_+ \rho_{11} + A_- \rho_{22}, \\ \dot{\rho}_{12} &= i\omega_{eg}\rho_{12} + \frac{1}{2}(A_- + A_+)\rho_{12} + B^* \rho_{21}, \\ \rho_{21} &= \rho_{12}^*, \qquad \rho_{22} = 1 - \rho_{11}, \end{aligned} \tag{8.46}$$

which imply that the stationary state of the atom (for which $\dot{\rho}_A = 0$), is described by a diagonal matrix with

$$\rho_{22} = \frac{A_+}{A_- + A_+}, \qquad \rho_{11} = 1 - \rho_{22}. \tag{8.47}$$

Substituting the population ρ_{22} above into 8.45, one obtains the stationary state photon emission rate

$$I_{ss} = \frac{2A_- A_+}{A_- + A_+}. \tag{8.48}$$

The proportion of this rate associated with the excited state $|e\rangle$ is only half the total rate; $A_- \rho_{22} = I_{ss}/2$. The other half is associated with the ground state $|g\rangle$. Expression 8.48 is proportional to A_+, because the off-resonant (virtual) excitation of the atom creates the stationary state population $\rho_{22} \neq 0$ in the first place.

Each representation incurs a different definition of bare "photon". Assuming that there exists a representation in which the bare photons are the physical photons observed in reality, then we can identify this representation as that which produces theoretical predictions closest to the experimental results.[51] If one requires that in the absence of external driving $I_{ss} \equiv 0$, then in the present context one concludes that the symmetric representation yields the most accurate master equation. The master equation it yields is the simplest special case

[51] A problem here is that there may be more than one empirical (i.e. experimental) constraint that we have to impose within our theory. For example, along with the (possible) requirement that $I_{ss} = 0$ we may require that Einstein causality holds in all physical interactions. It may not always be possible to obtain a theory within the standard framework, that satisfies all such requirements simultaneously (cf. chapter 9).

of the general equation given in 8.29;

$$\dot{\rho}_A = -i\omega_{eg}[\sigma_z, \rho_A] + \frac{1}{2}A_- \left(2\sigma^- \rho_A \sigma^+ - \sigma^+\sigma^- \rho_A - \rho_A \sigma^+ \sigma^-\right), \tag{8.49}$$

which is nothing but the Born-Markov master equation with a decay rate A_- instead of Γ.

To determine the natures of the nonzero rates associated with the Coulomb and Poincaré gauges we need some numbers. A typical transition frequency in the optical regime is $\omega_{eg} = 3.7 \times 10^{15}\text{s}^{-1}$ corresponding to a wavelength of 500nm. A possible estimate for the upper cut-off frequency is $\omega_u = 3.7 \times 10^{19}\text{s}^{-1}$ corresponding to the Bohr radius.[52] An estimate for the environmental-response time Δt is the time it takes a photon to reach the walls of the laboratory. Assuming that photons travel at the speed of light and that the walls of the laboratory are about 3m away yields $\Delta t = 10^{-8}\text{s}$. Finally a typical spontaneous decay rate is $\Gamma = 10^7\text{s}^{-1}$.

Using these estimates one obtains a stationary state photon emission rate I_{ss} of about 1.5 photons per second in the Coulomb gauge. This is well below typical detector dark count rates of about 500 photons per second and more or less impossible to observe experimentally. Using the same parameters in the Poincaré gauge one obtains an A_+ of about 4×10^6 photons per second, which clearly shows that the master equation associated with the Poincaré gauge can't be valid.

A way of obtaining higher stationary emission rates (in any gauge) is to move the photon-absorbing environment closer to the atom. The reason for this is that A_+ scales essentially as $1/\Delta t$, while A_- remains more or less the same when Δt changes. A photon-absorbing environment 10cm away from the atom implies $\Delta t \approx 3 \times 10^{-10}\text{s}$ and using the same values as above one obtains an I_{ss} of about 40 photons per second in the Coulomb gauge.

One could also consider atomic systems with a relatively large spontaneous decay rate Γ and a relatively small transition frequency ω_{eg}, like the ones used in recent experiments with single quantum dots and colour centers in diamond. Matthiesen *et al.* (2011) have studied the fluorescence from Gallium Arsenide with a single layer of self-assembled Indium Arsenide at a temperature of 4.2K and measured a lifetime of 760ps for an excited electronic state with a transition wavelength of about 950nm. This corresponds to a decay rate Γ of about 10^9s^{-1} and a transition frequency ω_{eg} of about $2 \times 10^{15}\text{s}^{-1}$. Assuming moreover that $\Delta t = 3 \times 10^{-10}\text{s}$, we obtain a Coulomb gauge I_{ss} of about 8400 photons per second.

Müller *et al.* (2011) have studied photon emission from an excited state using chromium-based colour centers in diamond with a lifetime of 1ns and a transition wavelength of 710nm at a temperature of 4K. These parameters correspond to $\omega_{eg} = 2.6 \times 10^{15}\text{s}^{-1}$ and $\Gamma = 10^9\text{s}^{-1}$. If we assume again a photon-absorbing environment which is 10cm or less away from the colour centre, the condition $\Gamma\Delta t \ll 1$ applies and the above calculations

[52] It should be noted that changing ω_u by a few orders of magnitude does not change A_+ significantly.

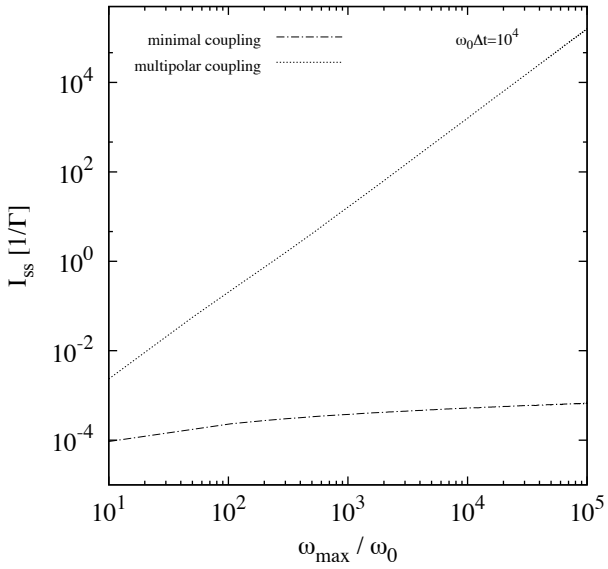


Figure 8.6: Logarithmic plot of the stationary state photon emission rate I_{ss} in the Coulomb and Poincaré gauges as a function of ω_u. The plots are the result of numerical solutions of 8.48 and 8.38.

hold. In this case the master equation associated with the Coulomb gauge predicts an I_{ss} of about 2600 photons per second.

8.5 Summary and discussion

According to the model employed in this chapter environmental interactions have the effect of continuously projecting the atom-field system onto a product state with the field in its vacuum state. For most representations of the atom-field system, the ground state of the total Hamiltonian is entangled with respect to the bare state basis. With respect to these Hamiltonians the field-environment interaction continually resets the atom-field system onto a state that is necessarily energetically higher than its ground state. Thus, the photon-absorbing environment constantly pumps energy into the system, which manifests itself as a nonzero stationary state photon emission rate even in the absence of external driving (Kurcz *et al.* (2010)). The only exception to this situation occurs when the bare ground state $|g;0\rangle$ coincides with the true ground state of the atom-field system, which is the case in the symmetric representation.

When the atom-field interaction V contains counter-rotating terms, one obtains a nonzero stationary state photon emission rate, which increases with decreasing Δt. One can offer a tentative explanation of this emission rate in terms of the virtual photon cloud (cf. 6.4); the counter-rotating terms cause virtual excitations of the atom-field system, which results in the virtual emission of photons. The environment can absorb these photons, which leaves the atom in an excited state with no possibility of virtually reabsorbing a photon to become de-excited. The atom must therefore decay via real emission. If Δt is the time taken for

a photon to interact with the environment, then by decreasing Δt one is, in effect, moving the environment closer to the atom. If the virtual cloud is localised around the atom, then moving the photon-absorbing environment closer to the atom will increase the frequency of virtual photon absorption. This will increase the frequency with which the atom is left excited, and thereby increase the stationary state emission rate. In summary, the emission rate increases with decreasing Δt—the distance of the environment from the atom—because decreasing Δt increases the exposure of the virtual cloud to the environment.

This qualitative analysis is consistent with the ideas of 6.4.2 and the energy-time uncertainty principle 6.91. According to 6.91 the environment is only able to resolve virtual emission events such that $\omega_{eg} + \omega < \Delta t^{-1}$, and therefore perceives the atom as dressed by photons with frequency $\omega_{eg} + \omega > \Delta t^{-1}$ (Compagno *et al.* (1995)). Decreasing Δt increases the bandwidth of frequencies that the environmental "measurements" are able to resolve.

Of course, the number of photons perceived by the environment also varies with the chosen atom-field coupling. Assuming that Δt is given by the environment, the coupling becomes the only free parameter and determines the extent to which the environment perceives a virtual cloud. Although I have focused on three main cases, in principle the $\{\alpha_k\}$ that determine the atom-field coupling could be chosen to generate *any* value of I_{ss} whatsoever. In this way, it becomes possible for the model to reproduce detector dark count rates and finite temperature effects.

CHAPTER 9

Subsystems and causality

I end here with a final rather short chapter in which I discuss the important subject of Einstein causality, and review how the concept relates to quantum subsystem relativity. Ever since the inception of quantum mechanics its interplay with the theory of relativity has been the subject of intense study. The elusive and often counter-intuitive nature of quantum nonlocality makes it one of the most important foundational aspects of the theory, yet to be fully understood. Given the nonlocal nature of quantum theory it isn't surprising that its consistency with Einstein causality (postulate 1, section 2.1) has frequently been called into question.

Since the literature on this subject is vast and ever increasing it would be hopeless to attempt to review it all. In this chapter I will review only simple "standard" results, and then focus entirely on the famous thought experiment of Fermi (1932) known as *Fermi's two atom problem*. The setup envisioned by Fermi offers a simple means by which to investigate questions regarding quantum nonlocality and Einstein causality. In particular, I will be interested in determining the role of virtual contributions in ensuring causal signal propagation, and the implications this has with regard to determining suitable subsystem decompositions.

9.1 A standard no-signalling theorem

Quantum entanglement leads to nonlocal correlations between spacelike separated systems. Bell (1964) showed that any hidden variable theory capable of reproducing the results of quantum mechanics must also be nonlocal. There are many "proofs" in the literature, that the nonlocality of quantum mechanics can't be used for superluminal communication. Since one *assumes* that subsystem operators take the form $A_1 \otimes I$ and $I \otimes A_2$ for subsystems 1 and 2 respectively, there are no (local) measurements that can be performed on one of the the subsystems alone, that will effect the statistics of the other. These no-signalling theorems

seem to be little more than tautologies amounting to the unremarkable statement that the identity operator does indeed leave a Hilbert space invariant.

In the general formulation of quantum measurement theory the act of measurement on a single subsystem is represented using Kraus operators (see for example, Kraus *et al.* (1983), Breuer & Petruccione (2007)). A measurement performed on subsystem 1 for example, has the effect

$$\rho \to \rho' := \sum_{i\mu} (K_{i\mu} \otimes I_2) \rho (K_{i\mu}^\dagger \otimes I_2). \tag{9.1}$$

where $\{K_{i\mu}\}$ denotes a set of Kraus operators, which satisfy

$$\sum_{i\mu} K_{i\mu}^\dagger K_{i\mu} = I_1. \tag{9.2}$$

Subsequently, the expectation value of an operator O_2 pertaining to subsystem 2 is

$$\mathrm{tr}(I_1 \otimes O_2 \rho') = \mathrm{tr}(I_1 \otimes O_2 \rho) \tag{9.3}$$

with the equality following from 9.2, the fact that operators pertaining to separate subsystems commute, and the cyclic property of the trace. It follows from 9.3 that the statistical predictions for the results of (local) measurements performed on subsystem 2 are unaffected by a (local) measurement of subsystem 1 made immediately beforehand. This shows that there can't be any *instantaneous* communication between distant observers based solely on local measurements.

9.2 Causality in quantum field theory

In order to properly investigate locality and microscopic causality in quantum theory one must encode these notions into well-defined conditions to be imposed on observables that are explicitly associated with regions (or points) in spacetime. One achieves this through the use of *quantum fields*. Attempts to put quantum field theory on a mathematically rigorous footing are ongoing. These attempts have come to be known as constructive quantum field theory and algebraic (or sometimes axiomatic) quantum field theory (AQFT).

The first attempt at specifying a precise set of axioms upon which quantum field theory could be built was given by Wightman (1964) (see also Haag (1996) and references therein). A field $\phi(x)$ at a point $x \in E^{1,3}$ is an operator valued distribution over a Hilbert space $\mathcal{H}$. An observable O associated with some $U \subset E^{1,3}$ is some polynomial of *operators* $\{\phi(f)\} \subset \mathcal{L}(\mathcal{H})$, which smear the fields over test functions $\{f\}$ whose support is U;

$$\phi(f) := \int d^4x \, \phi(x) f(x). \tag{9.4}$$

The space of test functions $FE^{1,3}$ is often taken as the space of smooth functions all of

whose derivatives approach zero faster than any positive power of x^{-1} as x approaches infinity. Causality is encoded into the theory through the requirement that

1. if the supports of the test functions f, g are spacelike separated then $[\phi(f), \phi(g)] = 0$ for bosons and $\{\phi(f), \phi(g)\} = 0$ for fermions.

Thus, all observables are compatible in two regions that can't be connected to each other by a causal signal.

There is also a notion of *primitive causality* built-in to AQFT, which assumes that physical equations of motion for fields are hyperbolic, so that solutions propagate with finite velocity $v \leq c$. Suppose we are given a region $\mathcal{R} \subset E^3$ taken with respect to some inertial frame $\mathcal{O}$, and that our Hilbert space $\mathcal{H}$ consists of states giving a complete physical description of physical phenomena in $\mathcal{O}$. Any two (in general distinct) states $|\psi\rangle$ and $|\psi'\rangle$ *look the same in a given region* $\mathcal{R}$ and at a given time t, if for all observables $O(t)$ (which are polynomials of the operators in 9.4 associated with $(t, \mathcal{R}) \subset E^{1,3}$[53]) one has

$$\langle\psi|O_{\mathcal{R}}(t)|\psi\rangle = \langle\psi'|O_{\mathcal{R}}(t)|\psi'\rangle. \tag{9.5}$$

In other words $|\psi\rangle$ and $|\psi'\rangle$ look the same in $\mathcal{R}$ if they can't be distinguished by any measurement made in $\mathcal{R}$, that is, by any measurement of observables associated with $(t, \mathcal{R})$. Now suppose that $\mathcal{R}$ denotes the ball of radius R centered at some $\mathbf{x} \in E^3$, and that we are given states $|\psi\rangle$ and $|\psi'\rangle$ satisfying 9.5 at, say, $t = 0$. Primitive causality is the requirement that equation 9.5 taken at time $t = 0$ implies that at time $t \in (0, R/c)$

$$\langle\psi|O_{\mathcal{S}}(t)|\psi\rangle = \langle\psi'|O_{\mathcal{S}}(t)|\psi'\rangle \tag{9.6}$$

where $\mathcal{S}$ is the ball of radius $R - ct$ centered on $\mathbf{x}$. This assumes that there is a one-to-one correspondence between observables associated with different time slices, so that if for example, energy can be defined in some region at a fixed time, then there is a corresponding unique energy associated with any other region at any other time. This is ensured by the Heisenberg equation, which implies

$$O(t) := e^{iHt} O e^{-iHt} \tag{9.7}$$

for some Hamiltonian H. Primitive causality is the direct encoding of Einstein causality into the field theoretic structure. It means that no causal influence (one that effects measurement outcomes) can move into $\mathcal{R}$ from its complement faster than light. Primitive causality necessarily holds—in the sense that 9.6 follows from 9.7 and 9.5—whenever the equations of motion governing the dynamics of the fields are hyperbolic (Buchholz & Yngvason (1994)).

There are very few (in fact, I'm not sure that there are any) interacting quantum field

[53] Since according to 9.4 observables have to be smeared over time and space, the notation $(t, \mathcal{R})$ should really be taken as shorthand for $\mathcal{R}_{t,\varepsilon} := \{(x^0, \mathbf{x}) \ : \ |x^0 - t| < \varepsilon, \ \mathbf{x} \in \mathcal{R}\}$ where ε is small.

theories used in practice, that can be cast into the algebraic/axiomatic framework, and certainly none as elaborate as a Yang-Mills gauge field theory such as QED. Those theories that can be put into the algebraic framework are predominantly free field theories. Most elementary textbooks on conventional quantum field theory seem content to formally verify that something like axiom 1 above holds for a handful of free theories and leave it at that. For example in scalar field theory one can show that (Ryder (1996))

$$[\phi(x), \phi^{\dagger}(x')] = [\phi(x), \phi(x')] = 0, \tag{9.8}$$

whenever $(x-x')^{\mu}(x-x')_{\mu} < 0$, i.e., for all points outside the lightcone of $x-x'$. Similarly, outside the lightcone the free Dirac field satisfies (Peskin & Schroeder (1995))

$$\{\psi^{\alpha}(x), \psi^{\dagger}_{\beta}(x')\} = \{\psi^{\alpha}(x), \psi^{\beta}(x')\} = 0, \tag{9.9}$$

the electric and magnetic fields in free QED satisfy (Cohen-Tannoudji *et al.* (1997))

$$[\mathbf{E}^{i}(x), \mathbf{B}^{j}(x')] = [\mathbf{E}^{i}(x), \mathbf{E}^{j}(x')] = [\mathbf{E}^{i}(x), \mathbf{B}^{j}(x')] = 0, \tag{9.10}$$

and in covariant formulations the four-potential satisfies (Cohen-Tannoudji *et al.* (1997))

$$[A_{\mu}(x), A_{\nu}(x')] = 0. \tag{9.11}$$

That the operators appearing in the above relations evolve freely (under the action of a free Hamiltonian), is what allows for the simple determination of their commutators/anti-commutators.

9.3 Fermi's two atom problem

Fermi (1932) imagined a setup consisting of two two-level atoms A and B. He posed the question; if atom A is excited and atom B is in its ground state then can atom B become excited before the time taken for a signal to propagate from A to B? He probably envisioned a scenario in which atom A decays via photon emission leading to a nonzero probability of excitation of atom B through absorption of the same photon. He most likely expected that this probability would be zero for times less than that taken for a signal to propagate from A to B. The general problem is that of identifying the nature of (electromagnetic) energy transfer between spatially separated material systems. This problem has received a good deal of attention over the years (see Fermi (1932), Biswas *et al.* (1990), Craig & Thirunamachandran (1992), Hegerfeldt (1994), Buchholz & Yngvason (1994), Milonni *et al.* (1995), Power & Thirunamachandran (1997), Sabín *et al.* (2011) and references therein).

On the face of it the *idea* of the Fermi problem seems to be quite straightforward (even if its solution is technically hard to find), but the problem is actually of a very subtle nature. First of all the setup envisioned by Fermi appears to presuppose that the atoms have

well-defined localisation properties, and that there is a parameter R giving the distance between them. That particles exist as localised objects in spacetime is far from clear however. A more modern perspective might be that localisation is only a property of interactions between field quanta and detection devices.

Even if the atoms are assumed to be fixed and separated by a distance R, the naive assumption that atom B can only become excited via the absorption of photons emitted by atom A is unwarranted. We know that bare ground state atoms can become spontaneously excited even in the absence of photons, due to the existence of counter-rotating terms in atom-field interaction Hamiltonians. Thus, we can't assume that a nonzero excitation probability of atom B for times less than R/c implies a violation of Einstein causality. Such an excitation might have nothing to do with atom A at all. This aspect of the problem will depend on the form of atom-field coupling chosen to model the problem. Actually the entire problem is clearly dependent on how one defines the atoms and field as physical subsystems. Separating out virtual excitations of atom B and real excitations caused by atom A, is a key step towards finding a solution.

Assuming an initial bare state $|e_A;g_B;0\rangle$ consisting of atom A excited, atom B in its ground state, and zero photons present, there are a number of excitation probabilities which could be perceived as relevant to the Fermi problem. The most naive approach would be to calculate the probability

$$P_1(t) := |\langle g_A;e_B;0|e^{-iHt}|e_A;g_B;0\rangle|^2 \tag{9.12}$$

in which the final state of all three systems is specified. Fermi found using approximations that this probability is causal, i.e., zero for $t < R/c$, but without approximation this result can't be achieved. This is not too surprising given that no attempt has been made to separate out virtual excitations. One might also calculate

$$\begin{aligned} P_2(t) &:= \langle e_A;g_B;0|e^{iHt}\left[\sum_n |n_A\rangle\langle n_A|\otimes|e_B\rangle\langle e_B|\otimes|0\rangle\langle 0|\right]e^{-iHt}|e_A;g_B;0\rangle \\ &= \sum_n |\langle e_A;g_B;0|e^{iHt}|n_A;e_B;0\rangle|^2, \end{aligned} \tag{9.13}$$

in which one finds the probability that atom B is excited *and* that there are no photons at time t, irrespective of the state of atom A. Similarly, one could calculate the probability to find atom A in its ground state and atom B excited without specifying the final state of the field. Again one would have to separate out the virtual and real excitations to obtain a relevant result. Evidently, the most general probability relevant to the problem is $P_A(t)$, *which is defined as the component of the probability*

$$P(t) := \sum_n \sum_m \sum_{\mathbf{k}\lambda} |\langle e_A;g_B;0|e^{iHt}|n_A;e_B;m_{\mathbf{k}\lambda}\rangle|^2 \tag{9.14}$$

that depends on atom A. The probability $P(t)$ to find atom B excited irrespective of the state

of the field and atom A will be the sum $P(t) = P_0(t) + P_A(t)$ where $P_0(t)$ denotes the virtual contribution independent of atom A. Hegerfeldt (1994) proved quite generally that if

1. the atoms are initially assumed to be localised in disjoint regions separated by R,
2. the probability $P(t)$ is given by the expectation value of a positive operator,
3. the energy (Hamiltonian) is bounded from below,

then $P(t)$ is nonzero for times $t < R/c$. It follows that a nonzero $P_0(t)$ is necessary in order to preserve the possibility that Einstein causality holds in the Fermi problem. This condition is necessary but certainly not sufficient to prove that Einstein causality holds. One must still employ an interaction Hamiltonian without instantaneous coupling terms. For this reason the Poincaré gauge Hamiltonian has been chosen in all previous formal proofs of causality in the Fermi problem.

In a simple quantum optical treatment in which one assumes the EDA, the fields at the position of each of the atoms are evaluated at the centre-of-mass positions $\mathbf{R}_A$ and $\mathbf{R}_B$ with $|\mathbf{R}_A - \mathbf{R}_B| =: R$. The Poincaré gauge electric field $\mathbf{E}(\mathbf{x})$ is equal to the transverse displacement $\mathbf{D}_\mathrm{T}(\mathbf{x})$ whenever $\mathbf{x} \neq \mathbf{R}_A, \mathbf{R}_B$, and the electromagnetic fields $\mathbf{D}_\mathrm{T}$ and $\mathbf{B}$ can be written formally as the sum of free and source components corresponding to each atom;

$$\mathbf{D}_\mathrm{T} = \mathbf{D}_\mathrm{T}^0 + \mathbf{D}_\mathrm{T}^A + \mathbf{D}_\mathrm{T}^B, \qquad \mathbf{B} = \mathbf{B}^0 + \mathbf{B}^A + \mathbf{B}^B. \tag{9.15}$$

It is easy to show that in the Poincaré gauge all observables of atom B depend on atom A either directly or indirectly through the transverse displacement field $\mathbf{D}_\mathrm{T}^A$, from which it follows using the retarded solution 6.30 that $P_A(t) = 0$ for $t < R/c$. Of course, due to the counter-rotating terms in the Poincaré gauge interaction Hamiltonian there is a nonzero probability $P_0(t)$ that the bare atom B is spontaneously excited out of the vacuum. Considering atom B alone, the state $|g_B; 0\rangle$ is not an eigenstate of the Poincaré gauge atom-field interaction Hamiltonian. Because of this the Poincaré gauge treatment in the EDA doesn't countenance an inconsistency with Hegerfeldt's theorem.

If $|g_A; g_B; 0\rangle$ were the ground state of the Hamiltonian, which would be the case if each atom coupled to the field via the symmetric coupling 6.84, and the atoms were not directly coupled to each other, then $P_0(t)$ would be zero and $P_B(t)$ would not be causal. Thus, the explicit presence of the virtual field in the Hamiltonian is necessary in order to preserve Einstein causality, meaning that the virtual cloud of photons can't be included within the initial atomic states (see for example Milonni *et al.* (1995) and references therein). This would seem to imply that, at least in quantum optics, a measurement of the energy of an atom constitutes a measurement of the *bare* Poincaré gauge atomic energy observable.

The paper of Hegerfeldt (1994) sparked a controversy at the time of publication, and a spate of responses followed the next year (see references given at the start of this section). The most common argument against the alleged causality problem was exactly that given above—that even if $P(t)$ is not causal, the *relevant* probability $P_B(t)$ *is* causal. However, this

does not seem to be something unbeknown to Hegerfeldt when he published his result. In fact the causal nature of $P_B(t)$ had already been verified using a simple model (Biswas *et al.* (1990)). Rather it seems that Hegerfeldt was posing the following question. If we require a nonzero $P_0(t)$ in order that $P_B(t)$ is causal, do we not then encounter a problem, *given that a nonzero* $P_0(t)$ *is surely itself unphysical*? He seems to be arguing that in attempting to renormalise a theory, spontaneous virtual excitations—described in the case of the Fermi problem by $P_0(t) \neq 0$—are precisely the kind of excitations one seeks to eliminate. His result shows that in such a successfully *renormalised* theory violations of Einstein causality necessarily occur if the seemingly reasonable conditions 1-3 above are satisfied. Most responses to Hegerfeldt's theorem seemed to ignore the issue that a nonzero $P_0(t)$ could in itself be viewed as presenting a serious problem of physical interpretation. In order to get around Hegerfeldt's theorem we must assume that either one or more of the conditions 1-3 are not valid (for example, the assumption that localised states as specified in condition 1 exist, may be invalid), or to accept that virtual excitations are a genuine physical occurrence.

The real problem we are faced with is how to construct a quantum theory in which unphysical violations of Einstein causality do not occur. This is one of the main problems AQFT confronts. The original ideas of Fermi about verifying Einstein causality by calculating the transition probability in 9.12 seem fairly far detached from a classical viewpoint involving Maxwell's equations. But in all of the proposed solutions to the Fermi problem equations of motion incurring retarded solutions play a key role. In the simple quantum optical solution one uses the retarded nature of the source component of the transverse displacement field. In AQFT there is a built-in primitive causality facilitated by the assumption that all physical equations of motion are hyperbolic. This suggests that a general formal proof of causality can be given within the framework of conventional QED without the use of any simplifying assumptions, by using Maxwell's equations directly in the quantum theory. Doing this in a mathematically rigorous and consistent fashion is probably far from straightforward, but it seems to be well-motivated on physical grounds.[54] It is perhaps amusing to note that in formulating QED we start right at the beginning with a theory in which *there are no violations of causality* when it comes to the action of charges on other charges—namely Maxwell electrodynamics. In trying to determine without approximation how to ensure that Einstein causality holds in the two atom problem we are naturally lead back to this beginning.

Through the direct use of Maxwell's equations one would be able to avoid the EDA, as well as any separation of charges into bound and free systems. Such a separation is based upon the ideas of macroscopic classical electromagnetism whereby the internal details of a bound system of charges are ignored, and one only retains interest in the source fields outside of the bound system itself. With this strategy in mind adopting the Poincaré gauge is natural, because the Poincaré gauge field canonical momentum is equal to the (negative

[54]For a discussion of Maxwell's equations in the context of AQFT see Ferrari *et al.* (1974), Ferrari *et al.* (1977).

of the) total electric field *outside* the system of charges. But with regard to fundamental questions concerning causality it is just as important that charges within a bound system are causally connected as it is that any two bound systems are themselves causally connected. Thus, to really ensure Einstein causality at the microscopic level the detailed structure of each bound system is important. Fundamentally each individual charge produces its own electric and magnetic fields.

Since the electric and magnetic fields afford retarded solutions we can ensure general microscopic causality through Poynting's theorem. This requires the use of the gauge-invariant definitions of material and electromagnetic energy densities $\mathscr{H}_M$ and $\mathscr{H}_{\rm EM}$ from 3.98. These definitions are quite natural given that the Hamiltonian is supposed to represent the total energy, but they do not specify the energies of bare subsystems with Hilbert spaces whose tensor product gives the composite system Hilbert space. In this particular sense they seem to be closer to the energies of renormalised subsystems of the type envisioned by Hegerfeldt (1994). No renormalisation procedure has been carried out however, and the (bare) vacuum expectation values of these energies are nonzero.

Poynting's theorem 4.38 along with the retarded solutions 4.10 ensure that changes in the energy density of the matter field at a point $(t,\mathbf{x})$ are independent of the matter field at all points, which can't be connected to $(t,\mathbf{x})$ by a causal signal. To work out the equation of motion for $\mathscr{H}_M$ explicitly I note that in the Coulomb gauge $\mathbf{A}=\mathbf{A}_{\rm T}$ and $\mathbf{E}=\mathbf{E}_{\rm T}+\mathbf{E}_{\rm L}=-\mathbf{\Pi}_{\rm T}-\mathbf{P}_{\rm L}$ where $\mathbf{P_L}$ is given by 2.37. With these identifications it is straightforward to show using the relations 3.45 and 3.99 that

$$\begin{aligned}[\mathscr{H}(\mathbf{x}),E^j(\mathbf{x}')] &= iJ^i(\mathbf{x})\left[\delta^{\rm T}_{ij}(\mathbf{x}-\mathbf{x}')+\partial_i g_{{\rm L},{\rm j}}(\mathbf{x}',\mathbf{x})\right] \\ &= iJ^i(\mathbf{x})\left[\delta^{\rm T}_{ij}(\mathbf{x}-\mathbf{x}')+\delta^{\rm L}_{ij}(\mathbf{x}-\mathbf{x}')\right] = iJ^j(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}').\end{aligned} \tag{9.16}$$

where $\mathbf{g}_{\rm L}$ is defined in 2.39 and $\delta^{\rm L}_{ij}(\mathbf{x}-\mathbf{x}')=\partial_i g_{{\rm L},{\rm j}}(\mathbf{x}',\mathbf{x})$ is the longitudinal delta function, which satisfies

$$\delta^{\rm T}_{ij}(\mathbf{x}-\mathbf{x}')+\delta^{\rm L}_{ij}(\mathbf{x}-\mathbf{x}')=\delta_{ij}\delta(\mathbf{x}-\mathbf{x}'). \tag{9.17}$$

The equation of motion for $\mathscr{H}_M$ is now easily found using 9.16;

$$\begin{aligned}\dot{\mathscr{H}}_{\rm M}(t,\mathbf{x}) &= -i[\mathscr{H}_M(t,\mathbf{x}),H]=\frac{1}{2}\left[\mathbf{J}(t,\mathbf{x})\cdot\mathbf{E}(t,\mathbf{x})+\mathbf{E}(t,\mathbf{x})\cdot\mathbf{J}(t,\mathbf{x})\right] \\ &= \frac{1}{2}\left[\left(\nabla\times\mathbf{B}(t,\mathbf{x})-\dot{\mathbf{E}}(t,\mathbf{x})\right)\cdot\mathbf{E}(t,\mathbf{x})+\mathbf{E}(t,\mathbf{x})\cdot\left(\nabla\times\mathbf{B}(t,\mathbf{x})-\dot{\mathbf{E}}(t,\mathbf{x})\right)\right]\end{aligned} \tag{9.18}$$

where 4.1b has been used in writing the second equality. Substituting the solutions 4.10 into the right-hand-side of 9.18 shows that the rate of change of the energy density of the matter field $\dot{\mathscr{H}}_{\rm M}(t,\mathbf{x})$, only depends on the matter field at other points $\mathbf{x}'$ at the retarded time

$t_r = t - |\mathbf{x} - \mathbf{x}'|$. The energy of the matter field in some closed region $\mathcal{R} \in \mathbb{R}^3$ is merely

$$H_M^{\mathcal{R}}(t) = \int_{\mathcal{R}} \mathrm{d}^3x \, \mathscr{H}_M(t, \mathbf{x}) \tag{9.19}$$

and the delta function in the commutation relation 9.16 ensures that $\mathscr{H}(t, \mathbf{x}')$ and $\mathbf{E}(t, \mathbf{x}')$ are compatible observables for $\mathbf{x} \neq \mathbf{x}'$. Moreover it ensures that the material and the electromagnetic energies are compatible in disjoint regions i.e.

$$[H_M^{\mathcal{R}}, H_{\mathrm{EM}}^{\mathcal{R}'}] \equiv \int_{\mathcal{R}} \mathrm{d}^3x \int_{\mathcal{R}'} \mathrm{d}^3x' \, [\mathscr{H}_M(\mathbf{x}), \mathscr{H}_{\mathrm{EM}}(\mathbf{x}')] = 0 \tag{9.20}$$

whenever $\mathcal{R} \cap \mathcal{R}' = \emptyset$. Ideally I would like to show that all of the observables are compatible outside the lightcone, but I don't know how.

Since $\mathscr{H}_{\mathrm{M}}$ is gauge-invariant the above result does not rely on the use of a particular gauge and avoids any approximations. Of course, the specifications of the electric and magnetic fields, as well as the specifications of the material and electromagnetic energy densities have been made with respect to a specific inertial frame. Therefore the comments regarding the covariance of Poynting's theorem made towards the end of section 4.2 continue to apply.

9.4 Summary and discussion

We have seen in this section that virtual contributions play a crucial role in ensuring causality in the Fermi problem. Dressed state (renormalised) models will necessarily lead to apparent violations of Einstein causality, which shows that they are either unphysical, or do not possess the localisation properties required in order that certain questions regarding Einstein causality make proper sense. If dressed states are not strictly localised, then what look like small violations of Einstein causality might inevitably show up in calculations.

The standard QED framework may well be insufficient for the purposes of investigating the delicate nature of particle localisation with which the idea of virtual clouds is intimately related. If, as the name suggests, virtual particles are not real, then neither are bare particles. It is then unclear how to use the standard framework in which all observables are built out of operators pertaining to bare particles, to describe *physical* particles in such a way that we can pose unambiguous questions about Einstein causality in *physical* interactions.[55]

One can, as has been shown, use traditional definitions of material and electromagnetic energy densities to give a "proof" of causality in the Fermi problem, which generalises standard proofs given in quantum optical treatments. These traditional energies don't constitute what in quantum theory one would call *free* energies pertaining to bare subsystems. In this sense they may be better termed *dressed* energies. If we agree that these definitions are in fact the correct ones, then we will have "come full circle". Starting out with these defini-

[55] I use the term "particle" here very loosely and for want of a better word. It seems increasingly likely that whatever the fundamental physical "objects" are, they are quite far removed from anything resembling what we traditionally mean by particles.

tions, we will have then quantised the theory and abandoned them in favour of the standard quantum mechanical interpretation of physical subsystems. We will then have decided that such bare subsystems are not actually physical, and that physical subsystems are made of dressed particles with dressed particle energies. Finally we will have decided that these dressed energies are nothing but the original energies that we had at the beginning. Our (somewhat lofty) goal would then be to construct a rigorous theory of QED based directly on these definitions without any reference to bare and virtual particles. This theory would have to replicate the undeniable practical success of conventional QED, and adhere to all the physical constraints imposed by fundamental principles like causality. Any attempts along these lines using constructive/axiomatic quantum field theory seem to have been unsuccessful so far.

Conclusions

The aim of this thesis has been to investigate the nature of different decompositions of composite light-matter systems into constituent subsystems. Because the notion of quantum subsystem is a relative one, there is considerable freedom in choosing such decompositions, and in QED this freedom is directly related to gauge freedom. In the classical setting gauge freedom has no consequences with regard to physical predictions. Material systems are specified through charge and current densities, and electromagnetic interactions are mediated by electric and magnetic fields. At the quantum level bare subsystems are defined in terms of gauge dependent operators, and predictions concerning bare states and canonical subsystem observables come out gauge dependent except in special cases such as scattering theory.

The crucial property ensuring gauge invariance of the S-matrix is free energy conservation. Upon recognising this we have at least two reasonable options regarding the physical interpretation of QED. The first option is to close the door on any hope of obtaining a meaningful ontology pertaining to QED. One stipulates that all observable quantities are encoded into the S-matrix, and that we can only assign *physical* meaning to scattering *processes* that lead to decay rates and cross-sections with direct *operational* meaning. Such a viewpoint has been advocated in the past by Heisenberg (1943) for example, but to me seems extremely limited. Not least because the current framework is mathematically ill-defined, but also because it places such an incredibly modest limit on the capability of physical theories. It implies that the best we can possibly hope to do is only *approximately* understand reality, as it would be if *all* processes occurred over infinite periods of time from $t = -\infty$ to $t = \infty$.

Our other option is to try and interpret QED in terms of traditional notions such as *particle*. In quantum optics one views bare particles as surrounded by clouds of virtual particles, but if virtual particles are not real then neither are bare particles, and our task is to identify what the real physical objects are. In other words we must provide an ontology, which clearly and unambiguously links the mathematical objects of the theory with physical objects occurring in reality. A somewhat vague idea along these lines is that physical particles are bare particles dressed with their virtual clouds. With this idea in mind I have obtained results using different atom-field coupling models in different physical situations. This has revealed that while using dressed states in certain situations eliminates unphysical divergences, their use necessarily leads to such things as violations of Einstein causality. Of course, this is only really a problem if we assume dressed states must have the requisite localisation properties in order that questions regarding Einstein causality can be properly posed. Turning this around it appears that dressed (i.e. physical) particles, must be

delocalised to some extent, which in a quantum theory is not overly shocking.

The original Maxwell theory of electrodynamics retains many desirable properties, such as the causal propagation of electric and magnetic fields and simple energy-momentum continuity equations. Perhaps this explains why the Poincaré gauge has been so successful at the quantum level in the treatment of spontaneous emission, level shifts and energy transfer (including Van der Waals interactions). Even in the Maxwell theory there is still an ambiguity regarding the nature of the infinite longitudinal field and the associated self energy. This is solved at the classical level using extended charge distributions and mass renormalisation. It should be noted however, that a mathematically rigorous *quantum* theory of Maxwell's equations/QED, in the sense of constructive/algebraic quantum field theory, has not been achieved.

In simple quantum optical models the Maxwell fields are expressed in terms of photon creation and annihilation operators, and photons appear to be seen as more fundamental. Models in which the fundamental processes are the absorption and emission of photons invariably suffer from additional infinite (often transient) virtual contributions, and often sacrifice the causal aspect of the original theory described in terms of Maxwell fields. This is the case, for example, in the Glauber (1963) theory of photodetection. At least part of the problem here (a large part in my opinion) seems to have its roots in the strategy of starting with free (non-interacting) quantum theories and obtaining the interacting theory by simply joining the free theories together using the tensor product of Hilbert spaces. This not only leads to field theories that are mathematically dubious—QED being a prime example—but also leads to strange physical notions such as the notion of virtual particle, which often proves difficult to sustain. The problem is that interacting systems are viewed as nothing but free systems whose interaction is described by a term appearing explicitly in the Hamiltonian. Infinities occur because interactions uncontrollably create *free* particles out of *free* Fock vacua, and very few of these infinities can be removed by normal-ordering.

Contrary to the above view regarding quantum subsystems, we must recognise that a subsystem of a composite system *with interactions*, is not a *free* subsystem, and we must proceed to build theories consistent with this realisation. Although this may have been recognised in the context of quantum field theory (see for example Haag (1996)), the statement seems applicable quite generally. This suggests a re-evaluation of the standard rules of quantum mechanics, such as the use of the tensor product in constructing a composite system's state space.

Appendices

APPENDIX A

Basic algebraic structures

The aim of the appendices is to identify and review the various mathematical structures, which are used throughout the thesis. I have attempted to introduce the material in as intuitive a way as I am able, but cover only the bare minimum of topics required to make full sense of the content in the chapters. This first appendix concentrates mostly on algebraic structures. I begin by reviewing fundamental concepts in set theory and then review some useful ideas from category theory. I go on to introduce the basic structures ubiquitous in physics, starting with groups and vector spaces.

The material I present has been drawn from a handful of textbooks and so I refer the reader to the following for more detailed expositions. For introductory set theory see Hassani (1999) part **0**. For the use of categories in mathematical physics see Geroch (1985) chapter 2. For the basics of groups and vector spaces see Hassani (1999) parts **I**, **II** and **VII**, and for a view with an eye toward quantum theory see Isham (1995) chapters $1-3$, 5 and 7.

A.1 Sets

A set A is a collection of things called *elements*. An element a could be anything from a physicist in a pickle to an event in space-time. I use the standard notation $a \in A$ to mean "a belongs to A", and the symbols $\exists$ and $\forall$ to mean "there exists" and "for all" respectively. A set B is said to be a *subset* of a set A if $a \in B \Rightarrow a \in A$, in this case one writes $B \subset A$. The *intersection* of two sets A and B is denoted $A \cap B$ and is defined as the set of elements belonging to both A and B. The *union* of A and B is denoted $A \cup B$ and is defined as the set of elements belonging either to A or to B. Finally the *cartesian product* of A and B is denoted $A \times B$ and is defined as the set of all ordered pairs (a,b) with $a \in A$ and $b \in B$.

A.1.1 Equivalence

It is useful in set theory to have a notion of equivalence as a means by which elements can be organised into subsets based on a particular property. Such a notion is afforded by the following definition.

Definition A.1.1 *A relation $\triangleright$ on a set A is a comparison test on the cartesian product $A \times A$. If (a, a') passes the test one writes $a \triangleright a'$ meaning "a is related to a'". An equivalence relation is a relation satisfying the following three conditions.*

1. $a \triangleright a$, $\forall a \in A$ *(reflexivity),*
2. $a \triangleright a' \Rightarrow a' \triangleright a$, $\forall a, a' \in A$ *(symmetry),*
3. $a \triangleright a'$ *and* $a' \triangleright a'' \Rightarrow a \triangleright a''$, $\forall a, a', a'' \in A$ *(transitivity).*

The set of all $a' \in A$ equivalent to a is denoted $[[a]]$ and is called the equivalence class of a.

An equivalence relation can be used to define a useful set called the quotient set.

Definition A.1.2 *A collection $\{B_\alpha\}$ of subsets of a set A is said to be a partition of A if they are mutually disjoint and cover A i.e. $B_\alpha \cap B_\beta = \emptyset$ and $\bigcup_\alpha B_\alpha = A$, where $\emptyset$ denotes the empty set and $\alpha \neq \beta$. The collection $A/\triangleright := \{[[a]] : a \in A\}$ of all equivalence classes of elements of A is a partition of A called the quotient set of A under the relation $\triangleright$.*

A.1.2 Maps

A map $f : A \to B$ from a set A to a set B is an assignment of an element $a \in A$ to an element of B denoted $f(a)$. The subset of points in B mapped from A under f is denoted $f(A)$. The set of all points in A, which are mapped by f into $C \subset B$ is denoted $f^{-1}(C)$. Three important properties of maps are defined in the following.

Definition A.1.3 *A map $f : A \to B$ is said to be injective if $\forall a, a' \in A, f(a) = f(a') \Rightarrow a = a'$. A map $f : A \to B$ is said to be surjective if $f(A) = B$. If f is injective and surjective it is said to be bijective.*

For our purposes a map will be invertible if and only if it is bijective. The inverse of $f : A \to B$ is denoted $f^{-1} : B \to A$ and is such that $(f \circ f^{-1})(b) = b$ and $(f^{-1} \circ f)(a) = a$. Here $\circ$ denotes the composition of maps defined as $(g \circ f)(a) := g(f(a))$ with $f : A \to B$, $g : B \to C$ and $f \circ g : A \to C$.

The only structure a set really has is its number of elements, or its *cardinality*. Two sets have the same cardinality if and only if there exists a bijection mapping from one to the other. In other words bijections are the structure preserving maps in the category of sets. This leads us nicely into a discussion of...

A.2 Some basic concepts in category theory

A.2.1 The idea of a category

Category theory provides, among other things, a convenient way to organise different mathematical structures and to identify their relationships. It allows one to identify certain constructions like sums and products, which pop up in separate areas of maths as being the same idea applied in two different places. Of particular use is the categorical classification of maps, which in some sense allows one to identify what a map does without reference to the particular branch of maths under consideration.

A category consists of three things; a collection of elements called objects, a set of morphisms which are the maps between objects, and a rule $\circ$ called composition, which assigns to two morphisms $\psi : A \to B$ and $\phi : B \to C$, a morphism denoted $\phi \circ \psi : A \to C$ from A to C. We have already encountered the most elementary category, which is the category of sets. The objects of any other category are generally obtained by equipping sets with certain additional structure. For example, if one gives a set a closed binary multiplicative operation, for which there exists inverses and an identity, one obtains a *group*. If the multiplication is commutative the group is *Abelian*. Providing an Abelian group with a notion of scalar multiplication one obtains a set with linear structure i.e. a linear space or *vector space*. These structures are each algebraic in nature. The other (complimentary) type of structure is *topological* structure, which we will encounter in due course.

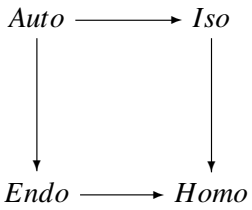
It is worth noting that there may be a great deal of overlap between any two categories. For example if one gives a vector space a certain kind of binary map called an *inner product* one obtains an *inner product space*. An inner product defines a *norm* on the vector space, so an inner product space is necessarily a *normed space*. A norm is simply a *metric* on a vector space and a *metric space* is necessarily a topological space with the *topology* induced by the metric. Thus, an inner product space is a topological space.

A.2.2 Morphisms

To conclude this section I have one thing left to do, and that is to examine the "structure preserving" morphisms in a category. We will see that such morphisms are of particular interest. Their classification is given in the following definition.

Definition A.2.1 *Let $\mathcal{O}$ and $\mathcal{O}'$ be any two objects in a category $\mathcal{C}$. A structure preserving map $\theta : \mathcal{O} \to \mathcal{O}'$ is called a homomorphism. When θ also happens to be a bijection, θ is said to be an isomorphism. When it happens that $\mathcal{O} = \mathcal{O}'$, then θ is said to be an endomorphism.*

If θ is both an isomorphism and an endomorphism it is said to be an automorphism.



The diagram illustrates the relationships between morphisms. The arrows are intended to signify inclusion.

As an example consider $(G,\cdot)$ and $(G',\star)$ in the category of groups. A group homomorphism $M : G \to G'$ is a map such that $\theta(g\cdot h) = \theta(g)\star\theta(h)$, $\forall g,h \in G$. Whether θ is an isomorphism, endomorphism or automorphism simply depends on whether θ is bijective, and/or whether the two groups are actually the same group. As I noted earlier often categories overlap with each other. As a result one must take care to identify the structure or structures with respect to which a morphism is a possible homomorphism. For example, it is quite possible that a morphism between topological groups preserves the topological structure, but isn't a group homomorphism.

There are important and useful examples in physics of each of the above types of morphism. *Linear operators* representing observables in quantum theory are the endomorphisms on vector spaces. The set of automorphisms on a vector space forms a group of transformations under composition, and nearly all of the groups in physics seem to be of this type. For example *unitary operators* used in quantum theory form the group of automorphisms on some inner product space.

The only morphisms I haven't really mentioned yet are the isomorphisms, which quite generally determine whether two separate objects can be identified. Roughly speaking isomorphic spaces can be thought of as abstractly "the same". I use the notation $\mathcal{O} \cong \mathcal{O}'$ to mean that the objects $\mathcal{O}$ and $\mathcal{O}'$ are isomorphic. A natural (or canonical) isomorphism is an isomorphism between spaces which is independent of any arbitrary choices. This could be for example, an isomorphism between vector spaces, which identifies elements in a way that is independent of any choice of bases for the spaces. The existence of a canonical isomorphism seems to signify that two spaces are really one and the same space, though this space might previously have been considered from two different points of view.

A.3 Groups and vector spaces

A.3.1 Basics

It seems that two of the most useful constructions in physics are groups and vector spaces.

Definition A.3.1 *A group is a set G together with a binary map $\cdot : G\times G \to G$ such that*

1. $g\cdot(g'\cdot g'') = (g\cdot g')\cdot g'' \quad \forall g,g',g'' \in G$,

2. $\exists e \in G \; s.t \; g \cdot e = e \cdot g = g \quad \forall g \in G$,

3. $\forall g \in G, \; \exists g^{-1} \in G \; s.t \; g \cdot g^{-1} = g^{-1} \cdot g = e$.

The element e is called the identity element and the element g^{-1} is called the inverse of the element g. If in addition to the above $g \cdot g' = g' \cdot g \; \forall g, g' \in G$, the group is said to be Abelian, in which case the map $\cdot$ is often written $+$ instead.

A vector space is obtained from an abelian group by equipping the set with a notion of linear scalar multiplication as follows.

Definition A.3.2 *A real (complex) vector space is an Abelian group $(V,+)$ for which the identity is usually denoted $\vec{0}$ and the inverse of $v \in V$ is usually denoted $-v \in V$. In addition it is equipped with a notion of real (complex) scalar multiplication defined by*

1. $\alpha(v+u) = \alpha v + \alpha u$,

2. $(\alpha+\beta)v = \alpha v + \beta v$,

3. $\alpha(\beta v) = (\alpha\beta)v$,

4. $0v = \vec{0}$ *and* $1v = v$,

$\forall u, v \in V$ *and* $\alpha, \beta \in \mathbb{R}(\mathbb{C})$. *A vector space with a binary multiplication map $\cdot : V \times V \to V$ is called an algebra.*

A variety of algebra, that pops up time and time again in physics is a *Lie Algebra*.

Definition A.3.3 *A Lie algebra consists of a vector space V together with a binary map $[\cdot,\cdot] : V \times V \to V$ called a Lie bracket, or commutator, such that*

1. $[v, \alpha u + \beta w] = \alpha[v,u] + \beta[v,w]$ *and* $[\alpha u + \beta w, v] = \alpha[u,v] + \beta[w,v]$,

2. $[v,v] = 0$,

3. $[v,[u,w]] + [w,[v,u]] + [u,[w,v]] = 0$ *(Jacobi identity),*

$\forall u, v, w \in V$ *and* $\alpha, \beta \in \mathbb{R}(\mathbb{C})$. *Points* 2 *and* 3 *above imply the commutator is antisymmetric* $[v,u] = -[u,v]$.

Maps on the cartesian product of vector spaces such as the commutator above are common. However, the cartesian product of vector spaces is not a vector space. This problem is rectified by defining the direct sum $V \oplus W$ of vector spaces V and W as the cartesian product $V \times W$ endowed with the natural vector space structure; $\alpha[(v,w) + (v',w')] = (\alpha[v+v'], \alpha[w+w'])$.

In practice, to specify a vector one chooses a *basis* for the vector space V. A set of N vectors $\{u_i\}_{i=1}^N \subset V$ is said to be *linearly dependent* if $\exists \alpha_1, ..., \alpha_N \in \mathbb{R}(\mathbb{C})$ such that

$$\sum_{i=1}^{N} \alpha_i u_i = \vec{0}, \tag{A.1}$$

otherwise they are said to be *linearly independent*. A vector space V is said to have dimension N if it contains a subset of N linearly independent vectors, but no subset of $N+1$ such vectors. A set of N linearly independent vectors in an N-dimensional vector space is called a *basis* of the vector space V. The elements u_i of the basis are said to *span* V. Any vector $v \in V$ can be written as a linear combination of basis elements;

$$v = \sum_{i=1}^{N} \alpha_i u_i. \tag{A.2}$$

Example A.3.1 *Every N-dimensional real (complex) vector space V is such that* $V \cong \mathbb{R}^n\,(\mathbb{C}^n)$, *where* $\mathbb{R}^n\,(\mathbb{C}^n)$ *denotes the set of all ordered n-tuples of real (complex) numbers. Thus, there is only really one finite-dimensional real (complex) vector space. Moreover as vector spaces we have* $\mathbb{C} \cong \mathbb{R}^2$, *so that an N-dimensional complex vector space can be viewed as a 2N-dimensional real vector space.*[1]

The dual space V^* of a real (complex) vector space V is the vector space of all maps $\psi : V \to \mathbb{R}\,(\mathbb{C})$, taking elements of V to its underlying field of numbers. Addition and scalar multiplication, which turn the set V^* into a vector space are defined in the obvious way. It happens that if $\dim V < \infty$ then $V \cong V^*$.

A.3.2 Inner product spaces

I have now covered most of the basics of vector spaces, but it seems that a bare vector space is often not enough to do any physics. A structure given to a vector space, which is of great importance is an inner product.

Definition A.3.4 *Let V be a complex vector space. A (positive definite) inner product on V is a map* $\langle\,,\,\rangle : V \times V \to \mathbb{C}$ *such that*

1. $\langle w, \alpha(v+u)\rangle = \alpha\langle w, v\rangle + \alpha\langle w, u\rangle$,
2. $\langle u, v\rangle = \langle v, u\rangle^*$,
3. $\langle v, v\rangle \geq 0$,

$\forall u, v, w \in V$ *and* $\alpha \in \mathbb{C}$. *A vector space with an inner product is called an inner product space. The map* $\|\cdot\| : V \to \mathbb{C}$ *defined by* $\|v\| := \langle v, v\rangle$ *is called the norm induced by the inner product. If two vectors* $v, u \in V$ *are such that* $\langle v, u\rangle = 0$ *they are said to be orthogonal and a basis* $\{u_i\}$ *such that* $\langle u_i, u_j\rangle = 0\ \forall i \neq j$ *is called an orthogonal basis. A vector* $v \in V$ *such that* $\|v\| = 1$ *is said to be normalised (to one), and a basis* $\{u_i\}$ *such that* $\langle u_i, u_j\rangle = \delta_{ij}$ *where* $\delta_{ii} = 1$ *and* $\delta_{ij} = 0$ *if* $i \neq j$, *is called an orthonormal basis.*

[1] It is important to recognise that $\mathbb{C}$ and $\mathbb{R}^2$ are only isomorphic as vector spaces, and not as fields of numbers. There is no natural multiplication of elements in the plane as there is for complex numbers. This is an example of an incidence when the warning I gave in section A.2.1 must be heeded.

In quantum mechanics one talks about Hilbert spaces rather than ordinary inner product spaces. A Hilbert space $\mathcal{H}$ is simply a complete inner product space, with completeness meaning that every Cauchy sequence converges (with respect to the norm) to a point inside the space. An infinite dimensional Hilbert space is said to be separable if it has a countably infinite dimension i.e. the indexing set $\{i\}$ of the basis $\{u_i\}$ has the same cardinality as the natural numbers $\mathbb{N}$. Every real (complex) separable Hilbert space is isomorphic to the space l^2 of square summable real (complex) sequences $\langle x_n \rangle$. A sequence is square summable if

$$\sum_{n=1}^{\infty} |x_n|^2 \leq \infty. \tag{A.3}$$

Example A.3.2 *The Hilbert space $L^2(\mathbb{R}^n)$, which is the space of all square integrable functions $\psi : \mathbb{R}^n \to \mathbb{C}$, is separable. A function ψ is said to be square integrable if*

$$\int_{-\infty}^{\infty} |\psi(x_1, ..., x_n)|^2 d^n x \leq \infty. \tag{A.4}$$

In quantum theory one often uses an alternative notation called Dirac notation. In Dirac notation the vector v is denoted $|v\rangle$, which is called a ket, and one uses $\langle u|v\rangle \equiv \langle u, v\rangle$ to denote the inner product. The so-called bra $\langle u|$ can be identified as an element of the dual space V^*, which maps a ket $|v\rangle$ to the value $\langle u, v\rangle \in \mathbb{C}$. In general infinite-dimensional vector spaces there may be many more bras than kets, but in a Hilbert space it turns out that they are in one-to-one correspondence.

A.3.3 Linear operators

Having defined the inner product we have almost everything needed to do some quantum physics stuff. The final ingredient is given by the maps on V preserving its structure. These are the endomorphisms, which in this context are called (linear) operators.

Definition A.3.5 *A linear operator (linear endomorphism or sometimes linear map) on a real (complex) vector space V is a map $L : V \to V$ such that*

1. $L(\alpha v + \beta u) = \alpha L(v) + \beta L(u)$

$\forall u, v \in V$ and $\alpha, \beta \in \mathbb{R}(\mathbb{C})$. For operators the standard map notation $A(v)$ is usually replaced by Av. The sum $A + B$ of operators A and B is itself an operator defined by $(A+B)v = Av + Bv$, and the product AB of A and B is an operator defined by $(AB)v = A(Bv)$.

Example A.3.3 *The space of all operators on a real (complex) vector space V is a real (complex) vector space denoted $\mathcal{L}(V)$. If $\dim V = n$ then $\dim \mathcal{L}(V) = n^2$ and since $V \cong$*

$\mathbb{R}^n\,(\mathbb{C}^n)$ *we have*

$$\mathcal{L}(V) \cong M(n,\mathbb{R})\,(M(n,\mathbb{C})) := \mathcal{L}(\mathbb{R}^n)\,(\mathcal{L}(\mathbb{C}^n)) \cong \mathbb{R}^{n^2}\,(\mathbb{C}^{n^2}) \tag{A.5}$$

where $M(n,\mathbb{R})\,(M(n,\mathbb{C}))$ *denotes the set of all real (complex)* $n \times n$ *matrices.*

An operator $A \in \mathcal{L}(\mathcal{H})$ has *eigenvector* $|a\rangle$ with *eigenvalue* a if

$$A|a\rangle = a|a\rangle. \tag{A.6}$$

An eigenvalue a_n is said to be d-fold degenerate if there exist d linearly independent eigenvectors $|a_n\rangle$ with the same eigenvalue a_n. The set of matrix elements of A is the set of numbers $\langle\psi, A\phi\rangle \equiv \langle\psi|A|\phi\rangle \in \mathbb{C}$. In particular, the matrix elements of A with respect to some orthonormal basis $\{e_i\} \equiv \{|i\rangle\}$ are the numbers $A_{ij} := \langle e_i, Ae_j\rangle \equiv \langle i|A|j\rangle$. The adjoint $A^\dagger$ of an operator A is defined by the condition

$$\langle\psi, A^\dagger\phi\rangle = \langle A\psi, \phi\rangle, \tag{A.7}$$

or in Dirac notation

$$\langle\psi|A^\dagger|\phi\rangle = \langle\psi|A|\phi\rangle^*. \tag{A.8}$$

I now give the definitions of three especially important types of operator.

Definition A.3.6 *An operator is said to be self-adjoint or Hermitian if*[2]

$$A = A^\dagger. \tag{A.9}$$

An operator A *is said to be anti-Hermitian if* $A^\dagger = -A$. *A result of the utmost importance in quantum theory is the spectral theorem for self-adjoint operators, which states that the eigenvalues of the self-adjoint operators are real numbers, and that the eigenvectors corresponding to distinct eigenvalues are orthonormal. Thus, the eigenvectors of self-adjoint operators often form orthonormal bases for a Hilbert space* $\mathcal{H}$.

Definition A.3.7 *Let* V *be an inner product space. An operator* $U : V \to V$ *is said to be unitary if it is invertible and*

$$\langle U\psi, U\phi\rangle \equiv \langle\psi|U^\dagger U|\phi\rangle = \langle\psi|\phi\rangle. \tag{A.10}$$

$\forall\psi,\phi \in V$. *The space of all unitary operators on* V *is denoted* $U(V)$ *and constitutes the set of automorphisms on* V *as an inner product space. The eigenvalues of a unitary operator*

[2] There is a subtle difference between what is meant by self-adjoint and Hermitian (see Reed & Simon (1975)), but I'm going to ignore this.

are complex numbers with absolute value 1. *Note that the definition above is equivalent to the requirement* $U^\dagger U = I$, *or* $U^{-1} = U^\dagger$.

Definition A.3.8 *A projection operator is any self-adjoint operator P such that*

$$P^2 = P. \tag{A.11}$$

Given a vector $|\psi\rangle$ we can write the projection operator onto the state $|\psi\rangle$ as $|\psi\rangle\langle\psi|$ such that $(|\psi\rangle\langle\psi|)|\phi\rangle := \langle\psi|\phi\rangle|\psi\rangle$. In particular the projection onto some orthonormal basis vector $|i\rangle$ is $|i\rangle\langle i|$. Now any $\psi \in \mathcal{H}$ can be written $\psi = \sum_i \alpha_i e_i$ or equivalently $|\psi\rangle = \sum_i \alpha_i |i\rangle$. Taking the inner product of both sides of this expression with $e_j \equiv |j\rangle$ gives $\langle j|\psi\rangle = \alpha_j$, because the $e_i \equiv |i\rangle$ are orthonormal. Thus we have $|\psi\rangle = \sum_i \langle i|\psi\rangle|i\rangle$, which can be viewed as the vector $|\psi\rangle$ multiplied by a *resolution of the identity*

$$I = \sum_i |i\rangle\langle i|. \tag{A.12}$$

One can use this to express an operator A with respect to a particular basis $\{|i\rangle\}$;

$$A = \sum_i |i\rangle\langle i|A\sum_j |j\rangle\langle j| = \sum_{ij} A_{ij}|i\rangle\langle j|. \tag{A.13}$$

If in particular the vectors $\{|i\rangle\}$ are eigenvectors of A with non-degenerate eigenvalues $\{a_i\}$, (A.13) becomes

$$A = \sum_i a_i |i\rangle\langle i|, \tag{A.14}$$

and this result is easily extended to the case of d-fold degenerate eigenvalues. The result (A.14) motivates the following definition

Definition A.3.9 *Let* $f : \mathbb{R}(\mathbb{C}) \to \mathbb{R}(\mathbb{C})$ *be some function, let V be a real (complex) vector space, and let* $A \in \mathcal{L}(V)$ *be an operator with non-degenerate eigenvalues* a_i *and corresponding eigenvectors* $|i\rangle$. *We define the function* $f : A \to f(A) \in \mathcal{L}(V)$ *of operator A, by*

$$f(A) := \sum_i f(a_i)|i\rangle\langle i|. \tag{A.15}$$

Again this result is easily extended to the case of degenerate eigenvalues.

Example A.3.4 *If* $A \in \mathcal{L}(V)$ *is self-adjoint then*

$$U := e^{iA} = \sum_i e^{ia_i}|i\rangle\langle i| \tag{A.16}$$

is unitary.

An extremely useful combinatorial formula involving a similarity transformation of an operator B by the exponential of an operator A is the *Baker-Campbell-Hausdorff formula*

$$e^A B e^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \frac{1}{3!}[A,[A,[A,B]]] + \ldots = \sum \frac{[[A]^n,B]}{n!} \tag{A.17}$$

where $[[A]^n,B]$ denotes the n-times nested commutator of A with B. The formula is quite general and works in infinite dimensions. When the commutator $[A,B]$ is central (proportional to the identity), like for example, the canonical commutation relation $[x^i,p_j] = \delta^i_j$, the series on the right-hand-side in A.17 terminates after the second term.

A.3.4 Operators with continuous spectrum

So far the assumption regarding the orthonormal basis $\{|i\rangle\}$ is that the label i is discrete. Quantum theories like wave mechanics use operators like the position operator $\hat{x}$ which have continuous spectrum. Strictly speaking, for an operator A with continuous spectrum there are no eigenvectors $|a\rangle$ corresponding to a single eigenvalue. However with due care it seems the rules for the discrete case can be extended to the continuous case, which ultimately justifies the heuristic formalism laid out by Dirac, in which one assumes that a relation $A|a\rangle = a|a\rangle$ *does*, in some sense, exist. The projection onto the eigenvalue a is then written $|a\rangle\langle a|da$. The orthonormality condition $\langle i|j\rangle = \delta_{ij}$ becomes $\langle a|b\rangle = \delta(a-b)$ where the Dirac delta function is defined for a given $f : \mathbb{R}(\mathbb{C}) \to \mathbb{R}(\mathbb{C})$, by

$$f(b) = \int da\, \delta(a-b) f(a) \tag{A.18}$$

whenever b is within the range of integration, otherwise the integral evaluates to 0.[3] Any vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \int da\, \psi(a)|a\rangle, \tag{A.19}$$

and the function of an operator A can be written

$$f(A) := \int da\, f(a)|a\rangle\langle a|. \tag{A.20}$$

Finally, any other operator $B \in \mathcal{L}(\mathcal{H})$ can be written in the eigenbasis of A as

$$B = \int da \int da'\, \langle a|B|a'\rangle |a\rangle\langle a'|. \tag{A.21}$$

A.3.5 Group action

So far I have talked mostly about vector spaces, but I began this section with the definition of a group. The *action* of groups on vector spaces seems to play a large role in most of

[3] As the definition clearly shows the so-called delta *function* is in fact a *measure*.

modern physics. Group action on a set is defined as follows.

Definition A.3.10 *Let G be a group with multiplication simply written gg', and let S be a set. A left action of G on S is a map $\Phi : G \times S \to S$ such that*

1. $\Phi(e,s) = s$,
2. $\Phi(g,\Phi(g',s)) = \Phi(gg',s)$,

$\forall g,g' \in G$ and $\forall s \in S$. Often the group action $\Phi(g,s)$ is written simply $g \cdot s$. A right action of G on S can be defined analogously.

The set S could be more than just a set. It might be a vector space or even G itself. In fact group multiplication *is* just the action of G on itself. In physical applications S is most often a vector space. A *representation* of G on V can be viewed as a collection of operators $T_g : V \to V$ defined by $T_g(v) := \Phi(g,v)$ for some action Φ.[4]

It will be useful to identify some particular types of group action. For example, an action is said to be free if the only element $g \in G$ such that $g \cdot s = s$ for any $s \in S$ is the identity e. A Particularly useful concept is the *orbit* of an element $s \in S$ due to the action.

Definition A.3.11 *The orbit of $s \in S$ is the set $\mathcal{O}_s$ defined by*

$$\mathcal{O}_s := \{s' \in S : \exists g \in G \; s.t \; g \cdot s = s'\}. \tag{A.22}$$

In other words the orbit of s consists of all the points in S that can be obtained by acting on s with G.

The action is called transitive if $\mathcal{O}_s = S$ for any $s \in S$ i.e., if any element of S can be obtained from some other element via the action of G on S. It is easy to verify that belonging to the same orbit $\mathcal{O}_s \subset S$ is an equivalence relation $\triangleright$ on S, and that the orbits are equivalence classes. One can therefore construct the quotient set under the equivalence relation $\triangleright$ as the collection of orbits; $S/\triangleright := \{\mathcal{O}_s : s \in S\}$.

A good deal of the useful actions of groups on a vector space V are by subgroups of the general linear group $GL(V)$.

Definition A.3.12 *The general linear group $GL(V) \subset \mathcal{L}(V)$ of a vector space V is the set of all invertible operators in $\mathcal{L}(V)$. For an n-dimensional real (complex) vector space $GL(V) \cong GL(\mathbb{R}^n)\,(GL(\mathbb{C}^n)) =: GL(n,\mathbb{R})\,(GL(n,\mathbb{C}))$.*

A subgroup of a group is a subset, that happens to be a group in its own right. The special linear group $SL(n,\mathbb{R})\,(SL(n,\mathbb{C}))$ is a subgroup of the general linear group consisting of matrices with determinant one. The orthogonal group $O(n) \equiv O(n,\mathbb{R}) \subset GL(n,\mathbb{R})$ is the group of orthogonal matrices i.e. matrices O such that $O^T = O^{-1}$ with the superscript ^{T}

[4] A representation T of G on V is in fact a group homomorphism $T : G \to GL(V)$ where $GL(V)$ is the general linear group on V. A group action on V defines a representation via $T_g(v) = \Phi(g,v)$.

denoting the matrix transpose. The unitary group $U(n) \equiv U(n,\mathbb{C}) \subset GL(n,\mathbb{C})$ is the set of all unitary matrices i.e. matrices U such that $U^\dagger = U^{-1}$, where the † denotes the adjoint (conjugate transpose, cf. A.3.3). One can show that the intersection of two subgroups is necessarily a subgroup. The special orthogonal and special unitary groups are defined as $SO(n) := SL(n,\mathbb{R}) \cap O(n)$, which consists of orthogonal matrices with determinant one, and $SU(n) := SL(n,\mathbb{C}) \cap U(n)$, which consists of unitary matrices with determinant one.

A.3.6 The tensor product of spaces

To describe composite quantum systems the *tensor product* is used. The full definition of the tensor product is quite involved, so I will just list its important properties. The tensor product of an n-dimensional vector spaces V and an m-dimensional vector space W is an nm-dimensional vector space denoted $V \otimes W$. The tensor product operation is linear in each slot, i.e.

$$(\alpha\psi + \beta\phi) \otimes \varphi = \alpha\psi \otimes \varphi + \beta\phi \otimes \varphi, \qquad \psi \otimes (\alpha\varphi + \beta\theta) = \alpha\psi \otimes \varphi + \beta\psi \otimes \theta \quad \text{(A.23)}$$

$\forall \psi, \phi \in V$, $\forall \varphi, \theta \in W$ and $\forall \alpha, \beta \in \mathbb{R}(\mathbb{C})$. If the vectors $e_i \equiv |i\rangle$ form a basis of V and the vectors $\varepsilon_\mu \equiv |\mu\rangle$ form a basis for W then $e_i \otimes \varepsilon_\mu \equiv |i\rangle \otimes |\mu\rangle$ is a basis vector in $V \otimes W$. Thus any vector $\psi \equiv |\psi\rangle \in V \otimes W$ can be written

$$|\psi\rangle = \sum_i^n \sum_\mu^m \psi_{i\mu} |i\rangle \otimes |\mu\rangle. \quad \text{(A.24)}$$

If V and W have inner products $\langle\cdot,\cdot\rangle_V$ and $\langle\cdot,\cdot\rangle_W$ then an inner product on $V \otimes W$ is naturally defined by

$$\langle \psi \otimes \phi, \varphi \otimes \theta \rangle := \langle \psi, \varphi \rangle_V \langle \phi, \theta \rangle_W. \quad \text{(A.25)}$$

If $A \in \mathcal{L}(V)$ and $B \in \mathcal{L}(W)$ then $A \otimes B \in \mathcal{L}(V \otimes W)$ is defined by

$$A \otimes B |\psi\rangle \otimes |\varphi\rangle := A|\psi\rangle \otimes B|\varphi\rangle. \quad \text{(A.26)}$$

With due care these results can be extended to the case of infinite-dimensional spaces and operators with continuous spectrum.

The type of space used in quantum field theory is called a *Fock space*. Fock spaces are built out of some "single particle" vector space V, using the tensor product and the direct sum operations. The so-called vacuum state belongs to $\mathbb{C}$. One adds to the vacuum space the single particle space V using the direct sum; $\mathbb{C} \oplus V$. To this one adds the "two particle space" $V \otimes V$. One continues in this way to obtain a space accommodating an arbitrary number of particles. To make the space usable one must take into account particle indistinguishability. This depends on the species of particle to be described, because different particles obey different statistics. The *bosonic* Fock space $\mathcal{F}_B(V)$ is obtained by symmetrising

(via isomorphism) the elements of each n-particle space. For example, $\psi \otimes \varphi \in V \otimes V$ goes to $\frac{1}{2}(\psi \otimes \varphi + \varphi \otimes \psi)$. The *fermionic* Fock space $\mathcal{F}_F(V)$ is obtained by anti-symmetrising each n-particle vector, so for example $\psi \otimes \varphi \in V \otimes V$ goes to $\frac{1}{2}(\psi \otimes \varphi - \varphi \otimes \psi)$.

In applications the single particle space V is usually a function space like $L^2(\mathbb{R}^3, \mathbb{C}^n)$. The value of the integer n depends on the field being described. For example $n = 1$ for a scaler field, $n = 2$ for a photon field, and $n = 4$ for a Dirac spinor field. Assuming for simplicity that $n = 1$ and considering the bosonic Fock space $\mathcal{F}_B$ one defines the inner product as

$$\langle \Phi, \Psi \rangle := \sum_{m=1}^{\infty} \int \prod_{i=1}^{m} d^3 k_i \, \phi^{(m)}(\mathbf{k}_1, ..., \mathbf{k}_m)^* \psi^{(m)}(\mathbf{k}_1, ..., \mathbf{k}_m). \tag{A.27}$$

The states $\Phi, \Psi \in \mathcal{F}_B$ are viewed as infinite sequences $\left(\phi^{(m)}\right)_{m=1}^{\infty}, \left(\psi^{(m)}\right)_{m=1}^{\infty}$ of the $\phi^{(m)}, \psi^{(m)} \in S_m[\bigotimes_{i=1}^{m} L^2(\mathbb{R}^3)]$, in which S_m denotes the symmetric subspace. In Dirac notation we can write a state with sharp momentum as $|\mathbf{k}_1, ..., \mathbf{k}_m\rangle$ and express the orthonormality of momentum basis states via

$$\langle \mathbf{k}_1, ..., \mathbf{k}_m | \mathbf{k}'_1, ..., \mathbf{k}'_{m'} \rangle = \mathcal{N} \delta_{mm'} \sum_{P} \delta(\mathbf{k}_1 - \mathbf{k}'_{P(1)}), ..., \delta(\mathbf{k}_m - \mathbf{k}'_{P(m')}). \tag{A.28}$$

The sum is over permutations of the integers $1, ..., m$. The constant $\mathcal{N}$ is a normalisation dependent on the number of the $\{\mathbf{k}_i\}$ and $\{\mathbf{k}'_i\}$ that are equal. For example, $\mathcal{N} = n!$ if this number is n.

One can define operators on $\mathcal{F}_B$, that create and destroy particles with particular momenta. The *creation* and *annihilation* operators, which are in fact operator valued measures, are defined by

$$\begin{aligned} a^\dagger(\mathbf{k}) \psi^{(m)}(\mathbf{k}_1, ..., \mathbf{k}_n) &= \sqrt{m+1} \, \psi^{(m)}(\mathbf{k}, \mathbf{k}_1, ..., \mathbf{k}_m) \\ a(\mathbf{k}) \psi^{(m)}(\mathbf{k}_1, ..., \mathbf{k}_m) &= \sqrt{m} \sum_{i=1}^{m} \delta(\mathbf{k} - \mathbf{k}_i) \psi^{(m)}(\mathbf{k}, \mathbf{k}_1, ..., \mathbf{k}_{i-1}, \mathbf{k}_{i+1}, ..., \mathbf{k}_m) \end{aligned} \tag{A.29}$$

where as before $\psi^{(m)}(\mathbf{k}_1, ..., \mathbf{k}_m)$ belongs to the m-particle (symmetric) subspace. In Dirac notation these definitions can be taken as applying to the momentum basis states and written

$$\begin{aligned} a^\dagger(\mathbf{k}) |\mathbf{k}_1, ..., \mathbf{k}_m\rangle &= \sqrt{m+1} |\mathbf{k}, \mathbf{k}_1, ..., \mathbf{k}_m\rangle \\ a(\mathbf{k}) |\mathbf{k}_1, ..., \mathbf{k}_m\rangle &= \sqrt{m} \sum_{i=1}^{n} \delta_(\mathbf{k} - \mathbf{k}_i) |\mathbf{k}_1, ..., \mathbf{k}_{i-1}, \mathbf{k}_{i+1}, ..., \mathbf{k}_m\rangle. \end{aligned} \tag{A.30}$$

The bosonic creation and annihilation operators obey the commutation relation

$$[a^\dagger(\mathbf{k}), a(\mathbf{k}')] = \delta(\mathbf{k} - \mathbf{k}'), \tag{A.31}$$

while in the fermionic case the commutator above must be replaced with the anti-commutator

to be consistent with the statistics fermions obey.

Supposing now that the momenta of a particle can only take discrete values, because the particles have been confined to a box with periodic boundary conditions, then we can label particle states differently. From the new point of view the notation $\mathbf{k}_i$ is intended to label the allowed values of momentum. The slots in the kets are taken to refer to these different values rather than to different particles. Conversely the labels in the slots denote the number of particles with the momentum value assigned to the slot. This is the *occupation number* representation of states, in terms of which the action of the creation and annihilation operators satisfy

$$\begin{aligned} a^\dagger_{\mathbf{k}_i}|n_1,...,n_m\rangle &= \sqrt{n_i+1}|n_1,...,n_i+1,...\rangle \\ a_{\mathbf{k}_i}|n_1,...,n_m\rangle &= \sqrt{n_i}|n_1,...,n_i-1,...\rangle, \end{aligned} \tag{A.32}$$

and the commutator A.31 can be written

$$[a^\dagger_{\mathbf{k}}, a_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}. \tag{A.33}$$

The orthonormality condition A.28 in the occupation number representation, takes the simple form

$$\langle n_1, n_2, ...|n'_1, n'_2, ...\rangle = \delta_{n_1 n'_1}\delta_{n_2 n'_2}.... \tag{A.34}$$

The construction above formally resembles the representation of a collection of harmonic oscillators with different frequencies. The number in each slot in the ket represents the number of oscillators with a particular frequency.

A.3.7 Tensors

Given a real vector space V an element ω of the dual V^* maps $v \in V$ to $\mathbb{R}$. Equally, we can view $v \in V$ as a map $\omega : V^* \to \mathbb{R}$ defined by

$$v(\omega) := \omega(v). \tag{A.35}$$

The tensor product of two dual vectors $\omega, \eta \in V^*$ denoted $\omega \otimes \eta$ is a map $\omega \otimes \eta : V \times V \to \mathbb{R}$. Similarly, the tensor product of two vectors $v, u \in V$ is denoted $v \otimes w$ and can be viewed as a map $v \otimes u : V^* \times V^* \to \mathbb{R}$. More generally, one can construct mixed maps such as $\omega \otimes v : V \times V^* \to \mathbb{R}$, and express them in terms of the bases $\{e_i\}$ and $\{\varepsilon^i\}$ for V and V^* respectively. To do this a most useful notational idea due to Einstein is used. Using the *Einstein summation convention* repeated indices, one upper and one lower, are implicitly assumed to be summed over. For example within the Einstein convention $e_i \otimes \varepsilon^i$ means $\sum_i e_i \otimes \varepsilon^i$. The basis $\{\varepsilon^i\} \subset V^*$ is said to be dual to the basis $\{e_i\} \subset V$ if $\varepsilon^i(e_j) \equiv e_j(\varepsilon^i) = \delta^i_j$ where δ^i_j equals 1 if $i = j$ and 0 otherwise.

Tensors are multilinear maps that take vectors and dual vectors to an underlying field of numbers.

Definition A.3.13 *Let V be a finite-dimensional real vector space, and let the r-times cartesian product of V with itself be denoted V^r. A real type $\binom{r}{s}$-tensor is a map $A : V^r \times V^{*s} \to \mathbb{R}$, which is linear with respect to each of its arguments. If $\{e_i\}$ is a basis in V and $\{\varepsilon^j\}$ is the dual basis in V^*, then within the Einstein summation convention any type $\binom{r}{s}$-tensor A can be written $A^{i_1\ldots i_r}_{j_1\ldots j_s} e_{i_1} \otimes \ldots \otimes e_{i_r} \otimes \varepsilon^{j_1} \otimes \ldots \otimes \varepsilon^{j_s}$ where $A^{j_1\ldots j_s}_{i_1\ldots i_r} \in \mathbb{R}$ are the components of A with respect to the bases $\{e_i\}$ and $\{\varepsilon^j\}$.*

The space of all $\binom{1}{0}$-tensors is V, the space of all $\binom{0}{1}$-tensors is V^*, and the space of all $\binom{1}{1}$-tensors is $T^1_1(V) \cong \mathcal{L}(V) \cong \mathcal{L}(V^*)$. The tensor product of an $\binom{r}{s}$-tensor and a $\binom{p}{q}$-tensor is an $\binom{r+p}{s+q}$-tensor. Thus, the space of all tensors together with the tensor product is an algebra called *the algebra of tensors*.

If swapping the indices in the components of a tensor leaves their values unchanged the tensor is called *symmetric*.

Definition A.3.14 *Let V be a finite-dimensional real vector space. The symmetric product of dual vectors $\omega, \eta \in V^*$ is a symmetric $\binom{0}{2}$-tensor defined as*

$$\omega\eta := \frac{1}{2}(\omega \otimes \eta + \eta \otimes \omega). \tag{A.36}$$

Any symmetric $\binom{0}{2}$-tensor g can be written $g = g_{ij}\varepsilon^i\varepsilon^j$ where $\{\varepsilon^j\}$ is a basis in V^*. If g is invertible it is called an inner product. A basis $\{e_i\} \subset V$ is said to be g-orthonormal *if $g(e_i, e_i) = 0, \pm 1$ and $g(e_i, e_j) = 0$ if $i \neq j$.*

By feeding an inner product g only one vector, we can view it as a map $g : V \to V^*$ such that

$$g(v) = g_{ij}\varepsilon^i\varepsilon^j(v^k e_k) = g_{ik}v^k\varepsilon^i =: v_i\varepsilon^i \in V^* \tag{A.37}$$

where I have defined $v_i := g_{ik}v^k$. The inverse of g is a map $g^{-1} : V^* \to V$ with components $(g^{-1})^{ij}$ such that $v^j = (g^{-1})^{ij}v_i$. In practice one usually omits the $^{-1}$ and simply writes $v^j = g^{ij}v_i$.

Example A.3.5 *The inner product space $E^{1,3}$ consisting of $\mathbb{R}^4$ together with the inner product $g : \mathbb{R}^4 \times \mathbb{R}^4 \to \mathbb{R}$ defined by*

$$g(x, x') := x^0x'^0 - x^1x'^1 - x^2x'^2 - x^3x'^3 \tag{A.38}$$

is called Minkowski space-time. It is easy to show that $x^0 = x_0$ and $x^i = -x_i$ for $i = 1, 2, 3$. The group of matrices Λ for which $g(\Lambda x, \Lambda x') = g(x, x')$ can be viewed as a generalisation of the orthogonal group $O(4)$ called the Lorentz group, and is denoted $O(1, 3)$. The

generalisation of this construction to any real $n = r + s$-dimensional vector space V is straightforward;

$$g(v,u) = v^1u^1 + ... + v^ru^r - v^{r+1}u^{r+1} - ... - v^{r+s}u^{r+s}. \tag{A.39}$$

The components of the bilinear form $g : V \times V \to \mathbb{R}$ above can be arranged in a matrix $\eta := diag(-1,...,-1,1,...,1)$ in which there are r lots of -1 and s lots of $+1$. It is easy to show that the matrices Λ belonging to $O(r,s)$ are those which satisfy $\Lambda^T\eta\Lambda = \eta$. It follows by taking the determinant of both sides that such matrices must satisfy $(det\Lambda)^2 = 1$, so that $det\Lambda = \pm 1$. The associated special group $SO(r,s)$ is the subgroup of matrices in $O(r,s)$ with unit determinant.

If swapping the indices in the component of a tensor multiplies its value by -1 then the tensor is called *anti-symmetric*.

Definition A.3.15 *Let V be a finite-dimensional real vector space. The anti-symmetric (or wedge) product of dual vectors $\omega, \eta \in V^*$ is an anti-symmetric $\binom{0}{2}$-tensor called a 2-form defined as*

$$\omega \wedge \eta := \omega \otimes \eta - \eta \otimes \omega. \tag{A.40}$$

Any 2-form g can be written $g = \frac{1}{2}g_{ij}\varepsilon^i \wedge \varepsilon^j$ where $\{\varepsilon^j\}$ is a basis in V^*. We can extend this idea to anti-symmetric type $\binom{0}{p}$-tensors, which are called p-forms. The space of all p-forms on V is denoted Λ^pV. Any p-form $\omega \in \Lambda^pV$ can be written

$$\omega = \frac{1}{p!}\omega_{i_1...i_p}\varepsilon^{i_1} \wedge ... \wedge \varepsilon^{i_p}. \tag{A.41}$$

Thus, $\{\varepsilon^{i_1} \wedge ... \wedge \varepsilon^{i_p}\}$ is a basis in Λ^pV.

Example A.3.6 *A two-form ω on a vector space V is said to be non-degenerate if $\forall v \in V$ $g(v,v') = 0 \Rightarrow v' = \vec{0}$. A non-degenerate two-form is called a symplectic form, and a vector space V together with a symplectic form is called a symplectic vector space.*

Symplectic spaces necessarily have even dimension. The matrix elements of a symplectic form with respect to a basis $\{e_i\} \subset V$ are defined by $\omega_{ij} := \omega(e_i, e_j)$. A famous result known as Darboux's theorem states that for a $2n$-dimensional symplectic space (V,ω) there exists a so-called canonical basis $\{(e_i, f_i)\} \subset V$, $i = 1,...,n$, with dual basis $\{(\varepsilon^i, \mu^i)\} \subset V^*$ such that

$$\omega = \sum_{i=1}^{n} \varepsilon^i \wedge \mu^i. \tag{A.42}$$

The matrix of ω with respect to the canonical basis has the form

$$(\omega_{ij}) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{A.43}$$

where I denotes the $n \times n$ identity matrix.

APPENDIX B

Differential geometry

This appendix is devoted to differential geometry including brief reviews of tensor analysis, Lie groups and fibre bundles. As in A the material I present has been drawn from a handful of textbooks. Two excellent books on differential geometry in physics are Fecko (2011) and Frankel (2011). For introductory tensor algebra, tensor analysis on manifolds and Lie group theory see Hassani (1999) part **VII** and **VIII**, chapters 27 and 28, Fecko (2011) chapters $1-6$, $10-14$ and $16-18$, Frankel (2011) part **I**, and finally Isham (1999) chapters $1-4$. For applications in mechanics and field theory see Marsden & Ratiu (2003) chapters 2 and 3. For an introduction to fibre bundles see Fecko (2011) chapters $19-21$, Frankel (2011) part **III**, Isham (1999) chapters 5 and 6, and for concrete applications in physics see Chruscinski & Jamiolkowski (2004) chapter 1.

B.1 Tensor Analysis

Usually in physics we are not merely interested in "static" vectors, but wish to know how objects change in space and time. The setting for such a description is a (smooth) *manifold*, which marries algebraic and topological structure. Manifolds are extremely rich structures supporting a vast number of useful constructions.

B.1.1 Manifolds

Loosely speaking an m-dimensional manifold is a topological space, which locally looks like $\mathbb{R}^m$, a flat m-dimensional vector space. There are some caveats in the definition of a manifold, which I will not touch on. I will give an adequate definition for our purposes, but first we must recall the definition of a topological space.

Definition B.1.1 *A topological space is a set X with a topology τ. A topology is a collection of subsets $U \subset X$ called open sets, such that*

1. *$X \in \tau$ and $\emptyset \in \tau$,*
2. *The union of two open sets is open,*
3. *The intersection of a finite number of open sets is open.*

A chart on a topological space M is a pair (U, ψ), where $\psi : U \to \mathbb{R}^m$ and U is an open set. Sometimes one refers to the map ψ alone as a chart. Each chart defines a set of coordinates $x^i : U \to \mathbb{R}$ on U such that $\psi(P) = (x^1(P), ..., x^m(P))$. We say that two charts (U, ψ) and (V, φ) have smooth structure if the map $\varphi \circ \psi^{-1} : \mathbb{R}^m \to \mathbb{R}^m$ is smooth (infinitely continuously differentiable).[5] In other words, if y^i are coordinates on V and x^i are coordinates on U then the $y^i(x^1, ..., x^m)$ are required to be smooth functions of the x^i. An atlas is a collection $\{(U_\alpha, \psi_\alpha)\}$, of such charts, which cover M i.e. they are such that $\bigcup_\alpha U_\alpha = M$. The topological space M together with such an atlas is a (smooth) manifold.

The useful maps on manifolds are the ones compatible with the smooth structure.

Definition B.1.2 *Let N and M be manifolds with dimension n and m respectively. A map $\phi : M \to N$ is said to be smooth if its coordinate representation $\varphi \circ \phi \circ \psi^{-1} : \mathbb{R}^m \to \mathbb{R}^n$ with respect to charts ψ and φ on M and N respectively, is smooth. A smooth bijective map $\phi : U \subset M \to \phi(U)$ with smooth inverse is called a local diffeomorphism. If $U = M$ then $\phi(U) = N$ and ϕ is called a diffeomorphism. Diffeomorphisms are the isomorphisms in the category of (smooth) manifolds.*

A submanifold is a subset U which is a manifold in its own right. A submanifold of M can be obtained simply by taking an open set U and restricting all of the charts on M to U. It seems we do not really lose any generality by defining maps globally on manifolds, because their local counterparts will just be their restriction to a submanifold.

Example B.1.1 *A function on a manifold M is a smooth map $f : M \to \mathbb{R}$, in other words a map such that $f \circ \psi^{-1}$ is smooth, where ψ is a chart on M. The set of all functions on M is denoted $F^\infty M$. The set of all functions at a particular point $P \in M$ is denoted $F^\infty\{P\}$.*

Example B.1.2 *A curve in a manifold M is a smooth map $\gamma : [a, b] \subset \mathbb{R} \to M$, in other words a map such that $\psi \circ \gamma$ is smooth, where ψ is a chart on M*

B.1.2 Tangents and cotangents

To do physics with manifolds we need to understand how the idea of a vector (e.g. position, velocity, momentum) fits into the manifold picture. The idea of a *tangent space* is to attach a vector to a point in a manifold. We will see that any such vector can be represented by a derivative acting on functions.

[5] The domain of the transition map $\varphi \circ \psi^{-1}$ is actually $\psi(U \cap V) \subset \mathbb{R}^m$, but I will usually abuse notation on this sort of thing and just write $\mathbb{R}^m$ instead.

If $\gamma : [a,b] \to M$ is a curve in a manifold M we define the tangent to γ at $P = \gamma(t)$ to be the map $X_P : F^\infty\{P\} \to \mathbb{R}$ such that $X_P(f) := df(\gamma(t))/dt$. The tangent measures the rate of change of f along γ. In fact there is a natural correspondence (canonical isomorphism) between basis vectors $\mathbf{e}_i$ in $\mathbb{R}^n$ and derivatives $\partial/\partial x^i$. The crucial features of the above example of a tangent to a curve are captured within the following general definition of a tangent vector.

Definition B.1.3 *A tangent at $P \in M$ is a map $X_P : F^\infty\{P\} \to \mathbb{R}$ such that*

1. $X_P(fg) = X_P(f)g + fX_P(g)$ *(derivation property),*
2. $X_P(\alpha f + \beta g) = \alpha X_P(f) + \beta X_P(g)$,

$\forall f,g \in F^\infty\{P\}$ and $\alpha,\beta \in \mathbb{R}$. The set of all tangents at P is denoted T_PM. By defining addition and scalar multiplication of tangents in the obvious way one sees that T_PM is an m-dimensional vector space.

To construct a basis of T_PM one uses the idea of a *coordinate curve*. The i'th coordinate curve through $P \in M$ is given by the inverse of a chart $\psi^{-1} : \mathbb{R}^m \to M$ with all but its i'th argument held frozen;

$$\gamma^i(u) := \psi^{-1}(x^1(P),...,x^{i-1}(P),u,...,x^m(P)) \tag{B.1}$$

where the x^i are the coordinates associated with ψ.

Definition B.1.4 *A tangent basis vector $\partial_{i,P} : F^\infty\{P\} \to \mathbb{R}$ at $P \in M$ is a tangent to a coordinate curve γ^i through P. If we let $\gamma^i(t) = P$ then*

$$\partial_{i,P} f = \frac{d}{dt} f(\gamma^i(t)) = \frac{\partial}{\partial x^i}(f \circ \psi^{-1})(x^1,...,x^m)\bigg|_P . \tag{B.2}$$

The $\partial_{i,P}$ form a basis for the tangent space T_PM, so any $X_P \in T_PM$ can be written $X_P = X^i(P)\partial_{i,P}$ with $X^i(P) \equiv X_P(x^i|_P)$.

To construct tensors we need to determine the vectors dual to tangents.

Definition B.1.5 *If $f \in F^\infty\{P\}$ then one can view f as a map on tangent vectors. In this case one writes $df : T_PM \to \mathbb{R}$, which is defined by*

$$df(X_P) := X_P(f). \tag{B.3}$$

The space of all such maps is the dual of T_PM denoted T_P^*M. The basis of T_P^*M dual to $\{\partial_{i,P}\} \subset T_PM$ is simply $\{dx^i_P\}$, where the x^i are the coordinate functions used to define the $\partial_{i,P}$. Thus, any cotangent $\omega_P \in T_P^*M$ can be written $\omega_P = \omega_i(P)dx^i_P$ with $\omega_i(P) \equiv \omega_P(\partial_{i,P})$.

Armed with tangents and cotangents we can define tensors of any type at a point $P \in M$. I won't bother to do this since I am only going to use vectors, one-forms and two-forms.

B.1.3 Vector fields and p-forms

In the previous chapter I defined tangents and cotangents as vectors *at a specific point* $P \in M$. By removing the restriction to the point P tangents and cotangents become *vector fields* and *one-forms* respectively.

Definition B.1.6 *The tangent bundle over a base manifold M is defined as the union of all of the tangent spaces at points in M*

$$TM := \bigcup_{P \in M} T_P M. \tag{B.4}$$

To specify a point in TM one must specify a point $P \in M$ and a vector $X_P \in T_P M$. Thus, the tangent bundle has dimension $2m = 2\dim M$. A vector field is a map $X : U \subset M \to TM$ such that [6]

$$X(P) := X_P \in T_P M. \tag{B.5}$$

The set of all vector fields on M is denoted χM. Any vector field can be written $X = X^i \partial_i$ where $X^i \in F^\infty U$, and $\partial_i \in \chi M$ is defined by $\partial_i(P) := \partial_{i,P} \in T_P M$.

Having defined vector fields it is easy to see how one-forms should be defined. I will define the more general p-forms of which one-forms are of course a special case. A p-form at a point $P \in M$ is an anti-symmetric map $\omega_P : T_P M^p \to \mathbb{R}$, and the space of all such maps is denoted $\Lambda^p_P M$. A basis for $\Lambda^p_P M$ is $\{dx^{i_1}_P \wedge \ldots \wedge dx^{i_p}_P\}$ where $\{dx^i_P\}$ is a basis in $T^*_P M$. The associated bundle is simply

$$\Lambda^p M := \bigcup_{P \in M} \Lambda^p_P M. \tag{B.6}$$

As with vector fields we define a p-form generally by "de-restricting" a p-form at $P \in M$, to all of $U \subset M$.

Definition B.1.7 *A p-form is a map $\omega : U \subset M \to \Lambda^p M$ such that*

$$\omega(P) := \omega_P \in \Lambda^p_P M. \tag{B.7}$$

Any p-form can be written in terms of its components $\omega_{i_1 \ldots i_p} \in F^\infty U$ in the basis $\{dx^i\}$ as

$$\omega = \frac{1}{p!} \omega_{i_1 \ldots i_p} dx^{i_1} \wedge \ldots \wedge dx^{i_p}, \qquad dx^{i_1} \wedge \ldots \wedge dx^{i_p}(P) := dx^{i_1}_P \wedge \ldots \wedge dx^{i_p}_P. \tag{B.8}$$

[6] Sometimes the tangent bundle is defined as the disjoint union $TM := \bigcup_P \{P\} \times T_P M$, which includes the point P explicitly. A vector field then takes $P \in M$ and gives a pair (P, X_P). This is in fact what I mean by a vector field in definition B.1.6, but it becomes tedious to continually have to write down the point P, which doesn't actually do anything! Within the notation I have opted for it must be implicitly understood that the P is there.

Example B.1.3 *The cotangent bundle dual to TM is simply*

$$T^*M := \bigcup_{P\in M} T_P^*M \equiv \Lambda^1 M, \tag{B.9}$$

so covectors at $P \in M$ are simply one-forms at $P \in M$. The space of smooth functions on M is

$$F^\infty M \equiv \Lambda^0 M, \tag{B.10}$$

meaning that functions are actually just zero-forms.

B.1.4 pushforward and pullback

It is conceivable that we should need to move vectors and p-forms around the manifold M, or even connect them to the same objects in a different manifold. The pushforward and pullback are maps taking a tensor at a point in M and giving a tensor of the same type at another point, possibly in a different manifold N. They are induced by some smooth map between the base manifolds M and N themselves.

Definition B.1.8 *Let M and N be manifolds and let $\phi : M \to N$. The pushforward of a vector $X_P \in T_PM$ by ϕ, is a map $\phi_{*P} : T_PM \to T_{\phi(P)}N$ defined by* [7]

$$(\phi_{*P}X_P)(f) := X_P(f \circ \phi|_P) \tag{B.11}$$

where $f \in F^\infty\{\phi(P)\}$ and $|_P$ denotes the restriction to $P \in M$. By removing the restriction on the point P we can view the pushforward as a map $\phi_* : TM \to TN$ written simply $\phi_*(X) := X(\cdot \circ \phi)$, whose restriction to P yields B.11.

Example B.1.4 *Let $\gamma : [a.b] \to M$ be a curve in M. Its pushforward $\gamma_{*t} : T_t\mathbb{R} \to T_{\gamma(t)}M$ is*

$$\gamma_{*t}\left(\frac{d}{dt}\right) = \frac{d}{dt}(\cdot \circ \gamma)(t), \tag{B.12}$$

which is just the tangent to γ at $\gamma(t)$. Choosing a chart φ with coordinates x^i on M, and writing $x^i(t) := x^i(\gamma(t))$ we have

$$\gamma_{*t}\left(\frac{d}{dt}\right)(f) := \dot{x}^i(t)\frac{\partial}{\partial x^i}\tilde{f}(x^1(t),...,x^m(t)) \tag{B.13}$$

where $\tilde{f} := f \circ \varphi^{-1} \in F^\infty\mathbb{R}^m$ is just the coordinate representation of f, and $\dot{x}^i(t) := dx^i/dt$ is a coordinate "velocity" component of the curve γ.

That's the pushforward, now for the pullback.

[7] The pushforward is also sometimes called the differential or even just the derivative.

Definition B.1.9 *Let M and N be manifolds and let $\phi : M \to N$. The pullback of a p-form $\omega_{\phi(P)} \in \Lambda^p_{\phi(P)}N$ by ϕ, is a map $\phi^{*P} : \Lambda^p_{\phi(P)}N \to \Lambda^p_P M$ defined by*

$$(\phi^{*P}\omega_{\phi(p)})(X_{1,P},...,X_{p,P}) := \omega_{\phi(P)}(\phi_{*P}X_{1,P},...,\phi_{*P}X_{p,P}) \tag{B.14}$$

where $X_{i,P} \in T_P M$. By removing the restriction to the point $\phi(P) \in N$ we can view the pullback as a map $\phi^* : \Lambda^p N \to \Lambda^p M$ given by $(\phi^*\omega)(X_1,...,X_p) := \omega(\phi_* X_1,...,\phi_* X_p)$, whose restriction to $\phi(P)$ yields B.14.

Example B.1.5 *In the case of one-forms definition B.1.9 reduces to*

$$(\phi^*\omega)(X) := \omega(\phi_* X) \;\; s.t \;\; (\phi^*\omega)(X)|_{\phi(P)} := \omega_{\phi(P)}(\phi_{*P}X_P). \tag{B.15}$$

The inverse maps of the pushforward and pullback $(\phi_{*P})^{-1} : T_{\phi(P)}N \to T_P M$ and $(\phi^{*P})^{-1} : T^*_P M \to T^*_{\phi(P)}N$ are such that $(\phi_{*P})^{-1} \equiv (\phi^{-1})_{*\phi(P)}$ and $(\phi^{*P})^{-1} \equiv (\phi^{-1})^{*\phi(P)}$.

Example B.1.6 *One of the most useful pullbacks is that of a zero-form $f \in F^\infty N$, which is defined simply as*

$$\phi^*(f) := f \circ \phi \;\; s.t \;\; \phi^*(f)|_P \equiv \phi^{*P}(f|_{\phi(P)}) := f|_{\phi(P)} \circ \phi|_P. \tag{B.16}$$

B.1.5 The Lie algebra of vector fields

A while back I defined vector fields, which it turns out are a bit special. A vector field $X : U \subset TM$ by its definition should be fed a point in M to give a vector in TM. But since a vector in TM is to be given a function (to yield a real number), *we can give the vector field the function without giving it the point*. Suppose we do this, by writing down $X(f)$. This object, upon receiving a point $P \in M$, spits out a real number; $X(f)(P) := X_P(f) \in \mathbb{R}$. In other words $X(f)$ is a function in $F^\infty M$, which means X can be viewed as taking functions to functions. This makes it possible for the set of vector fields χM to become an algebra. Vector fields are unique in this respect, because no other tensor fields afford this possibility.

A natural first guess at a multiplication map for χM would be to take straightforward composition of vector fields. A quick calculation shows that $X \circ Y$ is not in general a vector field, because it doesn't satisfy the derivation property. On the other hand $[X,Y] := X \circ Y - Y \circ X$ *is* a derivation.

Definition B.1.10 *The set χM of vector fields on a manifold M equipped with the Lie bracket (commutator) $[\cdot,\cdot] : \chi M \times \chi M \to \chi M$ defined by*

$$[X,Y] := X \circ Y - Y \circ X \tag{B.17}$$

is a Lie algebra called the Lie algebra of vector fields.

An idea that I will make use of in B.3.2 is that of ψ-*related* vector fields. Given manifolds M and N, and a smooth map $\psi : M \to N$, the vector fields $X \in \chi M$ and $Y \in \chi N$ are said to be ψ-related if $\psi_* X = Y$. If ψ is a diffeomorphism then $\psi_* X$ is defined on the whole of N. An important property of the Lie bracket B.17 is that, if $X_i \in \chi M$, $i = 1,2$ is ψ-related to $Y_i \in \chi N$, then the Lie brackets $[X_1, X_2]$ and $[Y_1, Y_2]$ are also ψ-related. More succinctly

$$\psi_* X_i = Y_i \quad \Rightarrow \quad \psi_*[X_1, X_2] = [Y_1, Y_2]. \tag{B.18}$$

B.1.6 Integral curves and flow

So a vector field can be thought of as a map taking functions to functions. It can also be though of as an assignment of a tangent to every point in M. An integral curve of a vector field X is a curve whose tangents at the points along it, make up the vector field X.

Definition B.1.11 *Let $\gamma : [a,b] \to M$ be a curve in a manifold M, and let $X : U \subset M \to TM$ be a vector field on $U \subset M$, γ is said to be an integral curve of X if*

$$\gamma_{*t}\left(\frac{d}{dt}\right) = X(\gamma(t)), \tag{B.19}$$

which in the coordinates specified in B.1.4, is equivalent to the requirement

$$\dot{x}^i(t) = \tilde{X}^i(x^1(t), \ldots, x^m(t)) \equiv X^i(\gamma(t)) \tag{B.20}$$

where $\tilde{X}^i := X^i \circ \varphi^{-1}$ is the coordinate representation of the component functions of $X = X^i \partial_i$.

Local integral curves of a vector field are unique up to reparametrisation. If γ and Γ are both integral curves of X such that $\gamma(0) = P$ and $\Gamma(0) = \gamma(a)$ for some $a \in \mathbb{R}$, then $\Gamma(t) = \gamma(t+a)$.

The image $\gamma([a,b])$ of an integral curve could represent the path of a classical particle in a configuration space M. It would be nice in this instance to have a map, which rather than taking a real number and giving a point in M, actually moves points to points, i.e. moves the particle around in $\gamma([a,b])$. This is the idea behind the flow of the vector field X.

Definition B.1.12 *Let $\gamma : [a,b] \to U$ be an integral curve of $X : U \subset M \to TM$, starting at $P \in M$ i.e., such that $\gamma(0) = P$. The flow of X is the set of maps $\{(F_t)_{t \in \mathbb{R}}\}$ with $F_t : U \to F_t(U) \subset M$ defined by*

$$F_t(P) = F_t(\gamma(0)) := \gamma(t). \tag{B.21}$$

If F_t is a local diffeomorphism then F_t^* and F_{t*} are vector space isomorphisms. Given the uniqueness of integral curves the following properties of the flow can be deduced

$$F_t \circ F_s = F_{t+s}, \qquad F_{-t} = F_t^{-1}, \qquad F_0 = I \tag{B.22}$$

where I denotes the identity map on M. Maps satisfying these properties form a so-called local one parameter group of transformations.

B.1.7 Derivatives

In this final subsection I discuss some useful derivatives of vector fields and p-forms. The first of these is the *Lie derivative* L_X, which measures the rate of change of a tensor field as it is infinitesimally transported along an integral curve of the vector field X, using the pullback of the associated flow.

Definition B.1.13 *From the more technical definition of a Lie derivative of a tensor field on a manifold M, (which I give for p-forms below) one can show that for a vector field on M, the Lie derivative with respect to a vector field $X \in \chi M$, is a map $L_X : \chi M \to \chi M$ such that*

$$L_X Y = [X,Y], \tag{B.23}$$

which serves well as a definition of the Lie derivative of a vector field on M.

For completeness I will give the definition of the Lie derivative of a p-form, which is a bit more involved.

Definition B.1.14 *Let ω be a p-form on M and $X \in \chi M$. The Lie derivative of ω with respect to X is $L_X\omega$ defined by*

$$L_X\omega := (F_t^*)^{-1}\frac{d}{dt}F_t^*\omega \quad s.t \quad L_X\omega|_{F_t(P)} \equiv L_X|_{F_t(P)}\omega_{F_t(P)} := (F_t^{*P})^{-1}\frac{d}{dt}F_t^{*P}\omega_{F_t(P)}. \tag{B.24}$$

In particular the Lie derivative of a zero-form $f \in F^\infty M$ is

$$L_X f = X(f). \tag{B.25}$$

The next derivative I will discuss is a derivative of p-forms called the *exterior derivative*. We have already encountered this derivative in the discussion of the relationship between functions and cotangents i.e., zero-forms and one-forms. Any zero-form f defines a one-form written df. The d here, is a map $d : \Lambda^p M \to \Lambda^{p+1}M$ called the exterior derivative.

Definition B.1.15 *The exterior derivative is a map $d : \Lambda^p M \to \Lambda^{p+1}M$ with the following properties*

1. $df(X) = X(f) \quad \forall X \in TM,\ f \in F^\infty M,$
2. $d(d\omega) = 0 \quad \forall \omega \in \Lambda^p M,$
3. $d(\omega+\eta) = d\omega + d\eta \quad \forall \omega,\eta \in \Lambda^p M,$
4. $d(\omega\wedge\eta) = (-1)^p d\omega\wedge\eta + (-1)^q \omega\wedge d\eta \quad \forall \omega \in \Lambda^p M,\ \eta \in \Lambda^q M.$

It follows that in coordinates

$$d\omega = d(\frac{1}{p!}\omega_{i_1\ldots i_p}dx^{i_1}\wedge\ldots\wedge dx^{i_p}) = \frac{1}{p!}d\omega_{i_1\ldots i_p}\wedge dx^{i_1}\wedge\ldots\wedge dx^{i_p} \tag{B.26}$$

for an arbitrary p-form ω.

The second property of d in the above definition makes it very interesting indeed. For regular vector fields on $\mathbb{R}^3$ this property can be seen to be equivalent to the vanishing of the curl of the gradient and of the divergence of the curl. It can also be seen as the cause of gauge freedom in electromagnetism.

The final derivative I wish to discuss is another derivative of p-forms called the interior product.

Definition B.1.16 *Let* $X \in TM$ *be a vector over a manifold* M *and* $\omega \in \Lambda^p M$*. The interior product is a map* $i_X : \Lambda^p M \to \Lambda^{p-1}M$ *defined by*

$$(i_X\omega)(X_1,\ldots,X_{p-1}) := \omega(X,X_1,\ldots,X_{p-1}), \tag{B.27}$$

which is just the contraction of X *with* ω*, in the first slot. The interior product can be classed as a derivative, because it satisfies the following property*

$$i_X(\omega\wedge\eta) = (i_X\omega)\wedge\eta + (-1)^p\omega\wedge(i_X\eta). \tag{B.28}$$

So that's all three derivatives covered. I end this section with some fun formulas relating them;

$$i_X(df) = L_X f = X(f) = df(X), \tag{B.29}$$

$$L_X = i_X\circ d + d\circ i_X, \tag{B.30}$$

$$L_{fX}\omega = fL_X\omega + df\wedge i_X\omega \tag{B.31}$$

where $\omega \in \Lambda^p M$, $X \in TM$ and $f \in F^\infty M$.

B.2 Symplectic Geometry

At the end of section A.3.7 I touched on the idea of a symplectic space, but this was within the purely algebraic setting. *Symplectic manifolds* are of immense importance, because they provide the setting for most classical physical theories. Since quantum theories are usually obtained from their classical counterparts in such a way as to preserve much of the classical structure, symplectic manifolds are important in physics quite generally.

B.2.1 Basics

Definition B.2.1 *A symplectic form ω on a $2m$-dimensional manifold M is a closed non-degenerate two-form. A two-form is said to be closed if*

$$d\omega = 0. \tag{B.32}$$

The so-called flat map $\omega^\flat : TM \to T^*M$ is defined as $\omega^\flat(X) := i_X(\omega) = \omega(X,\cdot)$, and the so-called sharp map $\omega^\sharp : T^*M \to TM$ is defined as $\omega^\sharp := \omega^{\flat\,-1}$. The two-form ω is symplectic if and only if $\omega^\flat$ and $\omega^\sharp$ are vector space isomorphisms (the musical isomorphisms). A map $\psi : M \to M$ is said to be symplectic if $\psi^*\omega = \omega$ i.e. if its pullback preserves the symplectic form.

Darboux's theorem guarantees the existence of a local chart on M with coordinates (x^i, p_i), $i = 1,\ldots,m$ such that [56]

$$\omega = dx^i \wedge dp_i, \tag{B.33}$$

which can be written $\omega = -d\theta$ where θ is the *canonical form* defined as

$$\theta := p_i dx^i. \tag{B.34}$$

In terms of the canonical coordinates any vector field $X \in \chi M$ can be written

$$X = X(x^i)\frac{\partial}{\partial x^i} + X(p_i)\frac{\partial}{\partial p_i}. \tag{B.35}$$

Using this expression one obtains the following expressions for the musical isomorphisms

$$\omega^\flat(X) = -X(p_i)dx^i + X(x^i)dp_i, \tag{B.36}$$

$$\omega^\sharp(X) = X(p_i)\frac{\partial}{\partial x^i} - X(x^i)\frac{\partial}{\partial p_i}. \tag{B.37}$$

where I assume repeated indices are summed over irrespective of their relative positions (upper or lower).

B.2.2 Hamiltonian systems

Definition B.2.2 *A Hamiltonian system is a triple (M,ω,H) where M is a manifold with even dimension, ω is a symplectic form and H is a distinguished function on M called the*

[56] The reason for denoting the second m coordinates with a lower rather than an upper index should become clear in what follows.

Hamiltonian. The Hamiltonian vector field X_H associated with H is defined as

$$X_H := \omega^\sharp(dH). \tag{B.38}$$

In canonical coordinates

$$X_H = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial x^i} - \frac{\partial H}{\partial x^i}\frac{\partial}{\partial p_i} \equiv \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial x^i}\right) \tag{B.39}$$

where the latter identification follows by identifying derivatives with basis vectors in $\mathbb{R}^m$.

If $\gamma : \mathbb{R} \to M$ is an integral curve of X_H and we define $x^i(t) := x^i(\gamma(t))$ and $p_i(t) := p_i(\gamma(t))$ it follows that

$$(\dot{x}^i(t), \dot{p}_i(t)) = X_H(\gamma(t)) = \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial x^i}\right), \tag{B.40}$$

which we recognise as Hamilton's equations of classical mechanics.

A formulation of these equations in terms of Lie-algebraic structure is most convenient when it comes to the question of how to quantise a classical theory. Such a formulation is afforded by defining the *Poisson bracket*.

Definition B.2.3 *Let the space of functions on a symplectic manifold (M, ω) be denoted $F^\infty M$. The Poisson bracket is a map $\{\cdot,\cdot\} : F^\infty M \times F^\infty M \to F^\infty M$ defined by*

$$\{f, g\} := \omega(X_f, X_g) = i_{X_g} i_{X_f} \omega = -i_{X_f} i_{X_g} \omega \tag{B.41}$$

where X_f and X_g are the Hamiltonian vector fields associated with the functions f and g respectively. In canonical coordinates this reads

$$\{f, g\} = \frac{\partial f}{\partial x^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x^i}. \tag{B.42}$$

When f and g coincide with the canonical coordinate functions x^i and p_j, B.42 yields the canonical Poisson bracket relation

$$\{x^i, p_j\} = \delta^i_j. \tag{B.43}$$

The function space $F^\infty M$ equipped with the Poisson bracket is a Lie algebra, i.e., the Poisson bracket satisfies the conditions in A.3.3.

I'm now set up to discuss *symmetries* of the Hamiltonian system. A *Cartan symmetry* of the Hamiltonian system (M, ω, H) is any *local* vector field $V : U \subset M \to TM$ whose local flow $F_t : U \to F_t(U)$ satisfies $F_t^* \omega = \omega$ and $F_t^* H = H$. This is equivalent to the requirement that $L_V \omega = 0$ and $L_V H = 0$. This condition in turn implies that $i_V \omega$ is closed i.e., $d i_V \omega = 0$. The most important Cartan symmetries are the exact ones.

Definition B.2.4 *A closed two-form ω on a manifold M is said to be exact if $\exists\theta \in \Lambda^1 M$ such that $d\theta = \omega$. An exact cartan symmetry $V \in \chi M$ of a Hamiltonian system (M,ω,H) is characterised by the fact that $i_V\omega$ is not only closed, but also exact. This requires the existence of a function $f \in F^\infty M$ such that $V = X_f \in \chi M$ is a global Hamiltonian vector field with global flow $F_t : M \to M$ satisfying $F_t^*\omega = \omega$ and $F_t^*H = H$. This is in turn equivalent to the requirement that*

$$-X_H(f) = X_f(H) = df(H) = i_{X_f}(\omega)(X_H) = \{f,H\} = 0. \tag{B.44}$$

Exact Cartan symmetries are in one-to-one correspondence with conservation laws. The function $f \in F^\infty M$ is called the conserved quantity.

So far I have dealt with finite-dimensional Hamiltonian systems. To be able to use the same ideas in field theory we must consider generalisations. The setting for classical field theories is usually a *Banach space*, which is a complete normed vector space (cf. A.3.2). I will only need to deal with Banach spaces which are function spaces over some $Y \in \mathbb{R}^m$. I will denote such a space FY and in the remainder of this section I will introduce constructions on FY similar to those above. The material I present has been adapted from Marsden & Ratiu (2003).

A *natural pairing* on real Banach spaces Z, Z' is just a map $\langle\cdot,\cdot\rangle : Z \times Z' \to \mathbb{R}$. A *vector field* X on A Banach space Z is just a linear operator $X : Z \to Z$. It can be seen that this is equivalent to the familiar definition from B.1.3 when Z is a manifold.

Definition B.2.5 *Let $Y \subset \mathbb{R}^m$ and let FY denote some function space on Y. The exterior derivative of $f \in FY$ is a map $d : FY \to M(Y,(\mathbb{R}^m)^*)$ defined by*

$$df(x) := df_x \in (\mathbb{R}^m)^* \tag{B.45}$$

where $M(Y,(\mathbb{R}^m)^*)$ denotes the set of maps from Y to $(\mathbb{R}^m)^*$. The gradient is a map $\nabla : FY \to M(Y,\mathbb{R}^m)$ defined by

$$\nabla f(x) := \nabla f_x \quad s.t \quad df_x = \langle \nabla f_x, \cdot \rangle \tag{B.46}$$

where $\langle\cdot,\cdot\rangle : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ is a natural pairing. Thus, the gradient can be viewed as the "dual" of the exterior derivative. An example of a gradient is given by the functional derivative.

Definition B.2.6 *Let $Y \subset \mathbb{R}^m$ and FY denote some function space on Y. Let a natural pairing on FY be defined by*

$$\langle f,g\rangle := \int_Y d^m x\, fg \tag{B.47}$$

$\forall f,g \in FY$. Let $L : FY \to \mathbb{R}$. The functional derivative of L with respect to g denoted

$\delta L/\delta g$, is a function in FY defined by

$$\left\langle \frac{\delta L}{\delta g}, f \right\rangle = \frac{d}{dt} L(g+tf)\bigg|_{t=0}. \tag{B.48}$$

The functional derivative is linear in its arguments and satisfies the usual product rule for differentiation. The chain rule for functional derivatives can be expressed in the form

$$\frac{\delta L[f(g)]}{\delta g} = \frac{\delta L[f(g)]}{\delta f}\frac{df(g)}{dg}, \tag{B.49a}$$

$$\frac{\delta f(L[g])}{\delta g} = \frac{\delta L[g]}{\delta g}\frac{df(L[g])}{dL[g]}. \tag{B.49b}$$

The evaluation map $E_y : FY \to \mathbb{R}$ is defined by $E_y(f) := f(y)$. In particular one finds for $x, y \in Y$

$$\frac{\delta E_y}{\delta f}(x) = \delta(x-y), \tag{B.50}$$

which is sometimes written simply

$$\frac{\delta f(y)}{\delta f(x)} = \delta(x-y). \tag{B.51}$$

I have intentionally left the nature of the function spaces such as FY in the above definitions somewhat vague. Sometimes the space of square-integrable functions $L^2(Y)$ will do fine. What one invariablly requires at the least is that FY consists of all functions *vanishing at the boundary of Y*. Often Y will be the whole of $\mathbb{R}^n$ and the functions will have to approach zero at infinity faster than some inverse power of the magnitude of $x \in \mathbb{R}^n$, in order that certain desired properties hold. Equally often Y will be a bounded region of E^3. In this case it will have to come with *(periodic) boundary conditions*, which ensure that the fields vanish there.

In chapter 3 states of the electromagnetic field are taken to be integral functionals φ of the classical vector potential $\mathbf{A} \in \chi E^3$, which is an ordered three-tuple of functions. The functional derivatives in this case are special cases of the functional derivatives in the following example.

Example B.2.1 *A general functional φ of several functions $f_i \in F\mathbb{R}^n$ and their derivatives can be written*

$$\varphi[f_i] \equiv \int d^n x \rho(\mathbf{x}, \{f_i(\mathbf{x})\}, \{\nabla f_i(\mathbf{x})\}) \tag{B.52}$$

where ∇f denotes the n-tuple $(\partial f/\partial x^1, ..., \partial f/\partial x^n)$. First I define

$$\nabla \cdot \frac{\partial \rho}{\partial \nabla f_i} := \nabla_j \frac{\partial \rho}{\partial \nabla_j f_i} \tag{B.53}$$

in which the repeated index j is summed. Now, to compute the functional derivative, we simply appeal to definition B.2.6;

$$\begin{aligned}\frac{d}{dt}\varphi[f_i+tg]\Big|_{t=0} &= \frac{d}{dt}\int d^n x\,\rho(\mathbf{x}, f_i(\mathbf{x})+tg(\mathbf{x}), \nabla f_i(\mathbf{x})+t\nabla g(\mathbf{x}))\Big|_{t=0} \\ &= \int d^n x \frac{\partial\rho(\mathbf{x})}{\partial f_i} g(\mathbf{x}) + \frac{\partial\rho(\mathbf{x})}{\partial\nabla f_i}\cdot\nabla g(\mathbf{x}) \\ &= \int d^n x \frac{\partial\rho(\mathbf{x})}{\partial f_i} g(\mathbf{x}) - \left(\nabla\cdot\frac{\partial\rho(\mathbf{x})}{\partial\nabla f_i}\right) g(\mathbf{x}) + \nabla\cdot\left(\frac{\partial\rho(\mathbf{x})}{\partial\nabla f_i} g(\mathbf{x})\right) \\ &= \int d^n x \left(\frac{\partial\rho(\mathbf{x})}{\partial f_i} - \nabla\cdot\frac{\partial\rho(\mathbf{x})}{\partial\nabla f_i}\right) g(\mathbf{x}) \end{aligned} \tag{B.54}$$

where by Stokes' theorem the integral over the total divergence on the third line is a surface integral, which vanishes because the functions vanish at infinity. Thus, according to B.2.6

$$\frac{\delta\varphi}{\delta f_i} = \frac{\partial\rho}{\partial f_i} - \nabla\cdot\frac{\partial\rho}{\partial\nabla f_i}. \tag{B.55}$$

Given a natural pairing on a Banach space one can easily construct a space with symplectic structure using the functional derivative.

Definition B.2.7 *Let FY be a Banach (function) space on Y. and $\langle\cdot,\cdot\rangle : FY^n \times FY^n \to \mathbb{R}$ be a natural pairing. Let $Z := FY^{2n}$. The map $\Omega : Z\times Z\to\mathbb{R}$ defined by*

$$\Omega((\varphi^\mu,\pi_\mu),(\varphi'^\mu,\pi'_\mu)) = -\langle\varphi'^\mu,\pi_\mu\rangle + \langle\varphi^\mu,\pi'_\mu\rangle,\quad \mu=1,\ldots,n \tag{B.56}$$

is a closed non-degenerate (i.e. symplectic) two-form in $\Lambda^2 Z$ provided the natural pairing $\langle\cdot,\cdot\rangle$ is not degenerate. A Hamiltonian vector field $X_G\in\chi Z$ for some function $G\in FZ$, is defined as usual by $\Omega^\flat(X_G) = dG = i_{X_G}\Omega = \Omega(X_G,\cdot)$. In terms of coordinates $\varphi^\mu,\pi_\mu\in FY^n$ this reads

$$X_G(\varphi^\mu,\pi_\mu) = \left(\frac{\delta G}{\delta\pi_\mu}, -\frac{\delta G}{\delta\varphi^\mu}\right). \tag{B.57}$$

As before an integral curve $z:\mathbb{R}\to Z$ of X_G satisfies $\dot z(t) = X_G(z(t))$. The associated flow is a collection of maps $\{F_t : Z\to Z\}$ defined by $F_t(z(0)) := z(t)$, which constitute a one-parameter group of transformations.

Definition B.2.8 *Let $Z = FY^{2n}$ where FY is a function space on $Y\subset\mathbb{R}^m$. Let $\langle\cdot,\cdot\rangle : FY^n \times FY^n\to\mathbb{R}$ be a natural pairing defined by*

$$\langle\varphi^\mu,\pi_\mu\rangle := \int_Y d^m x\,\varphi^\mu\pi_\mu,\quad \mu=1,\ldots,n. \tag{B.58}$$

Let $\Omega : Z\times Z\to\mathbb{R}$ be defined as in definition B.2.7. The Poisson bracket of $F,G\in FZ$ is a

map $\{\cdot,\cdot\} : FZ \times FZ \to FZ$ *defined by*

$$\{F,G\}|_{(\varphi^\mu,\pi_\mu)} := \Omega(X_F|_{(\varphi^\mu,\pi_\mu)}, X_G|_{(\varphi^\mu,\pi_\mu)}) = \int_Y d^m x \left(\frac{\delta F}{\delta \varphi^\mu} \frac{\delta G}{\delta \pi_\mu} - \frac{\delta G}{\delta \varphi^\mu} \frac{\delta F}{\delta \pi_\mu} \right). \tag{B.59}$$

As before a conserved quantity is one which is in involution (i.e. Poisson commutes) with a distinguished function $H \in FZ$ *assumed to be the generator of dynamics.*

B.3 Lie Groups

Groups always play a role in the description of symmetries. In a gauge field theory the gauge group is used to describe the gauge symmetry. Gauge groups are subgroups of the general linear group(s) $GL(n,\mathbb{R})$ $(GL(n,\mathbb{C}))$. These groups are not only groups, but also manifolds for which matrix elements act as coordinates. They are in fact *Lie groups*, which means that the group operations of multiplication and inversion respect the smooth manifold structure. In general, matrix multiplication produces matrix elements that are polynomials of the elements of the matrices being multiplied and which are therefore smooth. The matrix elements of inverted smooth matrices are also smooth. Thus, finite-dimensional matrix groups are Lie groups.

B.3.1 Basics

Definition B.3.1 *A Lie group G is a (smooth) manifold, which is also a group, such that the multiplication map* $m : G \times G \to G$ *and the inversion map* $i : G \to G$ *are both smooth. An r-parameter local Lie group is a Lie group on* $U \subset \mathbb{R}^r$ *with* $m : U \times U \to \mathbb{R}^r$ *and* $i : U_0 \subset U \to \mathbb{R}^r$*. Given a manifold M, a local group of transformations on M is a Lie group G with action* $\Phi : U \to M$ *where* $\{e\} \times M \subset U \subset M \times G$*, and*

1. $g \cdot (h \cdot P) = (gh) \cdot P$,
2. $e \cdot P = P$,
3. $g^{-1} \cdot (g \cdot P) = P$

where $g \cdot P := \Phi(g,P)$.

The left (right) action of a Lie group on itself is called *left (right) translation*. For example, left translation on the Lie group G is the map $L : G \times G \to G$ defined by $L(g,h) = gh =: L_g(h)$ where $L_g : G \to G$ is a diffeomorphism. For each translation there are useful pushforward and pullback maps, which move tangents and cotangents around G. For example, the pushforward $L_{g*} : TG \to TG$ (such that $L_{g*}|_h =: L_{g*h} : T_hG \to T_{gh}G$) is used to define an especially important type of vector field on G called a *left-invariant vector field*.

Definition B.3.2 *Let G be a Lie group. A vector field $\xi \in \chi G$ is said to be left-invariant if it is L_g-related to itself, that is,*

$$L_{g*}\xi = \xi, \tag{B.60}$$

$\forall g \in G$. Restricted to some $h \in G$ this reads $L_{g*h}\xi_h = \xi_{gh}$. The subset of χG consisting of all left-invariant vector fields is denoted $\mathfrak{g}$.

Right-invariant vector fields can be defined analogously, using right translation. The set of left (right)-invariant vector fields $\{\xi_a\}$ is a *frame* for the vector space χG, which means that any $X \in \chi M$ can be written

$$X = \alpha^a \xi_a \tag{B.61}$$

where $\xi_{a,g} = e^i_a(g)\partial_{i,g}$ and $\alpha^a, e^i_a \in F^\infty G$.

Through analogy with the definitions of left and right-invariant vector fields one can define left and right-invariant one-forms.

Definition B.3.3 *A left-invariant one-form on a Lie group G is a one-form $\omega \in \Lambda^1 G$ such that*

$$L^*_g \omega = \omega, \tag{B.62}$$

$\forall g \in G$. A one-form ω is left-invariant if and only if $\omega(\xi)$ is a constant function in $F^\infty G$ for any $\xi \in \mathfrak{g}$.

B.3.2 The Lie Algebra of a Lie group

Since given a Lie group G, the map $L_g : G \to G$ is a diffeomorphism, $L_{g*}\xi$ is defined on all of G. This means $L_{g*h}\xi_h = (L_{g*}\xi)_{gh}$ is a well defined tangent in $T_{gh}G$. Furthermore if $\xi \in \mathfrak{g}$ then $L_{g*}\xi = \xi_{gh}$, and so according to B.18 we have

$$L_{g*}[\xi_1, \xi_2] = [L_{g*}\xi_1, L_{g*}\xi_2] = [\xi_1, \xi_2], \tag{B.63}$$

$\forall \xi_1, \xi_2 \in \mathfrak{g}$. In other words if $\xi_1, \xi_2 \in \mathfrak{g}$, then $[\xi_1, \xi_2] \in \mathfrak{g}$, which means that $(\mathfrak{g}, [\cdot,\cdot])$ is a *Lie subalgebra* of χG.

Definition B.3.4 *Let G be a Lie group. The Lie algebra $(\mathfrak{g}, [\cdot,\cdot])$ of left-invariant vector fields on G is called the Lie algebra of the Lie group G. If $\{\xi_i\}$ is a basis for $\mathfrak{g}$ then one can show that*

$$[\xi_i, \xi_j] = c^k_{ij}\xi_k \tag{B.64}$$

where the c_{ij}^k are called structure constants satisfying

$$c_{ij}^k = -c_{ji}^k, \qquad c_{ij}^k c_{kl}^m + c_{jl}^k c_{ki}^m + c_{il}^k c_{kj}^m = 0. \tag{B.65}$$

The basis fields ξ_i are often called generators of the Lie algebra.

Suppose that given $\xi \in \mathfrak{g}$, we define $\xi_e \in T_eG$ by $\xi_g \equiv L_{g*e}\xi_e \ \forall g \in G$, then one can show that the map $\iota : T_eG \to \mathfrak{g}$ defined by $\iota(\xi_e) := \xi$ is a vector space isomorphism. Thus, (quite remarkably) these spaces can be identified; $\mathfrak{g} \cong T_eG$. This means that $\mathfrak{g}$ is a *finite-dimensional* subalgebra of χG, whose elements are completely determined by their values at the identity element $e \in G$.

The flows of elements of $\mathfrak{g}$ are each one parameter subgroups, and every one parameter subgroup is the flow of some $\xi \in \mathfrak{g}$. The integral curves of the elements of $\mathfrak{g}$ are unique and complete i.e., they are defined on the whole of $\mathbb{R}$. The map relating the Lie algebra $\mathfrak{g}$ to the Lie group G is called the exponential map.

Definition B.3.5 *Let G be a Lie group with Lie algebra $\mathfrak{g}$. The exponential map $\exp : \mathfrak{g} \to G$ is defined by*

$$\exp(t\xi) := \gamma(t) \tag{B.66}$$

where $\gamma : \mathbb{R} \to G$ is the integral curve of $\xi \in \mathfrak{g}$. Conversely, if $\gamma : \mathbb{R} \to G$ defines a one parameter subgroup then

$$\xi_e := \gamma_{*e}\left(\frac{d}{dt}\right)\Big|_{t=0} \tag{B.67}$$

defines the associated left-invariant vector field ξ.

Of particular importance is the concept of *infinitesimal generators*, which are the vector fields on some manifold M induced by a local group of transformations.

Definition B.3.6 *Let G be a local group of transformations on M a manifold. Let $X_e \in T_eG$. The infinitesimal generator of transformations is a vector field $\xi^X \in \chi M$ defined by*

$$\xi_P^X(f) := \frac{d}{dt} f(P \cdot \exp(tX))\Big|_{t=0}. \tag{B.68}$$

The associated flow consists of maps F_t^X such that $F_t^X(P) = P \cdot \exp(tX)$. The map $\rho' : \mathfrak{g} \cong T_eG \to \chi M$ defined by $\rho'(X) = \xi^X$ is a Lie algebra homomorphism.[57]

Example B.3.1 *A particular case of the above definition is that in which $M = G$ and the action of G on M is simply right translation. It is then easy to show that $\xi^X \equiv X$, which*

[57] This means that ρ defines a *representation* (cf. B.3.7).

shows that the left-invariant vector fields are the infinitesimal generators induced by the right action of G on itself.

B.3.3 Subgroups of the general linear group and their Lie algebras

I come now to the important matter of Lie groups and Lie algebras acting on a vector space V. The most general Lie group acting on a vector space V is the general linear group $GL(V)$ consisting of the invertible operators (endomorphisms) $A : V \to V$. If the dimension of V is n, then one can identify V with $\mathbb{R}^n$ if it is real, or $\mathbb{C}^n \cong \mathbb{R}^{2n}$ if it is complex. One can therefore represent the operators in $\mathcal{L}(V)$ with real or complex matrices. It is easy to verify that the action of $GL(V)$ on V is a group action as defined by A.3.10.

Here I turn my attention to the identification of the Lie algebras of $GL(V)$ and its subgroups. We saw in B.3.2 that an element ξ of a Lie algebra $\mathfrak{g}$ defines a one-parameter subgroup $\gamma^\xi(t) = e^{t\xi}$, which takes values in the associated Lie group G. This means one can obtain the Lie algebra of G by first differentiating the one-parameter subgroups at the unit element $t = 0$ to obtain a unique element of T_eG (cf. B.67), and then using the pushforward to find the associated left-invariant vector field in $\mathfrak{g}$.

To properly see how this works let's consider the case $G \subset GL(V)$. Since we are dealing with matrices it's natural to take matrix elements as coordinates. Explicitly, one writes $x^i_j(A) = a^i_j$ where (a^i_j) is the matrix representation of $A \in GL(V)$. Defining the one-parameter subgroup $\gamma^{\xi_A}(t) := e^{t\xi_A}$ whose initial velocity is denoted $A := \dot{\gamma}^{\xi_A}(0)$, we seek the associated left-invariant vector field $\xi^A \in \mathfrak{g}$. Note that $A \in \mathcal{L}(V)$ need not be invertible, it is a completely arbitrary operator. We have according to B.67

$$\xi^A_e = \frac{d}{dt}\left(\cdot \circ \gamma^{\xi_A}(t)\right)\Big|_{t=0} = \dot{x}^i_j(\gamma^{\xi_A}(0))\partial^j_{i,e} = a^i_j\partial^j_{i,e}, \tag{B.69}$$

which gives us the element ξ^A_e of $T_eGL(V)$ associated with A. Now we use the pushforward to find $\xi^A \in \mathfrak{g}$;

$$\xi^A_g = L_{g*e}\xi^A_e = (\xi^A_g)^i_j\partial^j_{i,g} \tag{B.70}$$

where

$$(\xi^A_g)^i_j = \xi^A_h\left(x^i_j(L_g(h))\right)\big|_{h=e} = a^k_l\left[\partial^l_{k,h}x^i_j(gh)\right]_{h=e} = a^k_l\frac{\partial g^i_n h^n_j}{\partial h^k_l} = a^n_j x^i_n(g)\partial^j_{i,g} \tag{B.71}$$

from which it follows that

$$\xi^A = a^n_j x^i_n \partial^j_i. \tag{B.72}$$

where it is understood that $\xi^A(g) = \xi^A_g$ is given by B.70. To check this construction has worked let $\gamma^{\xi_A}(t)$ denote the integral curve of ξ^A starting at the identity; $\gamma^{\xi_A}(0) = e \equiv I \equiv$

(δ_i^j). We have

$$\xi^A_{\gamma^{\xi^A}(t)} = \dot{x}^i_j(\gamma^{\xi^A}(t))\partial^j_{i,\gamma^{\xi^A}(t)} = a^k_j x^i_k(\gamma^{\xi^A}(t))\partial^j_{i,\gamma^{\xi^A}(t)}, \tag{B.73}$$

which using the abbreviation $x(t) := x(\gamma^{\xi^A}(t))$ implies

$$\dot{x}^i_j(t) = a^k_j x^i_k(t) \quad \Leftrightarrow \quad \dot{x}(t) = Ax(t). \tag{B.74}$$

In particular we have $\dot{x}(0) = Ax(0) = Ax(e) = AI = A$, and from this it follows that $\xi^A_e = a^i_j \partial^j_{i,e}$, which takes us back to B.69. Since $A \in \mathcal{L}(V)$ is arbitrary, what the above calculations have established is a three-way canonical identification $\mathcal{L}(V) \cong T_eGL(V) \cong \mathfrak{gl}(V)$;

$$\begin{array}{ccccc} \mathcal{L}(V) & \longrightarrow & T_eGL(V) & \longrightarrow & \mathfrak{gl}(V) \\ \downarrow & & \downarrow & & \downarrow \\ A & \longrightarrow & \xi^A_e & \longrightarrow & \xi^A \end{array}$$

For the general linear group there are no restrictions on the operators (matrices) A, which is why the Lie algebra is the whole of $\mathcal{L}(V)$. Taking subgroups of $GL(V)$ means imposing conditions on its elements, and this leads to concurrent restrictions on the vector fields that make up the Lie algebra of the subgroup. The above method can be used to determine the Lie algebra $\mathfrak{g}$ of any Lie subgroup $G \subset GL(V)$. Take, for example, the orthogonal group $O(V) \cong O(n.\mathbb{R})$, which acts on the real n-dimensional vector space $V \cong \mathbb{R}^n$. Letting $\gamma : \mathbb{R} \to O(V)$ be a curve that starts at $e \equiv I$ (a subgroup always contains the identity) and writing in coordinates $x(t) := x(\gamma(t))$ we have by definition of the orthogonal group $x(t)x(t)^T = I$, where ^{T} denotes the matrix transpose. Thus,

$$0 = \frac{dI}{dt}\bigg|_{t=0} = \frac{d}{dt}x(t)x(t)^T\bigg|_{t=0} = \dot{x}(0) + \dot{x}(0)^T \quad \Leftrightarrow \quad \dot{x}(0) = -\dot{x}(0)^T. \tag{B.75}$$

If we let $A := \dot{x}(0)$ then we can identify $\xi^A_e \in T_eO(V)$ and $\xi^A \in \mathfrak{o}(V)$ as follows

$$\xi^A_e = a^i_j \partial^j_{i,e}, \qquad \xi^A = a^k_j x^i_k \partial^j_i, \qquad \text{where} \qquad A = -A^T. \tag{B.76}$$

So, the general recipe for finding the Lie algebra $\mathfrak{g}$ of the Lie group G is as follows; let $\gamma : \mathbb{R} \to G$ start at e and let $A := \dot{x}(0)$, then, based on the fact that $x(t) \in G$ must satisfy certain properties defining of the subgroup, deduce the properties that A must possess through simple differentiation.

In B.76 we have established the identifications $\mathfrak{o}(V) \cong T_eO(V) \cong o(n,\mathbb{R})$ where $o(n,\mathbb{R})$ denotes the set of all anti-symmetric real $n \times n$ matrices. These matrices are necessarily traceless which means that $o(n,\mathbb{R}) \equiv so(n,\mathbb{R}) := o(n,\mathbb{R}) \cap sl(n,\mathbb{R})$, where $sl(n,\mathbb{R})$ is (isomorphic to) the Lie algebra $\mathfrak{sl}(V)$ of the Lie group $SO(V)$ consisting of orthogonal

operators (matrices) with unit determinant. The Lie algebra $sl(n,\mathbb{R})$ simply consists of traceless real matrices, which can be checked easily with the help of the matrix identity $d/dt(\det x(t))|_{t=0} = \mathrm{tr}\dot{x}(0)$ and the recipe used above.

Another important subgroup is the pseudo-orthogonal group $O(r,s)$, which consists of real matrices leaving the symmetric bilinear form $g : V \times V \to \mathbb{R}$ defined in A.3.5 invariant. The associated special group $SO(r,s)$ consists of those elements of $O(r,s)$ having unit determinant. There are also the unitary and special unitary groups $U(n)$ and $SU(n)$ acting on the n-dimensional complex vector space. Our general recipe allows us to obtain all of the Lie algebras associated with these subgroups, which are collected below

$GL(n,\mathbb{R})$, $GL(n,\mathbb{C})$	$\det A \neq 0$	invertible matrices
$SL(n,\mathbb{R})$, $SL(n,\mathbb{C})$	$\det A = 1$	unimodular matrices
$Sp(2n,\mathbb{R})$	$A^T JA = J$	symplectic matrices
$O(r,s)$	$A^T \eta A = \eta$	pseudo-orthogonal matrices
$SO(r,s)$	$A^T \eta A = \eta$, $\det A = 1$	pseudo-orthogonal, unimodular matrices
$O(n,\mathbb{R})$	$A^{-1} = A^T$	orthogonal matrices
$SO(n,\mathbb{R})$	$A^{-1} = A^T$, $\det A = 1$	orthogonal, unimodular matrices
$U(n,\mathbb{C})$	$A^{-1} = A^\dagger$	unitary matrices
$SU(n,\mathbb{C})$	$A^{-1} = A^\dagger$, $\det A = 1$	unitary unimodular matrices

in which the matrix η is defined in A.3.5 and the matrix J in A.43. The corresponding Lie algebras are

$\mathcal{L}(n,\mathbb{R})$, $\mathcal{L}(n,\mathbb{C})$		all matrices
$sl(n,\mathbb{R})$, $sl(n,\mathbb{C})$	$\mathrm{tr}A = 0$	traceless matrices
$sp(2n,\mathbb{R})$	$A^T J = -JA$	symplectic pseudo-antisymmetric matrices
$o(r,s) \equiv so(r,s)$	$A^T \eta = -\eta A$	pseudo-antisymmetric matrices
$o(n,\mathbb{R}) \equiv so(n,\mathbb{R})$	$A = -A^T$	anti-symmetric matrices
$u(n,\mathbb{C})$	$A = -A^\dagger$	anti-hermitian matrices
$su(n,\mathbb{C})$	$A = -A^\dagger$, $\mathrm{tr}A = 0$	anti-hermitian, traceless matrices

B.3.4 Representations of Lie groups and Lie Algebras

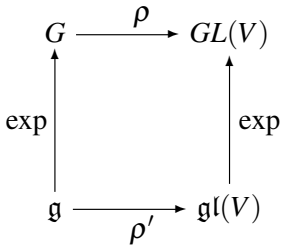
Often of interest in physics are the *representations* of certain Lie groups and Lie algebras on vector spaces.

Definition B.3.7 *A representation of a Lie group G on V is a Lie group homomorphism $\rho : G \to G' \subset GL(V)$. Similarly a representation of a Lie algebra $\mathfrak{g}$ on V is a Lie algebra homomorphism $\rho' : \mathfrak{g} \to \mathfrak{g}' \subset \mathfrak{gl}(V)$, which is a map such that $\rho'(\xi^A + \lambda\xi^B) = \rho'(\xi^A) + \lambda\rho'(\xi^B)$ and $[\rho'(\xi^A), \rho'(\xi^B)] = \rho'\left([\xi^A, \xi^B]\right)$.*[58] *This definition implies that a Lie algebra representation necessarily maps generators to generators and therefore preserves structure constants.*

If $\dim\mathfrak{g} = \dim\mathfrak{g}'$ then $\mathfrak{g} \cong \mathfrak{g}'$ if and only if there exist bases of each algebra for which the structure constants are the same.

[58] Note that ρ' is itself linear with respect to its argument *and* the images of ρ' are linear maps on V.

The exponential map maps a Lie algebra to its Lie group. Thus, a Lie group representation induces a Lie algebra representation and vice versa. A Lie group representation $\rho : G \to G'$ and its *derived representation* $\rho' : \mathfrak{g} \to \mathfrak{g}'$ are related by the following *commutative diagram*[59]



Explicitly ρ and ρ' are related by

$$\rho(e^{\xi}) = e^{\rho'(\xi)}, \qquad \rho'(\xi) = \frac{d}{dt}\rho(e^{t\xi})\bigg|_{t=0}. \tag{B.77}$$

If $\rho : G \to G'$ and $G' \subset GL(V)$ is defined by some set of conditions, then the derived representation will have properties induced by the conditions imposed on ρ. For example, if $\rho : G \to O(r,s)$ then for g defined in A.3.5 we have $g(\rho(h)v, \rho(h)u) = g(v,u)$. The derived representation $\rho' : \mathfrak{g} \to \mathfrak{o}(r,s)$ must therefore satisfy $g(\rho'(\xi)v, u) = -g(v, \rho'(\xi))$.

Two important properties of representations are *irreducibility* and *equivalence*.

Definition B.3.8 *If a representation $\rho : G \to GL(V)$ is such that $\forall w \in W \subset V$, $\rho(g)w \in W$ then W is said to be an invariant subspace of V with respect to ρ. The spaces V and $\{0\}$ are necessarily invariant subspaces, but if no other invariant subspaces exist then the representation ρ is said to be irreducible, otherwise it is said to be reducible.*

Definition B.3.9 *Two representations $\rho_1 : G \to GL(V_1)$ and $\rho_2 : G \to GL(V_2)$ are said to be equivalent if there exists an isomorphism $A : V_1 \to V_2$ such that $\rho_2(g) = A\rho_1(g)A^{-1}$.*

The nature of the isomorphism depends on the spaces V_1 and V_2. If, for example, they are complex inner product spaces $A : V_1 \to V_2$ must be unitary. The equivalence of Lie group representations implies the equivalence of the derived representations ρ_1' and ρ_2' with $\rho_2'(\xi) = A\rho_1'(\xi)A^{-1}$.

B.3.5 Rotations, spinors and the Lorentz group

I have now developed all of the machinery necessary in order to properly understand the action of important physical groups on important physical vector spaces, and how these

[59] In a *diagram* an arrow represents a map and the vertices are objects in a category. Combining arrows to make a longer route from one object to another represents composition of maps. A diagram is said to *commute* if whenever there are two different routes from one object to another the two maps representing those routes are equal.

actions might be related. Often the relationships between Lie algebras are more simple than those between Lie groups, the latter necessarily containing more information.

$SO(3)$ rotations and $SU(2)$

An important relationship in physics is the relationship between $SO(3)$ the rotation group and $SU(2)$ the special unitary group generated by the Pauli matrices. I will start by considering the corresponding Lie algebras.

The algebra $su(2) = \{2\times 2 \text{ matrices } A : A = -A^\dagger \text{ and } \mathrm{tr}A = 0\}$ possesses a basis

$$s_i = -i\sigma_i/2, \quad i = 1,2,3, \quad \text{such that} \quad [s_i, s_j] = \varepsilon_{ijk} s_k \tag{B.78}$$

where the σ_i are the Pauli matrices

$$\sigma_1 \equiv \sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 \equiv \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 \equiv \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{B.79}$$

The structure constants are evidently $c_{ij}^k = \varepsilon_{ijk}$ where ε_{ijk} is the Levi-Civita symbol, which takes the value $+1$ for cyclic permutations of 123, the value 0 if any of the indices are equal, and the value -1 otherwise. The most general element of $su(2)$ is a linear combination of the generators S_i and can therefore be expressed as

$$A = -\frac{i}{2}\theta\hat{n}_i\sigma_i = -\frac{i}{2}\theta\hat{\mathbf{n}}\cdot\vec{\sigma} \tag{B.80}$$

where $\theta\hat{\mathbf{n}} \in \mathbb{R}^3$ is a three-vector and $\vec{\sigma} := (\sigma_x, \sigma_y, \sigma_z)$. The matrix A is the generator corresponding to the group element $e^A \in SU(2)$;

$$A = \frac{\partial}{\partial\theta} e^{A(\theta)}\bigg|_{\theta=0}. \tag{B.81}$$

In fact the most general element of $SU(2)$ can be written

$$B = b_0 - i(\mathbf{b}\cdot\vec{\sigma}) = \cos(\theta/2) - i(\hat{\mathbf{n}}\cdot\vec{\sigma})\sin(\theta/2) = e^A \tag{B.82}$$

where the second equality follows from the definition of $SU(2)$, which requires that $b_0^2 + \mathbf{b}^2 = 1$ of which the most general solution is $b_0 = \cos(\theta/2)$, $\mathbf{b} = \hat{\mathbf{n}}\sin(\theta/2)$. Thus, in this case the exponential map covers the whole Lie group.

A similar analysis of the group $SO(3)$ and it's Lie algebra $so(3)$ can be performed. As generators of $so(3)$ one can take the matrices $\{l_i\}$ such that $(l_i)_{jk} = -\varepsilon_{ijk}$. Explicitly we

have

$$l_3 \equiv l_z := \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad l_2 \equiv l_y := \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad l_1 \equiv l_x := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{B.83}$$

The structure constants are again the ε_{ijk}, i.e.

$$[l_i, l_j] = \varepsilon_{ijk} l_k, \tag{B.84}$$

and the most general element of $so(3)$ can be written $\theta \hat{\mathbf{n}} \cdot \vec{l}$ where $\vec{l} := (l_1, l_2, l_3)$. This is the generator corresponding to the element

$$e^{\theta \hat{\mathbf{n}} \cdot \vec{l}} \equiv e^A, \qquad \hat{\mathbf{n}} \cdot \vec{l} = \frac{d}{d\theta} e^{A(\theta)} \bigg|_{\theta=0} \tag{B.85}$$

of $SO(3)$, which is the most general expression of an $SO(3)$ group element. It actually corresponds to a rotation by an angle θ about the vector $\hat{\mathbf{n}}$. The Lie algebras $su(2)$ and $so(3)$ are clearly isomorphic;

$$su(2) \cong so(3), \qquad -\frac{i}{2}\sigma_i \leftrightarrow l_i, \tag{B.86}$$

which establishes a representation of $so(3)$ on $\mathbb{C}^2$, as well as a representation of $su(2)$ on $\mathbb{R}^3$.

Unlike the Lie algebras the Lie groups $SU(2)$ and $SO(3)$ are not isomorphic. In fact $SU(2)$ covers $SO(3)$ twice. A 2-to-1 surjective representation of $SU(2)$ on $\mathbb{R}^3$ is established via the representation $\rho : SU(2) \to SO(3)$ defined by

$$\rho(\pm e^{-i\theta \hat{\mathbf{n}} \cdot \vec{\sigma}}) = e^{\theta \hat{\mathbf{n}} \cdot \vec{l}}. \tag{B.87}$$

The representation is established in the following way. Let $H_0(2)$ denote the set of 2×2 complex Hermitian matrices with unit determinant. Next define the vector space isomorphism $\psi : \mathbb{R}^3 \to H_0(2)$ by

$$\psi(\mathbf{x}) := \mathbf{x} \cdot \vec{\sigma}. \tag{B.88}$$

It is easily checked that $\det\psi(\mathbf{x}) = -\mathbf{x}^2$ and $\psi(\mathbf{x})^2 = I\mathbf{x}^2$. Now define the map $L : SU(2) \times H_0(2) \to H_0(2)$ by $L(A,H) \equiv L_A(H) := AHA^\dagger$, which it is readily verified preserves the determinant and Euclidean metric;

$$\det L_A(\psi(\mathbf{x})) = 1, \qquad L_A(\psi(\mathbf{x}))^2 = I\mathbf{x}^2. \tag{B.89}$$

It follows that the matrix R^A such that

$$R^A\mathbf{x} := [\rho(A)](\mathbf{x}), \qquad \rho(A) := \psi^{-1} \circ L_A \circ \psi \tag{B.90}$$

belongs to the orthogonal group $O(3)$. Now, we have from B.88 that $A\psi(\mathbf{x})A^\dagger = A\sigma_i A^\dagger x_i$, so that if we now suppose R^A is given by $R^A_{ij}\sigma_j = A\sigma_i A^\dagger$ then according to this definition

$$R^A_{ij}x_i = \psi^{-1}(R^A_{ij}\sigma_j x_i) = \psi^{-1}(A\sigma_i A^\dagger x_i). \tag{B.91}$$

This last expression is precisely $[\rho(A)](\mathbf{x})$ with ρ as defined in B.90. Thus $R^A := \rho(A)$ defined in B.90 also satisfies $R^A_{ij}\sigma_j = A\sigma_i A^\dagger$. This implies that $\det R^A = 1$, and therefore that R^A actually belongs to $SO(3)$. It is also implies that $R^A = R^{-A}$, meaning that the representation $\rho : SU(2) \to SO(3)$ given in B.90 is 2-to-1.

The Lorentz group and $SL(2,\mathbb{C})$

The relationship between a particular component of the Lorentz group $O(1,3)$ and $SL(2,\mathbb{C})$ is similar to the relationship between $SO(3)$ and $SU(2)$ covered above. The Lorentz group is defined in A.3.5. It consists of four connected mutually disjoint components;

$$O(1,3) = \mathcal{L}^\uparrow_+ \cup \mathcal{L}^\uparrow_- \cup \mathcal{L}^\downarrow_+ \cup \mathcal{L}^\downarrow_-, \qquad \mathcal{L}_+ \cap \mathcal{L}_- = \emptyset = \mathcal{L}^\uparrow \cap \mathcal{L}^\downarrow \tag{B.92}$$

where

$$\begin{aligned}
\mathcal{L}^\uparrow_+ &:= \{\Lambda \in O(1,3) : \Lambda^0_0 \geq 1,\ \det\Lambda = +1\},\\
\mathcal{L}^\uparrow_- &:= \{\Lambda \in O(1,3) : \Lambda^0_0 \geq 1,\ \det\Lambda = -1\},\\
\mathcal{L}^\downarrow_+ &:= \{\Lambda \in O(1,3) : \Lambda^0_0 \leq 1,\ \det\Lambda = +1\},\\
\mathcal{L}^\downarrow_- &:= \{\Lambda \in O(1,3) : \Lambda^0_0 \leq 1,\ \det\Lambda = -1\}.
\end{aligned} \tag{B.93}$$

The component $\mathcal{L}^\uparrow_+$ is called the *proper orthochronous subgroup* and consists of the regular Lorentz boosts and rotations in $SO(3)$. The other components can be obtained from $\mathcal{L}^\uparrow_+$ by reversing time and space through the time-reversal and parity matrices defined by $\mathcal{T} := \mathrm{diag}(-1,1,1,1)$ and $\mathcal{P} := \mathrm{diag}(1,-1,-1,-1)$ respectively. Explicitly

$$\mathcal{L}^\uparrow_- = \mathcal{P}\mathcal{L}^\uparrow_+, \qquad \mathcal{L}^\downarrow_+ = \mathcal{T}\mathcal{L}^\uparrow_+, \qquad \mathcal{L}^\downarrow_- = \mathcal{P}\mathcal{T}\mathcal{L}^\uparrow_+. \tag{B.94}$$

I'll now show that the Lie algebra $so(1,3)$ is isomorphic to $sl(2,\mathbb{C})$, while the Lie group $L^\uparrow_+$ is covered twice by $SL(2,\mathbb{C})$ analogously to the situation with $SO(3)$ and $SU(2)$. The generators of the Lorentz group can be taken as the sets of matrices $\{l_i\},\{b_i\}$ defined for

$i = 1,2,3$ by

$$l_i := \begin{pmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & l_i^3 \end{pmatrix}, \qquad b_i := \begin{pmatrix} 0 & \mathbf{n}_i^T \\ \mathbf{n}_i & 0_3 \end{pmatrix} \tag{B.95}$$

where the l_i^3 are the matrices defined in B.83, 0_3 denotes the 3×3 zero-matrix, and the $\mathbf{n}_i$ are defined by $(\mathbf{n}_i)_j := \delta_{ij}$. The structure constants with respect to these generators are given by

$$[l_i, l_j] = \varepsilon_{ijk} l_k, \qquad [b_i, b_j] = -\varepsilon_{ijk} l_k, \qquad [l_i, b_j] = -\varepsilon_{ijk} b_k. \tag{B.96}$$

The most general proper orthochronus Lorentz transformation can be written $\Lambda = \Lambda_R \Lambda_B$ where Λ_R is a rotation and Λ_B is a boost. The most general rotation as we have already seen in B.85 can be written $\Lambda_R = e^{\theta \hat{\mathbf{n}} \cdot \vec{l}}$.[60] A general boost with velocity $\mathbf{v}$ is

$$\Lambda_B = \begin{pmatrix} \gamma & \gamma \mathbf{v}^T \\ \gamma \mathbf{v} & I_3 + \frac{(\gamma - 1)}{|\mathbf{v}|^2} \mathbf{v}\mathbf{v}^T \end{pmatrix}. \tag{B.97}$$

where $\gamma := (1 - |\mathbf{v}|)^{-1/2}$. Defining the *rapidity* $\phi := |\mathbf{v}|/c = |\mathbf{v}|$ so that $\mathbf{v} = \phi \hat{\mathbf{n}}$ one obtains $\cosh \phi = \gamma$ and $\sinh \phi = \gamma |\mathbf{v}|$. The boost in B.97 can then be written

$$\Lambda_B = \begin{pmatrix} \cosh \phi & \hat{\mathbf{n}}^T \sinh \phi \\ \hat{\mathbf{n}} \sinh \phi & I_3 + (\cosh \phi - 1) \hat{\mathbf{n}}\hat{\mathbf{n}}^T \end{pmatrix} = e^{\phi \hat{\mathbf{n}} \cdot \vec{b}} \tag{B.98}$$

from which we see that the exponential map covers the entire set of boosts.[61] Since any $A \in SL(2,\mathbb{C})$ can be written $A = UH$ where $U \in SU(2)$ and $H \in H_0(2)$, to obtain a representation $\rho : SL(2,\mathbb{C}) \to \mathcal{L}_+^\uparrow$ it suffices to find representations mapping from each of $SU(2)$ and $H_0(2)$ into $\mathcal{L}_+^\uparrow$. A basis for $su(2)$ are the $-i\sigma_i/2$ and a basis for $h_0(2)$ (the Lie algebra of $H_0(2)$) are the matrices $\sigma_i/2$. The procedure used to find the representation $\rho : SU(2) \to SO(3)$ in B.90 can be adapted to find the representation $\rho : SL(2,\mathbb{C}) \to \mathcal{L}_+^\uparrow$ being sought. The 2-to-1 surjective representation found can be written

$$\rho(\pm e^{-i\vec{\sigma} \cdot (\vec{\theta} - i\vec{\phi})/2}) = e^{\vec{\theta} \cdot \vec{l} + \vec{\phi} \cdot \vec{b}}. \tag{B.99}$$

Between the Lie algebras $so(1,3)$ and $sl(2,\mathbb{C})$ we can construct two isomorphisms labelled 1 and 2 below;

$$l_i \overset{1}{\leftrightarrow} -\frac{i}{2}\sigma_i, \quad b_i \overset{1}{\leftrightarrow} \frac{1}{2}\sigma_i, \qquad l_i \overset{2}{\leftrightarrow} -\frac{i}{2}\sigma_i, \quad b_i \overset{2}{\leftrightarrow} -\frac{1}{2}\sigma_i. \tag{B.100}$$

Viewed as representations these isomorphisms are *inequivalent* according to B.3.9. Their

[60] In this expression the 3×3 matrices from B.85 must of course be replaced by the 4×4 matrices from B.95.

[61] Note that the subset of boosts *doesn't* constitute a subgroup.

exponentiation induces inequivalent Lie algebra representations denoted $\rho_{0,1/2}$ and $\rho_{1/2,0}$: $\mathcal{L}_+^\uparrow \to SL(2,\mathbb{C})$, and defined by

$$\rho_{1/2,0}(e^{\vec{\theta}\cdot\vec{l}+\vec{\phi}\cdot\vec{b}}) = e^{-i\vec{\sigma}\cdot(\vec{\theta}+i\vec{\phi})/2}, \tag{B.101a}$$

$$\rho_{0,1/2}(e^{\vec{\theta}\cdot\vec{l}+\vec{\phi}\cdot\vec{b}}) = e^{-i\vec{\sigma}\cdot(\vec{\theta}-i\vec{\phi})/2}. \tag{B.101b}$$

Each representation defines an action of the (proper orthochronus) Lorentz group on $\mathbb{C}^2$. The two distinct sets of Complex vectors transforming under Lorentz transformations according to B.101a and B.101b are called *right and left (Weyl) spinors* respectively.

B.3.6 Representations on function spaces

In quantum mechanics we don't deal with spin degrees of freedom only, but also with square-integrable wavefunctions. Quantum states of actual (non-interacting) particles are usually taken to be $\mathbb{C}^n$-valued square integrable functions, a prescription through which we seek to combine the ideas of wave mechanics with the notion of spin. More precisely, a spinor field is a field over spacetime, which takes values in a vector space that supports an irrecducible representation of $\mathcal{L}_+^\uparrow$.[62] For this reason we need to extend the formalism of representations on finite-dimensional vector spaces to vector-valued function spaces. First I will consider representations on scalar function spaces.

Definition B.3.10 *Let FM be a function space over a manifold M.*[63] *Let G be a Lie group and $R : G \times M \to G$ be a right action; $R(g,P) \equiv R_g(P) \equiv P \cdot g$. A representation of G on FM is a map $\rho : G \to GL(FM)$ defined by $[\rho(g)\psi](P) := \psi(P \cdot g)$.*

In order that ρ defines a representation, i.e. a left action on FM, one requires a right action of G on M. The representation ρ is in fact nothing but the pullback induced by R_g; $\rho(g)\psi = \psi \circ R_g = R_g^*\psi$. As such $\rho(g)$ is an associative algebra automorphism $\rho(g)(\psi\phi) = \rho(g)\psi\rho(g)\phi$ with respect to the point-wise product on FM, meaning $\rho : G \to \mathrm{aut}(FM) \subset GL(FM)$. The Lie algebra of $\mathrm{aut}(FM)$ turns out to be χM the set of vector fields on M.

Definition B.3.11 *Let $\rho : G \to GL(FM)$ be a representation. The derived representation is a map $\rho' : \mathfrak{g} \to \chi M$ denoted $\rho'(X) = \xi^X$, where ξ^X is the infinitesimal generator (cf. B.3.6) associated with $X \in \mathfrak{g}$ at the point $P \in M$ defined by*

$$[\xi^X(P)](f) \equiv \xi^X_P(f) := \frac{d}{dt}\left(f(P \cdot e^{tX})\right)\Big|_{t=0} \tag{B.102}$$

[62] One usually adds to $\mathcal{L}_+^\uparrow$ the spacetime translation group, which means the full symmetry group for spinor fields is actually the restricted Poincaré group.

[63] In physical applications M will typically denote Euclidean 3-space or Minkowski space-time, and FM will denote the space of square-integrable functions $L^2(M)$. There are however, many other spaces we might also be interested in, the smooth functions $F^\infty M$ for example. For this reason it is good to keep the function space FM general.

for a given $f \in FM$. If $\{E_i\}$ is a basis in $\mathfrak{g}$ then we write $\xi^{E_i} =: \xi^i$.

To bring these definitions to life let's consider the case of a wave-mechanical particle and the rotation group. In this example $M = E^3$, $FM = L^2(E^3)$, $G = SO(3)$, $\mathfrak{g} = so(3)$, and $R : E^3 \times SO(3) \to E^3$ is defined by $R(\mathbf{r}, A) = A^{-1}\mathbf{r}$. The group representation $\rho : SO(3) \to GL(L^2(E^3))$ is given simply by $[\rho(A)\psi](\mathbf{r}) = \psi(A^{-1}\mathbf{r})$. To obtain the derived representation we let $X \in so(3)$ and find the associated infinitesimal generator in χE^3. Letting x^i be coordinates on E^3 such that $x^i(\mathbf{r}) := r_i$ and letting $\psi : E^3 \to \mathbb{C}$ be an arbitrary wavefunction we have[64]

$$\xi^X_{\mathbf{r}}(\psi) = \xi^X_{\mathbf{r}}(x^i)\partial_{i,\mathbf{r}}\psi, \qquad \xi^X_{\mathbf{r}}(x^i) = \frac{d}{dt}x^i(e^{-tX}\mathbf{r})\bigg|_{t=0} = -X^{ij}r_j. \tag{B.103}$$

In particular we can look at the infinitesimal generator associated with the generators l_i of $so(3)$ defined in B.85;

$$\xi^{l_i}_{\mathbf{r}} = -(l_i)_{jk}r_k\partial_{j,\mathbf{r}} = \varepsilon_{ijk}r_k\frac{\partial}{\partial r_j} = -(\mathbf{r}\times\nabla)_i, \tag{B.104}$$

which we recognise, to within a factor of i, as the angular momentum operator in wave mechanics.[65]

I'm now in a position to extend these ideas to deal with vector valued wavefunctions.

Definition B.3.12 *Let $F(M,V)$ denote a function space consisting of vector-valued functions on a manifold M. Let G be a Lie group. If $\bar{\rho} : G \to GL(FM)$ is a representation on FM, and $\hat{\rho} : G \to GL(V)$ is a representation on V then we can define a representation $\rho : G \to GL(F(M,V))$ on $F(M,V)$ by $[\rho(g)\psi](m) := [\hat{\rho}(g)](\psi(m\cdot g))$ where $\psi(m\cdot g) = [\bar{\rho}(g)\psi](m)$.*

If $\{E_i\}$ is a basis for V then $\psi \in F(M,V)$ can be written $\psi = \psi^i E_i$ where $\psi^i \in FM$. The action of the representation ρ on ψ can therefore be written

$$[\rho(g)\psi](m) = \left([\bar{\rho}(g)\psi^i](m)\right)\hat{\rho}(g)E_i = \psi^i(m\cdot g)\hat{\rho}(g)E_i. \tag{B.105}$$

The derived representation $\rho' : \mathfrak{g} \to \mathrm{aut}F(M,V)$ is defined as follows

Definition B.3.13 *Given the definitions in B.3.12 let $\bar{\rho}' : \mathfrak{g} \to \chi M$ denote the derived representation associated with $\bar{\rho}$ and let $\hat{\rho}' : \mathfrak{g} \to \chi M$ denote the derived representation associated with $\hat{\rho}$. The derived representation $\rho' : \mathfrak{g} \to \mathrm{aut}F(M,V)$ can be written $\rho' = \bar{\rho}' + \hat{\rho}'$, or equivalently $\rho(X) = \xi^X + \hat{\rho}(X)$. More precisely, letting $\psi = \psi^i E_i$, the action of $\rho'(X)$*

[64] note that in this example $m\cdot e^{tX} = \mathbf{r}\cdot e^{tX} = e^{-tX}\mathbf{r}$.

[65] To obtain the actual angular momentum operator $L := -i\mathbf{r}\times\nabla$ one simply has to replace the l_i used in B.104 with the *generators of angular momentum* $J_i := il_i$.

on a vector-valued wavefunction ψ can be written

$$\rho'(X)\psi = (\xi^X \psi^i)E_i + \psi^i \hat{\rho}'(X)E_i. \tag{B.106}$$

Simply put, the derived representation ρ' consists of two components. The first one consists of a normal representation (in the sense of B.3.7) acting on the basis vectors E_i, multiplied by the component functions ψ^i, which are unchanged. The second one consists of a normal representation (in the sense of B.3.11) acting on the component functions ψ^i multiplied by the basis vectors E_i, which remain unchanged. Since $\rho'(X) : F(M,V) \to F(M,V)$ we can write $\rho'(X)\psi = (\rho'(X)\psi)^i E_i$, and if the E_i are canonical basis vectors such that $(E_i)^j = \delta_i^j$, then the components $(\rho'(X)\psi)^i$ are easily verified to be

$$(\rho'(X)\psi)^i = \xi^X(\psi^i) + \psi^j(\hat{\rho}'(X))^i_j \tag{B.107}$$

where $\hat{\rho}'(X) : V \to V$ is represented by a matrix.

As an example consider the two-component wave-mechanical spinor under the action of rotations. The spaces are the same as those specified above for the wave-mechanical particle without spin. The only difference is that the wavefunctions take values in $\mathbb{C}^2$.

Example B.3.2 *A spinor wavefunction ψ can be written $\psi = \psi^1 E_1 + \psi^2 E_2 = (\psi^1, \psi^2)^T$, where $E_1 = (1,0)^T$ and $E_2 = (0,1)^T$ are canonical basis vectors. The representation $\hat{\rho} : SO(3) \to SU(2)$ is given by $\hat{\rho}(e^{\theta\hat{\mathbf{n}}\cdot\vec{I}}) = e^{-i\theta\hat{\mathbf{n}}\cdot\vec{\sigma}/2}$, and the representation $\bar{\rho} : SO(3) \to GL(L^2(E^3))$ is given as in B.3.10 by $[\bar{\rho}(X)(\psi^i)](\mathbf{r}) = \psi^i(X^{-1}\mathbf{r})$. The representation ρ is therefore given by*

$$[\rho(e^{\theta\hat{\mathbf{n}}\cdot\vec{I}})\psi](\mathbf{r}) = \psi^i(e^{-\theta\hat{\mathbf{n}}\cdot\vec{I}}\mathbf{r})e^{-i\theta\hat{\mathbf{n}}\cdot\vec{\sigma}/2}E_i. \tag{B.108}$$

The derived representation $\hat{\rho}' : so(3) \to su(2)$ is just the isomorphism $\hat{\rho}'(l_i) = -i\sigma_i/2$ from B.86, and the derived representation $\bar{\rho}' : so(3) \to \chi E^3$ is given as in B.104 by $[\bar{\rho}'(l_i)](\mathbf{r}) = \xi^{l_i}_{\mathbf{r}} = -(\mathbf{r}\times\nabla)_i$. The derived representation ρ' is therefore given by

$$[\rho'(l_i)\psi](\mathbf{r}) = -(\mathbf{r}\times\nabla)_i\psi(\mathbf{r}) - \frac{i}{2}\sigma_i\psi(\mathbf{r}) \equiv -i(L_i + S_i)\psi(\mathbf{r}) =: -iJ_i\psi(\mathbf{r}). \tag{B.109}$$

Here $L_i = -i\mathbf{r}\times\nabla$ is the i^{th} component of the *orbital angular momentum operator*. It differentiates the component functions without mixing them up. On the other hand $S_i = \sigma_i/2$ is the i^{th} *spin operator*, which scrambles the components but leaves their $\mathbf{r}$ dependence unchanged. The operator J_i is the i^{th} component of the *total angular momentum operator*.[66]

The final example I wish to look at are the representations of $\mathcal{L}^\uparrow_+$ on spinor wavefunctions. As we saw in B.101 their are actually two inequivalent representations, which serve to define two distinct types of spinor.

[66] If we use the generators of angular momentum il_i instead of the l_i in B.109 we get $[\rho'(il_i)\psi](\mathbf{r}) = J_i\psi(\mathbf{r})$. As it must be by definition, ρ' is linear with respect to il_i, so $\rho'(il_i) = i\rho'(l_i)$.

Example B.3.3 *The right spinors are those which transform under a Lorentz transformation* $\Lambda = e^{\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})}$ *according to the representation* $\hat{\rho}_{1/2,0}$ *from B.101a. The left spinors transform according to* $\hat{\rho}_{0,1/2}$ *in B.101b. The associated inequivalent representations* $\rho_{1/2,0}$ *and* $\rho_{0,1/2}$ *acting on two-component wavefunctions are given by*

$$\left[\rho_{1/2,0}(e^{\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})})\right]\psi_R(\mathbf{r}) = \psi_R^i(e^{-\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})}\mathbf{r})e^{-i\hat{\mathbf{n}}\cdot\vec{\sigma}(\theta+i\phi)/2}E_i, \tag{B.110a}$$

$$\left[\rho_{0,1/2}(e^{\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})})\right]\psi_L(\mathbf{r}) = \psi_L^i(e^{-\hat{\mathbf{n}}\cdot(\theta\vec{l}+\phi\vec{b})}\mathbf{r})e^{-i\hat{\mathbf{n}}\cdot\vec{\sigma}(\theta-i\phi)/2}E_i. \tag{B.110b}$$

B.4 Fibre bundles

Fibre bundles play a central role in modern gauge field theories. Intuitively speaking a fibre bundle consists of the assignment of a manifold called a *fibre* to each point in some base manifold. Requiring that each fibre be diffeomorphic to some manifold called the *typical fibre*, means a fibre bundle is locally trivial, but might have a very rich global structure. I am primarily interested in *vector bundles* and *principal bundles*. Vector bundles, as the name suggests are fibre bundles made out of vector spaces. We have already encountered two paradigmatic examples, the tangent and cotangent bundles over some base manifold M. Principal bundles are made out of Lie groups.

B.4.1 Basics

Definition B.4.1 *A fibre bundle is a collection* (E,π,M,F) *where* E *is a manifold called the total space,* M *is manifold called the base space,* $\pi : E \to M$ *is a surjective smooth map, and* F *is a manifold called the typical fibre such that* $F \cong \pi^{-1}\{x\}\ \forall x \in M$*. The pre-image* $\pi^{-1}\{x\}$ *is called the fibre over the point* $x \in M$*.*[67] *Sometimes the total space* E *itself is referred to as the fibre bundle rather than* (E,π,M,F)*.*

A real (complex) vector bundle is a fibre bundle for which each fibre $\pi^{-1}\{x\}$ has the structure of a real (complex) vector space. A trivial bundle is one for which $E \equiv M \times F$ and $\pi \equiv \mathrm{pr}_1$ with pr_1 defined as the map that projects out the first element of an ordered pair. Given a covering $\{O_\alpha\}$ of the base manifold M $(= \bigcup_\alpha O_\alpha)$, a local trivialisation of the bundle E is a collection of maps $\{\psi_\alpha\}$ such that

$$\psi_\alpha(\pi^{-1}\{O_\alpha\}) = O_\alpha \times F \qquad \text{and} \qquad \mathrm{pr}_1 \circ \psi_\alpha = \pi. \tag{B.111}$$

Each ψ_α maps the portion of E over O_α to the trivial bundle such that the fibre above every point $x \in O_\alpha$ is the typical fibre F. Every fibre bundle is locally trivial i.e., given any E

[67] One could instead write $E := \bigcup_{x\in M} E_x$ with $\pi^{-1}\{x\} := E_x := \{x\} \times F_x$ and call F_x the fibre over x. Then E is just the collection of all points in M each glued to a fibre $F_x \cong F$. This way of doing things perhaps yields a more intuitive picture of what a fibre bundle is. However, as I noted in B.1.3 the point x doesn't actually do anything, so we can identify $E_x := \{x\} \times F_x$ with F_x itself, provided we understand that the point x is implicitly present when working with E_x.

there always exists a local trivialisation.

I'll now review some useful constructions on fibre bundles.

Definition B.4.2 *Let (E,π,M) be a fibre bundle and let $w_\zeta \in T_\zeta E$. The tangent w_ζ is said to be vertical if*

$$\pi_{*\zeta} w_\zeta = 0. \tag{B.112}$$

The subspace of all vertical vectors is denoted $V_\zeta E$

Example B.4.1 *Suppose $E \equiv TM$ for some base manifold M. As coordinates on TM we can take the (x^i, v^i) where $TM \ni v_x = v^i(x)\partial_{i,x}$ and the x^i are local coordinates on M. A general vector $w_{(x,v_x)} \in T_{(x,v_x)}TM$ can be written*

$$w_{(x,v_x)} = w_{(x,v_x)}(x^i)\frac{\partial}{\partial x^i} + w_{(x,v_x)}(v^i)\frac{\partial}{\partial v^i_x}. \tag{B.113}$$

Since $\pi_*(\partial/\partial v^i)(f) = \partial(f\circ\pi)/\partial v^i = 0$ for any $f \in F^\infty M$ it follows that

$$\pi_{*(x,v_x)} w_{(x,v_x)} = 0 \quad \Leftrightarrow \quad w_{(x,v_x)} = w_{(x,v_x)}(v^i)\frac{\partial}{\partial v^i_x}. \tag{B.114}$$

A *section* of a fibre bundle is an important map, which loosely speaking can be viewed as doing the opposite to the projection π.

Definition B.4.3 *Let (E,π,M) be a fibre bundle. A local section $\psi : U \subset M \to E$ is a smooth map such that*

$$\pi \circ \psi = I \tag{B.115}$$

where I denotes the identity. The collection of sections on E is denoted ΓE.

Example B.4.2 *The sections on a tangent bundle M are nothing but the local vector fields, i.e., $\Gamma E \equiv \chi M$.*

B.4.2 Vector bundles and connections

Here, following Frankel (2011), I consider vector bundles in more detail. Suppose we are given a bundle (E,π,M,F), and a covering $\{U_\alpha\}$ of M. In a vector bundle each fibre has the structure of a vector space, so we can take $F = \mathbb{R}^k$ (recalling that $\mathbb{C}^k \cong \mathbb{R}^{2k}$). The local diffeomorphisms (local trivialisations) are then $\phi_U : U \times \mathbb{R}^k \to \pi^{-1}(U)$. Now, we denote by $\{e^U_a : U \to E\}$ a collection of smooth sections, which are independent for each $x \in U$, and we assume these sections constitute a *local frame* in the sense that any section from U can be written $\psi_U = \psi^a_U e^U_a$. We can use this frame to define the diffeomorphisms ϕ_U as

$\phi_U(x,\psi_U^a E_a) := \psi_U(x)$ where $\psi = \psi_U^a E_a \in \mathbb{R}^k$ and $\{E_a\}$ denotes a basis in $\mathbb{R}^k$. In particular we have

$$\phi_U(x,E_a) = e_a^U, \quad x \in U, \quad \{E_a\} \text{ a basis in } \mathbb{R}^k. \tag{B.116}$$

The map ϕ_U effectively turns the basis $\{E_a\} \subset \mathbb{R}^k$ into a basis $\{e_a^U\}$ of the abstract fibre $\pi^{-1}(U)$, which sits over $U \subset M$. Of course $\pi^{-1}(U)$ is supposed to be identifiable with $\mathbb{R}^k$, but we don't make this identification until the point $x \in U$ has been specifed. Then we use ϕ_U to make the identification.

With the maps $\{\phi_U : U \subset M\}$ we can define *transition maps* $c_{VU} : V \cap U \times \mathbb{R}^k \to \mathbb{R}^k$ with V and U open in M, by

$$c_{VU}(x)\psi_U(x) := \phi_V^{-1}(\phi_U(x,\psi_U^a E_a)) \qquad \Rightarrow \qquad \psi_V^a(x) = c_{UV}(x)_b^a \psi_U^b(x) \tag{B.117}$$

where naturally $c_{VU}(x) : \mathbb{R}^k \to \mathbb{R}^k$ belongs to a group $G \subset GL(k,\mathbb{R})$. This extremely important group is called the *structure group* of the vector bundle and the most general structure group is just the general linear group itself. Note that from the definition B.117 of the transition maps a couple of important properties follow;

$$c_{UV}c_{VW}c_{WU} = I, \qquad c_{UV}(x) = c_{VU}(x)^{-1}. \tag{B.118}$$

If we arrange the components ψ_U^a of ψ_U into a column vector $\mathbf{\Psi}_U := (\psi_U^1,...,\psi_U^k)^T$ we can express the definitions above in terms of these columns. In particular we can write

$$\psi_V^a(x) = c_{UV}(x)_b^a \psi_U^b(x), \qquad \Leftrightarrow \qquad \mathbf{\Psi}_V(x) = c_{UV}(x)\mathbf{\Psi}_U(x) \tag{B.119}$$

To define a connection on the bundle we need the notion of an *E-valued one-form*.

Definition B.4.4 *An E-valued one-form is a map that assigns to each point in M, a cotangent that maps tangent vectors over M to points in E. More concisely an E-valued p-form ω is a map $\omega : M \to T^*(M,E)^p$ where $T_x^*(M,E)^p \ni \omega_x : T_xM^p \to E$. The collection of such p-forms is denoted $\Lambda^p(M,E)$, and in particular $\Lambda^1(M,E) \equiv \Lambda(M,E) \cong E \otimes \Lambda M$. Thus, locally in U, any E-valued one-form can be written*

$$\omega = \omega_i^a e_a^U \otimes dx^i. \tag{B.120}$$

Definition B.4.5 *A connection on E is a map $\nabla : \Gamma E \to \Lambda(M,E)$ such that for any $f \in F^\infty M$*

$$\nabla(\psi f) = (\nabla\psi)f + \psi \otimes df. \tag{B.121}$$

According to B.120, locally in U, $\nabla\psi \in \Lambda(M,E)$ can be written $\nabla\psi = (\nabla\psi)_\mu^a e_a^U \otimes dx^\mu$,

and in particular

$$\nabla e_a^U = \omega_{a,\mu}^b e_b^U \otimes dx^\mu = e_b^U \otimes \omega_a^b \qquad \Leftrightarrow \qquad \nabla e^U = e^U \otimes \omega \tag{B.122}$$

where the $\omega_a^b = \omega_{a,\mu}^b dx^\mu$ *are viewed as matrix elements of* ω*, which is called the connection one-form.*

The gauge potential in electromagnetism can be identified as a connection one-form. To see how we need to look at what the two definitions above can tell us. Using B.121 and B.122 we have

$$\nabla \psi_U = \nabla(e_a^U \psi^a) = e_a^U \otimes \left[\psi_U^b \omega_b^a + d\psi_U^a\right] \equiv e_a^U \otimes \nabla \psi_U^a \tag{B.123}$$

where

$$\nabla \psi_U^a := \psi_U^b \omega_b^a + d\psi_U^a. \tag{B.124}$$

Using $\omega_b^a = \omega_{b,\mu}^a dx^\mu$ and $d\psi_U^a = \partial_\mu \psi_U^a dx^\mu$ (cf. B.1.5) we have

$$\nabla \psi_U^a = \left[\psi_U^b \omega_{b,\mu}^a + \partial_\mu \psi_U^a\right] dx^\mu \equiv [D_\mu^U \psi_U^a] dx^\mu \tag{B.125}$$

where

$$D_\mu^U \psi_U^a := \psi_U^b \omega_{b,\mu}^a + \partial_\mu \psi_U^a. \tag{B.126}$$

The derivative D_μ^U is sometimes called the *covariant derivative*. Using B.121 and B.122 again we obtain

$$\nabla e_a^V = \nabla(e_b^U (c_{UV})_a^b) = e_c^U \otimes \left[\omega_b^c (c_{UV})_a^b + d(c_{UV})_a^c\right] = e_d^V \otimes \left[(c_{VU})_c^d \omega_b^c (c_{UV})_a^b + d(c_{UV})_a^d\right]. \tag{B.127}$$

Equating the right-hand-side of B.127 with $\nabla e_a^V = e_d^V \otimes \omega'^d_{\ a}$ where ω' denotes the connection one-form on $V \subset M$, and using $c_{VU} = c_{UV}^{-1}$, we obtain on the overlap $U \cap V$

$$\omega'^b_{\ a} = (c_{UV}^{-1})_c^b \omega_d^c (c_{UV})_a^d + (c_{UV}^{-1})_c^b d(c_{UV})_a^c, \tag{B.128}$$

which can be written simply

$$\omega' = c_{UV}^{-1} \omega c_{UV} + c_{UV}^{-1} dc_{UV}. \tag{B.129}$$

Example B.4.3 *In electrodynamics* $M = E^{1,3}$*,* E *is the trivial bundle* $E^{1,3} \times \mathbb{C}^n$*, the structure group* G *is* $U(1) \cong SO(2)$*, and sections are wavefunctions* $\psi : E^{1,3} \to \mathbb{C}^n$*. It is easiest to consider each component* $\psi_U^\alpha = \psi_U^{\alpha,1} + i\psi_U^{\alpha,2}$ *seperately and identify such a component as*

the real two-tuple $(\psi^{\alpha,1}, \psi^{\alpha,2})$. *There are then two real basis vectors to consider in each* $U \in E^{1,3}$. *These are* $e_1^U \leftrightarrow e^U$ *and* $e_2^U \leftrightarrow ie^U$ *where* e^U *is to be viewed as a frame for the complex line bundle. We have using B.122 that*

$$\nabla e^U = e^U \otimes eA^U, \qquad eA^U := \omega_1^2 = -\omega_2^1 \tag{B.130}$$

where e *denotes the elementary charge unit, and for each component we have* $\psi_U^\alpha(x) = c_{UV}(x)\psi_V^\alpha(x)$ *where* $c_{UV}(x) := e^{ie\lambda(x)}$. *In real terms we identify* $c_{UV}(x) \in SO(2)$ *as*

$$c_{UV}(x) = \begin{pmatrix} \cos e\lambda(x) & -\sin e\lambda(x) \\ \sin e\lambda(x) & \cos e\lambda(x) \end{pmatrix}. \tag{B.131}$$

Equation B.129 along with $eA^U := \omega_1^2$ *then yields for* $x \in U \cap V$

$$A^V = A^U + d\lambda, \qquad A_\mu^V = A_\mu^U + \partial_\mu \lambda(x), \tag{B.132}$$

which is the same as 3.57, while B.126 yields

$$D_\mu^U \psi_U^\alpha = \partial_\mu \psi_U^\alpha + ieA_\mu^U \psi_U^\alpha \tag{B.133}$$

which is the same as 3.54.

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