The de Broglie-Bohm Causal Interpretation of Quantum Mechanics and its Application to some Simple Systems

by

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Abstract

The de Broglie-Bohm causal interpretation of quantum mechanics is discussed, and applied to the hydrogen atom in several contexts. Prominent critiques of the causal program are noted and responses are given; it is argued that the de Broglie-Bohm theory is of notable interest to physics. Using the causal theory, electron trajectories are found for the conventional Schrödinger, Pauli and Dirac hydrogen eigenstates. In the Schrödinger case, an additional term is used to account for the spin; this term was not present in the original formulation of the theory but is necessary for the theory to be embedded in a relativistic formulation. In the Schrödinger, Pauli and Dirac cases, the eigenstate trajectories are shown to be circular, with electron motion revolving around the z-axis. Electron trajectories are also found for the $1s-2p_0$ transition problem under the Schrödinger equation; it is shown that the transition can be characterized by a comparison of the trajectory to the relevant eigenstate trajectories. The structures of the computed trajectories are relevant to the question of the possible evolution of a quantum distribution towards the standard $|\psi|^2$ distribution (quantum equilibrium); this process is known as quantum relaxation. The transition problem is generalized to include all possible transitions in hydrogen stimulated by semi-classical radiation, and all of the trajectories found are examined in light of their implications for the evolution of the distribution to the $|\psi|^2$ distribution. Several promising avenues for future research are discussed.

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Introduction

1.1 Introduction

The foundations of quantum mechanics are a matter of some controversy; indeed, quantum mechanics is a rare field in that there is more than one competing interpretation, and there are several different formalisms leading to the same numerical predictions. All of these are in agreement with experimental evidence. It is the general assumption in science that in this event, one or more interpretations and/or formalisms are eventually ruled out by experimental testing. However, in the case of quantum mechanics, this has not yet been the case; despite the age of standard quantum mechanics (almost a century) there remain not only competing formal accounts of quantum theory, but competing interpretations of the various formal accounts as well.

The mathematical formalism quantum mechanics has been extremely well confirmed experimentally. It is able to predict such quantities as the frequencies of spectral lines with great accuracy. It also accounts for the discreteness of some physical quantities, such as spectral line frequencies and spin. One may also predict the black-body emissions spectrum in terms of the emission and absorption of *quantized* radiation. But at the same time quantum mechanics is able to account for the wave-like properties of matter seen in diffraction

experiments. The theory's extremely successful formalism thus became accepted at first without a clear physical interpretation; the interpretation in physical terms grew later and continues to be the subject of debate [82, 92].

Despite the notable successes of the quantum formalism, standard quantum mechanics in its usual form is considered inadequate as a physical theory by some thinkers– philosophers as well as physicists. Briefly speaking, it does not describe in unambiguous terms the *reality* of the quantum world; some have argued that this is impossible. It also gives no *explanatory* description of the mysteries of the quantum world, from the two-slit experiment to the now increasingly observed quantum nonlocality. Even in the context of predicting probabilities of measurements it is unclear in the standard view whether the wave ψ is to represent an individual system, as has been the practice of some texts, or an ensemble of similar systems (the statistical interpretation).

Because some features of what has become the standard interpretation of quantum theory are considered fundamentally questionable, there is motivation for the investigation of alternatives, and in fact the standard view of quantum mechanics has itself been 'upgraded' since its original conception near the turn of the 20th century. There are features physicists would ideally like a quantum theory to have. One, which may not be possible, is to give an account of quantum phenomena that is consistent with relativity. Another would be to give rise to an intelligible story about measurement– a topic about which there is much controversy. Yet another would be to give rise, in the classical limit of the theory, to classical physics in some generally describable way.

All of these questions have been prioritized to varying degrees in the search for a new interpretation, theory, or formalism of quantum mechanics, which must be consistent with standard quantum mechanics to the extent (quite a broad one) that standard quantum mechanics has been experimentally confirmed.

The controversies surrounding the foundations of quantum mechanics revolve around the question of what a theory should be able to do, and why. One's views this topic typically

comes from one's philosophical perspectives, though many physicists do not explicitly think about this. Rather, they absorb the philosophical attitudes of their teachers and their community, and do 'what works' in terms of computations. However, as will be argued here in the case of quantum mechanics, this approach may leave important concerns unanswered. Many physicists are now aware of this, and the foundations of quantum mechanics is a growing area of research despite the fact that the standard quantum formalism has given very successful results. See for example the work of [27], [8, 7], [48, 47], [42] for various perspectives on the foundations of quantum mechanics, and more specific work by Sprung *et al.* [94, 96], Valentini [89, 88, 86, 87], Holland [61] and Hiley [55, 18, 56].

Followers of the standard interpretation of quantum mechanics often claim that it is sufficient that the theory generates very good predictions of quantities such as the frequencies of spectral lines and the probabilities of measurements of spin and other observable quantities. If a more detailed structure cannot possibly be observed, they argue (according to the uncertainty principle), what value can there be in seeking a physical theory that describes it? This identification of what should be discussed with what is *real*, and of what is real with what can be observed, has been termed a *positivist* point of view. However, it can be argued that even within a positivist point of view, there is motivation for seeking an alternative interpretation of quantum mechanics and/or an alternative formalism. This motivation might be, for example, to find a version of quantum mechanics that could handle the questions of observer-independence and the classical limit better than the standard theory.

Physicists who take, in opposition to the positivist view, a *realist* view, might like a quantum theory to provide an ontological description of matter at the quantum scale. Such a description would be about what is 'really'– for example, in the absence of an observer– happening at the quantum scale; what the electron really is (particle, wave, other entity), whether it has location, how it moves, and what forces guide it. A realist approach would not identify what can be measured with what exists; this leaves room for the existence of unobservable things.

These unobservable things have been referred to in the literature as hidden variables [12] because they would contain information not contained in standard quantum mechanics but would not be observable. It was long believed that there could be no realistic account of quantum phenomena using hidden variables [90]. This understandably left the positivist approach in a much more favourable light. However, Bell in [10] was able to clarify the matter of hidden variables theories; it is now accepted that one can account for quantum phenomena using *nonlocal* hidden variables.

This thesis will examine a realistic alternative formulation of quantum mechanics, namely the de Broglie-Bohm causal theory, and its application to hydrogen. This so-called causal theory is a realistic theory in that it is focused on giving an ontological description of quantum phenomena. In addition to discussing the direct application to the hydrogen atom, the question of the necessity of the axiomatic assumption that the particles are always distributed according to the usual quantum distribution $\rho = |\psi|^2$ will be discussed. It is hoped that some insights can be gained about the causal theory and its applications to physical systems, and that some interesting physics and applied mathematics may result.

In order to make a convincing argument for the significance of alternative versions of quantum mechanics in general, and for the causal program in particular, it is necessary to present a version of what is considered the standard interpretation of quantum mechanics, along with some of the central reasons that physicists are considering other interpretations. This will be the topic of the next section; the de Broglie-Bohm causal theory will be introduced in the remainder of this chapter.

1.1.1 The Copenhagen Interpretation

For future reference, it is useful here to present the central axioms of quantum mechanics, which are the basis of the Copenhagen interpretation and which are important in the alternative interpretations of quantum mechanics as well. This discussion is adapted from Griffiths [50]; see also such standard texts as Schiff [82] and Messiah [75].

Axiom 1 *The states of a quantum mechanical system are described by normalized rays* $|\psi\rangle$ *in a Hilbert space* $\mathcal{H}$*.*

Here, the ray $|\psi\rangle$ corresponds to a differentiable, complex-valued, square-integrable function defined on the coordinate space in question. It is normalized when its square integral over the space on which it is defined is equal to 1. The coordinate space is simply $\mathbb{R}^3$ for a single particle, but is $\mathbb{R}^{3N}$ for N particles. It can be shown that a Hilbert space whose elements are functions with these properties can be constructed [82, 49]. The inner product on the Hilbert space $\mathcal{H}$ is defined as follows:

$$\langle\psi|\phi\rangle = \int_{space} \psi^* \phi d\mathbf{x}, \quad \forall \psi, \phi \in \mathcal{H}.$$

Axiom 2 *To each quantum mechanical observable there corresponds a linear Hermitian operator acting in* $\mathcal{H}$*.*

If we denote the classical position and momentum by $\mathbf{x}$ and $\mathbf{p}$ respectively, then observable quantities $Q(\mathbf{x}, \mathbf{p}, t)$ are represented by operators formed by replacing $\mathbf{p}$ with $-i\hbar\nabla$, i.e. $\hat{Q} = \hat{Q}(\mathbf{x}, -i\hbar\nabla, t)$. If the coordinates and momenta of the k^{th} particle of a quantum mechanical system are characterized by operators $\hat{x}_k$ and $\hat{p}_k$, then this axiom can be shown to give rise to the central commutation relation

$$[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}\hat{I}.$$

Axiom 3 *Any measurement of the physical quantity corresponding to the operator* $\hat{A}$ *yields an eigenvalue* a_n *of* $\hat{A}$*. Furthermore, immediately after the measurement the system is in an eigenstate of* $\hat{A}$*,*

$$|\psi\rangle = |\phi_n\rangle$$

where

$$\hat{A}\,|\phi_n\rangle = a_n\,|\phi_n\rangle\,.$$

If one represents the original state as a linear combination of eigenstates of the operator $\hat{A}$,

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle ,$$

then the probability of obtaining the value a_n is equal to the magnitude of the relevant coefficient:

$$P(a_n) = \sum_i |c_{n_i}|^2$$

where the c_{n_i} are coefficients of the degenerate eigenstates ϕ_{n_i} of $\hat{A}$ with eigenvalue a_n.

Axiom 4 *With any physical system we can associate a Hermitian operator $\hat{H}$, called the Hamiltonian, which determines the time evolution of the system according to*

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle . \tag{1.1}$$

In the nonrelativistic case, the Hamiltonian operator $\hat{H}$ is in general constructed by

$$\hat{H} = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V$$

and in this case (1.1) is known as the Schrödinger equation. V denotes the classical potential and $\mathbf{p}$ has been replaced by the quantum mechanical momentum operator, $-i\hbar\nabla$. V may in general depend on both $\mathbf{x}$ and t, and is often an approximation of the interactions between the system particle(s) and a large group of other particles forming the environment, which are simulated by the given potential.

In practice, in addition to the axioms given above, one must specify a potential function. This is done through analogy with classical potentials. One must also specify an initial wave function which then evolves according to the Schrödinger equation, or a relativistic equation, depending on the context of the problem. These specifications are typically made using a combination of physical intuition and experience with quantum mechanics; there is

no generally accepted axiomatic statement about how to choose initial wave functions given the kind of system one would like to represent, though there are generally approved choices such as Gaussian packets.

With these caveats, these four postulates express the basics of standard 'Copenhagen' quantum mechanics. Note that it is assumed that the relationship between the state function $|\psi\rangle$ and the real world of measured physical quantities is that the probability of obtaining an eigenvalue a_n is given by the square of the amplitude of the $|\phi_n\rangle$ component of the total wave function $|\psi\rangle$. This means that quantum theory can be said to generate probabilities of various possible results of the measurement of any observable, rather than predictions of them.

There are some distinct differences between the axioms presented above and the axioms of other physical theories, such as the theory of special relativity. There, from physical principles such as the invariance of the theory under changes of (inertial) reference frame, the central equations of the theory can be derived. In quantum theory, we do not have equally physical, intuitive, axioms. Bell wrote that 'quantum mechanics is a theory for which we know the equations, but not the principles' and called this state of affairs 'a scandal' [12].

Note that there is no assumption in the above axioms about quantum reality in and of itself; indeed, Bohr thought that quantum systems were not separable from the measurement context in which they were observed, and thus that there was no unambiguous way to refer to 'quantum reality' [20]. Thus, any axiomatic description of quantum reality from which the equations of quantum mechanics could follow (in the manner that they do in special relativity) would not be meaningful as it could not refer to a specific measurement context (see the discussions in [92], [18] and [12]). This view was reinforced by the positivist philosophical approach taken by Bohr: if one cannot observe a quantum system in the absence of a measurement context, and because the system's properties seem to depend so strongly on the measurement context, then any inherent, underlying quantum reality cannot be observed, and thus is not worth including in the physical theory.

For these reasons, the physical nature of a system in the absence of a measurement context is not described at all in standard quantum theory, and in fact, the real nature of a system in a measurement context is not described either. Thus, it was not Bohr's view, nor is it the view of many practicing physicists, that an electron *is* a wave in some situations and *is* a particle in other situations. Instead of giving, or even presupposing, a version of the nature of reality, the above axioms tell us how to generate probabilities of measurements given an element of a Hilbert space. Some physicists, including Bohr according to some accounts [92] even would claim that this is all we can *ever* have in a quantum theory of individual systems.

An illustration of this aspect of quantum mechanics is the uncertainty principle. Let P and Q denote physical quantities with associated quantum mechanical operators $\hat{P}$ and $\hat{Q}$ respectively. Also let ΔP and ΔQ denote the spread in measured values of the associated physical quantities, which is thus a measure of the uncertainty in the quantities. Then, in general,

$$\Delta P \Delta Q \geq \left| \frac{1}{2i} \langle [P, Q] \rangle \right|^2 . \tag{1.2}$$

The knowledge of the quantities P and Q at a given time is thus constrained whenever the operators do not commute; for further accuracy in one must necessarily lose accuracy in the other. Perhaps the most famous statement of the uncertainty principle involves the position x and momentum p and reads

$$\Delta x \Delta p \geq \frac{\hbar}{2}.$$

In general, the uncertainty limit represents a restraint on what can be known at a given time; in the above it is applied to the position and momentum and implies that both cannot be known arbitrarily precisely at any time. The constraint on possible knowledge applies to any two observables whose corresponding operators do not commute.

In the context of the standard interpretation of quantum mechanics, which as noted does not discuss a reality existing in and of itself in some unambiguous way, the uncertainty principle implies that (for example) a particle cannot even have a well-defined position and momentum at any one time. Different and incompatible measurement contexts are necessary to measure the position and the momentum; physical quantities do not have meaning in and of themselves in the absence of a measurement context, and therefore position and momentum are not simultaneously well-defined concepts. This in effect becomes a statement not about what *is* in a quantum system, but about what *is not*, namely simultaneous position and momentum. Of course, it applies not only to position and momentum but to any pair or set of observables represented by Hermitian operators that do not commute with each other. The uncertainty principle is generally understood to refer not to what we can *know*, but to the extent to which the system is (in and of itself) *defined*.

In addition to the question of describing, or not describing, physical reality at the quantum level, it is worth briefly discussing the high profile given to the role of measurement in many axiomatic versions of quantum theory such as the one given above. Axiom 3 states the essential feature of quantum measurement: after a measurement, the wave function is said to be in one of the eigenstates of the relevant Hermitian operator, and the probabilities of the various possible measurements are the squares of the coefficients as given in the axiom.

For example, measurements of the spin of quantum objects, such as silver atoms, were found to yield only two values (up and down, simply stated), no matter in which direction the measurement apparatus was aligned. Classically, this would not be the case as spinning objects would have a continuous range of spin values. But if measurement outcomes are assumed to be eigenvalues of operators, the mathematical tools are there to describe various kinds of discreteness. In fact, the Copenhagen interpretation does an excellent job of describing the measurement outcomes of experiments on quantum systems, and its success in the non-relativistic regime cannot be overstated.

Yet it is somewhat enigmatic that measurement should be so prominent in an *axiomatic* statement of a theory. This is an outcome of the fact that quantum systems behave differently in different measurement contexts, unlike classical systems. However, the prominence of measurement brings about some controversial points about the standard theory, which will be discussed further in subsequent chapters. At this point, it is simply worth noting that in the axiomatic framework given in Section 1.1.1, the evolution (during measurement) of ψ to an eigenstate ϕ_n is given as a separate statement and it is not argued that this particular time evolution follows from the Schrödinger equation. Thus, it could be argued that the axiomatic statement of quantum theory given in Section 1.1.1 presupposes a classical scale on which the measurement apparatus exists. Note, however, that this axiomatic statement of 'standard' or Copenhagen quantum theory, though a commonly found one [49, 82] is a simplification.

There are some significant objections to the standard interpretation of quantum mechanics as presented here and in various standard texts. This is due in part to the fact that some features of the Copenhagen interpretation are counter-intuitive. There is also criticism based on the lack of an explicit description of the physical reality of the quantum scale; if one does not subscribe to the idea that the prediction of measurement probabilities is all we even *can* have in terms of a quantum theory of individual systems, then there is a call for something more.

1.1.2 Objections to the standard interpretation

One of the most prominent objections to the standard interpretation, and one shared even by its followers, is that it relies on the collapse of the wave function upon measurement (See Axiom 3). The word 'collapse' refers to the process by which the wave function changes from

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

to

$$|\psi\rangle = |\phi_i\rangle\,;$$

This process is in general not consistent with the Schrödinger equation (or the Pauli, Dirac, or Klein-Gordon equations, depending on the problem at hand), and hence it is not consistent with Axiom 4. It is not clear why *any* imaginable 'measurement' interaction would necessarily cause precisely this change in the wave function, particularly because the axiomatic statements of quantum theory do not clearly define what kind of experimental setup constitutes a measurement.

The requirement that the wave function undergo this collapse when, and only when, a measurement– a type of interaction that has yet to be clearly defined, but that must presumably involve some kind of interaction with the classical scale– is performed, therefore can be said to presuppose a classical scale on which matter must behave fundamentally differently than matter at the quantum scale. It would be this classical interaction that would distinguish measurement processes from 'purely' quantum processes, and allow them to violate Axiom 4. However, the presupposition of the classical scale is not ideal; ideally, the classical scale, and classical physics, would emerge from the quantum theory.

One approach to this problem is to adopt what is called the statistical interpretation [8, 7]; this has become the approach of the followers of standard quantum mechanics. According to this approach, the wave function does not represent an individual system, but an ensemble of similar systems. When the wave function collapses upon measurement, there is no difficulty with the non-Schrödinger evolution of a single system. Rather than describing the individual time evolution of a single system at all, in the statistical interpretation the collapse of the wave function is interpreted as follows: any measurement yields information about which element of an ensemble of systems has been observed. Further measurements are then correctly predicted by the collapsed wave function, which represents another ensemble, all of whose elements have the property specified in the first measurement.

However, the statistical interpretation leaves something to be desired from the point of

view of the realist. If our *most fundamental* theory of the world at small scales is based on ensembles, what are these ensembles composed of? Are we not assuming the existence of individual things, with which we compose hypothetical ensembles, and then essentially stating that the individuals themselves can have no satisfactory representation? To the physicist committed to building understanding about the quantum world, who acknowledges that individual electrons (for example) can be observed, this restriction might well seem unsatisfying. The statistical interpretation thus replaces the problem of the collapse of the wave function with a different, but still significant, problem.

Another objection to the standard view, whether in the statistical interpretation or in the framework of an individual wave function that undergoes a 'collapse', is that the theory requires *any* kind of measurement interaction in order to be well-posed. This, it has been argued, is not really a feature of the mathematical theory, but is a consequence of the positivist philosophical underpinning. This has led to the identification of what exists with what can be observed, and thus to the conclusion that if two operators do not commute, the corresponding physical observables have no simultaneous existence. If some (or all) quantities do not exist independently of observation, then it would seem that a classical observer is required in order to make the universe, or the relevant subsystem, collapse into an unambiguous state of existence.

This has been the source of much discussion of quantum mechanics and of whether it inherently depends on conscious observers (see for example [93, 70]). Many physicists who are at some level committed to a realist point of view find this conclusion quite troubling; the Earth seems to have been here before human or animal life, for example, and it seems quite vain to imagine that we are necessary in order to collapse its wave function. However, if we ourselves are not necessary, then in this theory we would need to specify what kind of system constitutes a measuring system, and hence draw the classical-quantum boundary. This has not satisfactorily been done for the standard theory, and certainly has not been done at the axiomatic level, while the classical scale is assumed at this level.

In addition to the question of conscious, or unconscious, observers, it has frustrated some thinkers that there are questions in standard quantum mechanics that are simply not considered well-posed, or are said to be meaningless. This is generally a result of the positivist approach in combination with the uncertainty principle, as discussed above; the question of what the position and momentum are at a given time is said to be meaningless. The question of tunnelling times through barriers also has this problem [68, 74, 67, 66]. The idea that such questions are inherently without meaning is hard to accept simply because we use our classical intuition even in quantum mechanics, and are tempted to think about momentum measurements via time-of-flight experiments, and to think that it must take some time to get through a barrier. In other fields, when one cannot find the answer to a question, one does not define the question to be meaningless. There is motivation to behave likewise in quantum mechanics.

It is worth pointing out that some authors have argued that the positivist assumption that we must identify what exists with what can be observed, and that it is not meaningful to talk about statements being 'true' or 'untrue' in the absence of observation, can *itself* not be observed. It could therefore be argued that the positivist assertion is self-defeating and therefore not a good standpoint with which to construct an axiomatic theory. This is a well-known point of view in the philosophy of science; see, for example, the discussion in [77] of Karl Popper's views on the matter.

It is possible to abandon the positivist assertion, and claim that the non-commuting observables *do* have existence independently of observation, but that their values cannot be known due to the uncertainty principle. In this case, one would want a theory that describes this underlying structure. Various theories under current consideration by the physics community take this approach.

Indeed, there are a variety of formulations of quantum theory being debated today, including the decoherent histories formulation of Gell-Mann and Hartle [42], the spontaneous localization theory of Ghirardhi, Rimini and Weber [43] and variants of these, as well as

others. Such theories reproduce the results of quantum mechanics in the regime in which quantum mechanics is known to be valid (and sometimes in general), and offer different interpretations of the quantum formalism and in some cases also a different formalism. Those that do not depend on the presence of observers to collapse the wave function are known as observer-independent formulations. A review of several such interpretations and extensions of quantum mechanics is given in [48, 47].

It is the purpose of this thesis to explore implications of one of these observer-independent theories, formulated originally by Louis de Broglie and later also by David Bohm [17, 16, 28]. The theory is referred to as the de Broglie-Bohm causal formulation of quantum mechanics. We will refer to is as the causal program, the causal theory or the causal interpretation, essentially interchangeably. It is hoped that its investigation will give rise both to interesting mathematics and a better understanding of topics in the foundations of quantum mechanics. Because the causal theory will be the central topic of this thesis, it is outlined in the following section.

1.2 The de Broglie-Bohm Causal Interpretation

In the de Broglie-Bohm formulation of quantum mechanics, there exist both a particle and a wave ψ. The wave evolves according to the Schrödinger equation (or the Pauli or Dirac equations, though the interpretation of these multicomponent wave functions is somewhat different) and propagates in space and time; the particle moves continuously and is guided by the wave.

Thus, already, the theory is radically different from the standard one, beginning with the ontological statement that there exist both a wave and a particle, and thereby directly discussing the properties of the quantum world. From the perspective of standard quantum theory, the existence of *both* the particle– one with a well-defined position and momentum at all times– and a wave, with real physical existence, is quite dramatic.

To motivate these possibly radical claims, Bohm began with a WKB-type form of the solution, inserting ψ in polar form into the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \tag{1.3}$$

where V is the usual classical potential. For simplicity, in this introduction to the theory we will limit ourselves to the single-particle Schrödinger equation. Writing $\psi = Re^{iS/\hbar}$, where R and S are real-valued functions of space and time, in the above, and separating the real and imaginary terms, yields two equations:

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = 0 \tag{1.4}$$

$$\frac{\partial R^2}{\partial t} + \nabla\cdot\left(R^2\frac{\nabla S}{m}\right) = 0 \tag{1.5}$$

The traditional WKB approximation assumes that, in the classical limit, the width of the wave packet is much greater than the wave length, and thus that the term $-\hbar^2\nabla^2 R/2mR$ is much smaller than the term $(\nabla S)^2/2m$ [18]. Neglecting this small term means that (1.4) reduces to

$$\frac{\partial S_c}{\partial t} + \frac{(\nabla S_c)^2}{2m} + V = 0 \tag{1.6}$$

where S_c refers to the classical generating function S which occurs in the classical Hamilton-Jacobi equation; indeed, (1.6) *is* the classical Hamilton-Jacobi equation representing a single particle moving with momentum $\mathbf{p} = \nabla S_c$.

Bohm's simple insight was that (1.4) can be rewritten in the same form as the classical Hamilton-Jacobi equation by introducing the quantum potential $Q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$, so that equation (1.4) becomes

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V + Q = 0. \tag{1.7}$$

Furthermore, (1.5) is the continuity equation; this means that we can interpret the density

$\rho = \psi^*\psi$ as a probability distribution of particles following trajectories given by $\mathbf{p} = \nabla S$.

Bohm's interpretation highlights the connection with the formalism of classical mechanics. Thus motivated, the theory describes particles which move along continuous trajectories of momentum

$$\mathbf{p} = \nabla S. \tag{1.8}$$

The particle is always guided by a field ψ, which obeys the Schrödinger equation. Furthermore, the forces on this particle are not simply the classical forces; there is an additional quantum force equal to $-\nabla Q$.

Noting that this law of motion for the particle admits arbitrary initial conditions, one is free to choose initial conditions that are compatible with a distribution proportional to $|\psi|^2(\mathbf{x}, 0) = R^2(\mathbf{x}, 0)$, so that the probability that a particle lies between $\mathbf{x}$ and $\mathbf{x} + d\mathbf{x}$ is $R^2(\mathbf{x}, t)d\mathbf{x}$. The continuity equation then guarantees preservation of this distribution under the evolution of the system; thus, the position distribution is consistent with standard quantum mechanics [18, 61].

The de Broglie-Bohm interpretation of quantum mechanics has been called the causal interpretation for the reason that once initial conditions are specified, the path of a particle is deterministic; furthermore, the path is caused by the usual potential acting together with the quantum potential. This is in contrast to the orthodox interpretation of quantum theory, in which the quantum world is fundamentally probabilistic. However, Bohm and Hiley do not argue that the universe is wholly deterministic [18]. They point to the idea that physical theories are still evolving; they do not claim to have discovered the ultimate theory of the universe and they recognize that theories have regimes in which they are valid; these are generally not the entire universe. They write

> So ultimately our overall world view is neither absolutely deterministic nor absolutely indeterministic. Rather it implies that these two extremes are abstractions which constitute different views or aspects of the overall set of appearances.

> Which view is appropriate in a given case will depend both on the unknown totality and on our particular mode of contact with it. ([18] p. 324).

In the causal theory, a particle has a precise momentum and position at any time. The uncertainty principle merely refers to how well the relevant variables can be measured:

> In our interpretation, what Heisenberg's principle refers to is not the actual momentum of the particle itself, but the value of the momentum that can be attributed to the particle after what is commonly called a measurement of the momentum. And because measurements are actually participatory, these two can differ ([18] p. 114).

In other words, the uncertainty principle refers to what we can measure, not to what exists. It is in this sense that the causal interpretation is a *realist* version of quantum theory, where the standard view of quantum theory is a *positivist* one. Note that both the causal theory and the standard one acknowledge that measurements affect quantum systems. The outcome of a measurement, furthermore, is not the same as the value of the measured quantity in the system as it was before measurement. Nevertheless, there *was* such a quantity, though it may not be reflected in the measurement due to the measurement interaction. The profound difference between the theories comes in whether the possible state of our knowledge of a system reflects possible states of its inherent existence.

It is instructive at this point to examine some simple consequences that occur in the causal formulation. First, consider the stationary wave

$$\psi = e^{i(kx-\omega t)} \tag{1.9}$$

which is an eigenstate of the momentum operator (in one dimension), with eigenvalue

$$p = \hbar k \tag{1.10}$$

in the x direction. This wave function is often used in simple problems to represent a free particle, as it is an eigenstate of the free particle hamiltonian.

If we apply the causal theory, we write $\psi = R(x,t)e^{iS(x,t)/\hbar}$, and thus obtain

$$S(x,t) = \hbar(kx - \omega t)$$

so that

$$\mathbf{p} = \nabla S = \hbar k \hat{e}_x.$$

This is consistent with standard quantum mechanics, and is a very simple illustration of how the causal theory yields intelligible results. However, in the causal interpretation, the primary meaning of (1.10) is not that the expectation value of the momentum, if it were to be measured, is $\hbar k$ (though this is the case). Primarily, (1.10) means that the free particle with wave function $\psi = e^{i(kx-\omega t)}$ travels in a straight line, beginning at some specified initial condition $x(0) = x_0$, with momentum $\hbar k$.

The causal theory is not always intuitive, especially in its original form. For example, one surprising consequence of the original de Broglie-Bohm framework occurs for some stationary states. Consider the time-independent Schrödinger equation:

$$H\psi = E\psi. \tag{1.11}$$

Suppose that $\psi_0(\mathbf{x})$ is a solution with eigenvalue E_0; then the time evolution is given by

$$\psi(\mathbf{x},t) = \psi_0(\mathbf{x})e^{-\frac{i}{\hbar}E_0 t} \tag{1.12}$$

which means that for the time-dependent wave function,

$$S(\mathbf{x},t) = S_0(\mathbf{x}) - E_0 t \tag{1.13}$$

so that the momentum equation is simply

$$\mathbf{p} = \nabla S(\mathbf{x}, t) = \nabla S_0(\mathbf{x}). \tag{1.14}$$

Since this is separable, barring any problems (zeroes, for example) with the function S, trajectories are integrable by a single quadrature for stationary states. So far, there is nothing necessarily unintuitive here, as one would expect the theory to be simpler for stationary states than for general states.

More surprisingly, though, is that when the stationary state is defined by a real function

$$\psi_0(\mathbf{x}) = R_0(\mathbf{x}), \tag{1.15}$$

then $S_0(\mathbf{x}) = 0$ and the momentum is identically zero. This would apply, for example, to all harmonic oscillator eigenstates.

As the original theory stands, and as it has been presented here, this result would apply to all s-states in atoms. Because of this the causal program originally gave a novel response to the well-known question of why an atom does not radiate electromagnetic radiation in its ground state: the electron is stationary.

However, it was shown [62, 54, 52] that the original guidance law (1.8) is not the non-relativistic limit of the Pauli theory in the case that the spin is non-zero. For spin particles, the momentum must instead be given by

$$\mathbf{p} = \nabla S + \nabla \log \rho \times \mathbf{s}, \tag{1.16}$$

where $\rho = |\psi|^2$ and $\mathbf{s}$ is the particle's spin. In order to preserve the current discussion, a derivation of this term from the Pauli equation for the case that the system is in an eigenstate of s_z is deferred until Section 4.1. This result and its implications will be discussed further in later chapters. However, it means that the momentum is no longer zero, even for real

stationary states. Since the additional term is divergence-free, the continuity equation, and hence the consistency of the statistics with standard quantum theory, is not affected. Note that the question of radiation from the atom remains. To fully address it, it would be necessary to take the full electromagnetic field into account.

With regard to the question of radiation, Holland argues that the account in the causal theory should be viewed in contrast to the usual interpretation, which he argues offers no physical explanation for the stability of matter at all, or at best allows for the interpretation of $|\psi|^2$ as a 'charge density' in a 'cloud of probability' ([61] p. 155). If we address the problem of why an atom does not give off electromagnetic radiation 'in isolation' with the claim that we cannot talk about the properties of matter 'in isolation' *at all*, the original question is not so much answered as denied. Holland further writes that "one has to be prepared to put aside expectations based on acquaintance with classical physics (i.e. habit and tradition) in order to develop a new intuition..." ([61] p. 155).

Another consequence of the causal theory, and one that has done much in the way of convincing physicists to take the causal theory seriously, is its trajectory treatment of the double slit experiment. This will be discussed in more detail in Chapter 2, but for now suffice it to say that the theory is able to reproduce the interference pattern by reproducing the standard quantum $|\psi|^2$ distribution, while attributing trajectories to the particles going through the slit system.

So far, the discussion of the causal theory and its implications has been limited to a particle's position and momentum, and indeed this is the original focus of the theory, though one may, of course, use it to discuss other quantities. However, Bell has argued that Bohm's focus on the position measurement is a strength rather than a drawback. For, he wrote,

> The only observations we must consider are position observations, if only the positions of instrument pointers. It is a great merit of the de Broglie-Bohm picture to force us to consider this fact. If you make axioms, rather than definitions and theorems, about the measurement of anything else, then you commit redundancy

and risk inconsistency" ([9], in [12] p. 166).

However, for the benefit of a more complete discussion and one that is more accessible to the quantum mechanics of real experiments, Holland gives a general discussion of the measurement [61] of other observables in the causal theory.

Usually in quantum mechanics, we have the expectation value of an operator

$$\langle A \rangle = \langle \psi | \, A \, | \psi \rangle = \frac{\int \psi^*(\mathbf{x}, t) A \psi(\mathbf{x}, t) d\mathbf{x}}{\int \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) d\mathbf{x}} \tag{1.17}$$

where $A = A(\hat{\mathbf{x}}, \hat{\mathbf{p}})$ is a Hermitian operator and is a function of the operators $\mathbf{x}$ and $\mathbf{p}$. If the wave function is normalized then the integral on the denominator is 1. The Hermiticity of A implies that the integral is real. Therefore, it makes sense to define the local expectation value, or the value of the quantity corresponding to A at each point along the trajectory, by

$$A(\mathbf{x}, t) = \frac{\mathrm{Re}\{\psi^*(\mathbf{x}, t) A \psi(\mathbf{x}, t) d\mathbf{x}\}}{\psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t)}. \tag{1.18}$$

With this definition, when it is assumed that the initial conditions $\mathbf{x}(0)$ are distributed according to $P = R^2 = \psi^* \psi$, Bohm's theory is consistent with conventional quantum theory.

Stating this explicitly, we can find the expectation value of an observable A as defined in (1.18) to be

$$\langle A \rangle = \int (\psi^* \psi)(\mathbf{x}, t) A(\mathbf{x}, t) d\mathbf{x} = \int (\psi^* \psi)(\mathbf{x}, t) \frac{\mathrm{Re}\{\psi^*(\mathbf{x}, t) A \psi(\mathbf{x}, t) d\mathbf{x}\}}{(\psi^* \psi)(\mathbf{x}, t)} d\mathbf{x}, \tag{1.19}$$

namely the integral over the space of the probability that the particle is at position $\mathbf{x}$– which is given by $\psi^* \psi$– times the local expectation value of the quantity at $\mathbf{x}$ given by (1.18). Since the operator is Hermitian, this real integral is equal to the expression in (1.17) when ψ is normalized.

Specifically, when

$$\psi = \sum_i c_i \phi_i \tag{1.20}$$

where a_n and ϕ_n are eigenvalues and eigenvectors of A respectively, and where the $|c_i|^2$ sum to unity, then the expectation value of A, calculated according to (1.18), is the same as the usual quantum expectation value

$$\langle A \rangle = \sum_i |c_i|^2 a_i.$$

There is also a more detailed theory of measurement in the causal program, which describes the process by which measurement of A will in general yield an eigenvalue a with probability $|c_a|^2$. This occurs because the wave ψ splits into non-overlapping packets corresponding to eigenfunctions of the operator A. The particle must then be in only one of the packets, and the measurement yields the corresponding eigenvalue. Which packet a particle enters depends on its initial position. The probabilities of the various measurement outcomes correspond to the standard quantum expectation values essentially because the initial spatial probability distribution is assumed to be $|\psi|^2$.

Despite the connection to the classical Hamilton-Jacobi equation, it should be noted that the causal interpretation of quantum theory is not a return to classical ideas. This can be concluded in part from the fact that the magnitude of the quantum potential, and therefore the action of the 'quantum force', does not change when the wave function ψ is multiplied by a constant factor. In other words, the behaviour of a system fails to change with overall scaling factors of ψ. Unlike classical fields for which the strength of the field is related to the strength of the field's effect, only the form and not the magnitude of this quantum field affects the motion.

Furthermore, the wave ψ propagates not in 3-dimensional space but in the composite 3N-dimensional space, known as configuration space, when there are N particles. The theory therefore has a fundamental nonlocality. Not only can a one-particle system be influenced by distant features of the environment (through their influence on ψ), but in systems with more than one particle the dependence of Q on all the positions means that the particles can

be strongly coupled ([18] p. 57). Bohm's position about this was that quantum systems are not simply collections of independent parts, interacting according to local information; they are indivisible wholes. This is similar, in fact, to Bohr's analysis of indivisibility in quantum measurement [18, 20]. Indeed, the degree of radical departure from classical physics will become increasingly clear, despite the fact that the causal theory shares some aspects of classical physics.

1.3 Why be interested in the Causal Theory?

The causal theory is of increasing interest in the physics community, even though its predictions statistically agree with the already well-known predictions of standard quantum mechanics. It does what was thought to be impossible [90]– it constructs a trajectory view of quantum particles consistent with standard quantum statistics. It is able to account for the quantization of spin in Stern-Gerlach experiments, and the strange 'wave-particle' duality of the double slit experiment [31, 80, 29]. Given that this also was long deemed impossible, it seems that there should be sufficient motivation for at least some examination of the theory as a possible contender.

Another significant source of interest in the theory are its philosophical underpinnings. While these are not typically the primary concern of physicists, there are many who find an appeal in being permitted to return to a classical paradigm in which particles are understood to be real, existing particles, in and of themselves.In the causal theory, particles are affected by our choices of measurement contexts but are not dependent on those for their 'objective' existence, or even for their description in physical theory.

The causal theory has some appeal beyond the appeal of a classical paradigm. It does not require the assumption of ensembles in order to describe quantum systems (as in the statistical interpretation which overcomes the problem of collapse). It offers an approach to the measurement problem in terms of non-overlapping packets, rather than using an

axiomatic statement about measurement such as the one given in Section 1.1.1. It also offers some connection to the classical scale, in that when the quantum potential Q is negligible, (1.7) becomes approximately the classical Hamilton-Jacobi equation.

In the causal theory, there are permissible questions that are not considered to be meaningful in the Copenhagen interpretation. Most obviously is the question of what a particle's position and momentum are at a given time– the trajectory of the particle. But there are others. It is possible, for example, using the local expectation value concept given in (1.18) to plot the spin vector along trajectories in a Stern-Gerlach experiment [80, 29] and hence visualize how the separation into packets of 'up' and 'down' spins occurs. Especially because this was thought to be impossible, examining the properties of 'Bohm trajectories', as they are often called, is interesting.

Another example of a question that is well-posed in the causal theory and not in the standard theory is the question of time. There has been considerable work done from the causal perspective on the question of quantum tunnelling [68, 74, 67, 66]. This is in part motivated by the fact that time is not a Hermitian operator, and hence, in standard quantum mechanics, the question of how long it will take a particle to tunnel through a barrier is not considered well-posed [68, 66]. However, if the particles follow trajectories, then one can predict the expected tunnelling time by computing how long the trajectories that go through the barrier spend inside it on average. There is no problem with time not being a Hermitian operator, because the realist approach of the theory yields a mechanism for defining the tunnelling time in other terms.

The causal theory's explanatory, realist approach to quantum nonlocality is also a source of interest. The exact extent and nature of nonlocality in quantum mechanics is still a source of debate, though there have been increasingly sophisticated experimental setups designed to test quantum nonlocality against Bell's inequalities [4, 5, 81] and many physicists now agree that it is likely, though not completely certain, that quantum nonlocality has been observed [12]. Because this is an important phenomenon in and of itself, and because the

associated entanglement is relevant to quantum computing, the fact that the causal theory offers a description of the way nonlocality comes about has increased physicists' interest in the theory.

Even in situations where standard quantum mechanics gives some satisfactory results, the causal program can be quite illuminating. One such situation is the question of tunnelling, as mentioned above. Another is the question of quantum chaos. The existence of a trajectory structure underlying quantum statistics allows the concept of quantum chaos to be defined in terms of chaotic quantum particle trajectories, and allows chaotic systems to be studied in more detail [97, 94].

In this thesis, the implications of the causal theory in some physically relevant contexts will be explored. The implication of the spin dependent term in the guidance equation (1.16) for the theory's application to the hydrogen atom will be discussed. Indeed, the theory is to be applied to the eigenstates of the hydrogen atom using the Schrödinger, Pauli and Dirac equations; the results of this application will show that the theory's application to hydrogen is consistent and intuitive.

In addition, the question of a quantum transition in hydrogen will be examined from the point of view of the causal theory. While the standard theory gives only a way to compute the probability, as a function of time, of detecting a transition via an energy measurement, the causal theory allows the computation of trajectories during the transition process– when usually the electron is said to be jumping mysteriously from one quantum state to another. It turns out that the transition problem shows interesting mathematical features, and in addition, the phenomenon of transition can be seen in the properties of the trajectories themselves.

The hydrogen atom is a simple and solvable one-particle system. It has more physical relevance than some other such systems, such as the one-dimensional potential problems of standard first texts in quantum mechanics (the infinite well, the square well, the square barrier). Unlike these potentials, the hydrogen atom potential, namely the Coulomb potential

representing the force from the proton, is not an approximation intended to represent many particles forming a wall or barrier. In addition, it seems meaningful to consider a hydrogen atom 'in isolation'. This is not meaningful under the statistical interpretation of standard quantum mechanics, as there would always be an ensemble of systems represented by any wave function. We have argued that it is an advantage of the causal theory that it describes individual systems, so it is of interest to apply to a system that exists in relative isolation.

In addition, the hydrogen atom is described in quantum mechanics using the Schrödinger, Pauli and Dirac equations, at varying levels of approximation. This means that there is quite a broad set of interrelated contexts in which to apply the causal theory, and these contexts are the limiting cases of one another. There is also quite a wealth of behaviour in the hydrogen atom, as one can consider linear combinations of eigenstates, which give rise to very different motion than single eigenstates, and one can consider transitions between eigenstates as well. Thus, the hydrogen atom is solvable, simple enough to have computable causal trajectories, but it has physical relevance and a broad range of behaviour. Also, because the electron has spin, the new term in (1.16) is non-zero. This term was not taken into account when the theory was first applied to hydrogen [19, 18, 61]. As we shall see, the spin term significantly changes the electron trajectories.

In the causal theory, one traditionally assumes that the particles are distributed according to $|\psi|^2$. However, if they are not so distributed, Bohm and Hiley [18] and others [89, 88, 86, 87] have suggested that the initial distribution will grow to approximate $|\psi|^2$ under time evolution, in a coarse-grained sense. But this process depends on the wave function having a certain degree of complexity, which is not the case for the hydrogen systems studied here. Thus, following the study of the hydrogen trajectories, the problem of relaxation is discussed for the purpose of moving towards a characterization of how much complexity would be required in order that the relaxation to $|\psi|^2$ occur.

In Chapter 2, we respond to some well-known criticisms of the causal program, and argue in favour of it, though we do not argue that it represents the ultimate physical theory of

the universe. We argue that it has advantages over the standard quantum theory, and that the computations presented here are relevant. We then turn to our application of the causal theory to the hydrogen atom. In Chapter 3 we present the application of the theory to Schrödinger eigenstates of hydrogen; Chapters 4 and 5 give the application to Pauli and Dirac eigenstates, comparing the trajectories in the relevant limits. In Chapter 6 we move back to the Schrödinger theory for the discussion of the application of the causal theory to the $1s-2p_0$ transition in hydrogen, stimulated by semi-classical radiation. Chapter 7 focuses on the question of the evolution of the initial probability distribution in the hydrogen systems of the earlier chapters, and generalizes the results of Chapter 6. Finally, in the concluding remarks we comment on the potential future insights to be gained from extensions of these topics in particular, and from the causal theory in general.

Chapter 2

Discussion of Relevant Literature

2.1 Introduction

In the previous chapter, it was argued that there are some well-established problems with the standard Copenhagen interpretation of quantum mechanics and that there are good reasons for examining other interpretations, including the causal program of Bohm and de Broglie. Not surprisingly, the causal program is itself not a perfect version of quantum mechanics, and there have been objections to it from physicists committed to the standard interpretation and from the physics community in general. In this chapter, we respond to some of the most common and most prominent objections to the causal interpretation, and argue that while there are objections that have merit, the points against the theory are not such that it should no longer be studied, nor do they imply that it is not a valid interpretation worth serious consideration.

Because it was long thought that no classical-style formulation could account for wave-particle duality, we discuss the two-slit experiment in Section 2.2. Following this, we respond to some general critiques of the causal theory in Section 2.3. In Section 2.4 we examine and respond to more specific accusations against the causal theory, which are based on its more detailed implications.

2.2 The Two-Slit Experiment

In the famous two-slit experiment, photons or particles are incident on a set of two (or many) parallel slits, and the pattern is viewed on a screen on the other side of the slits. When only one slit is open, the result is a smooth distribution of 'hits' on the screen, with the most 'hits' directly opposite the open slit. However, when both slits are open, the resultant pattern is not simply the sum of the patterns from two single slits, as would be expected if many particles simply went through either one slit or the other. Instead, there is an interference pattern more characteristic of waves going through slits and diffracting than of particles going through one slit or the other. This is in itself somewhat surprising, for it shows that matter has wave-like properties. In addition, when detectors are placed in front of the slits, in an effort to determine which slit the particle has gone through, the interference pattern is lost. So not only does matter have wave-like properties, these properties vanish upon observation!

Feynman referred to this as *the only mystery* in quantum mechanics, [41] and acknowledged that the description given by quantum theory does not amount to an intuitive understanding, only to a description that accurately represents the results of the two-slit experiment, and of course many others such as the Stern-Gerlach experiment.

It was argued that there could be no way to describe the experiment using a trajectory interpretation– one of the earliest objections to any kind of quantum trajectories. For if the particle really goes through either one slit or the other, then when some go through one slit, and some through the other, they cannot interfere like waves. For if they do, when both slits are open and the particle goes through the first slit, how does it 'know' whether the other slit is open, in order to 'know' whether to interfere? Surely, it was thought, no trajectory-based theory could duplicate the wave/particle duality, because distribution from the two-slit (or multi-slit) system in quantum mechanics is not the sum of the distributions from the slits taken separately.

It is likely that the mystery of the two-slit experiment, which pointed to the mystery of

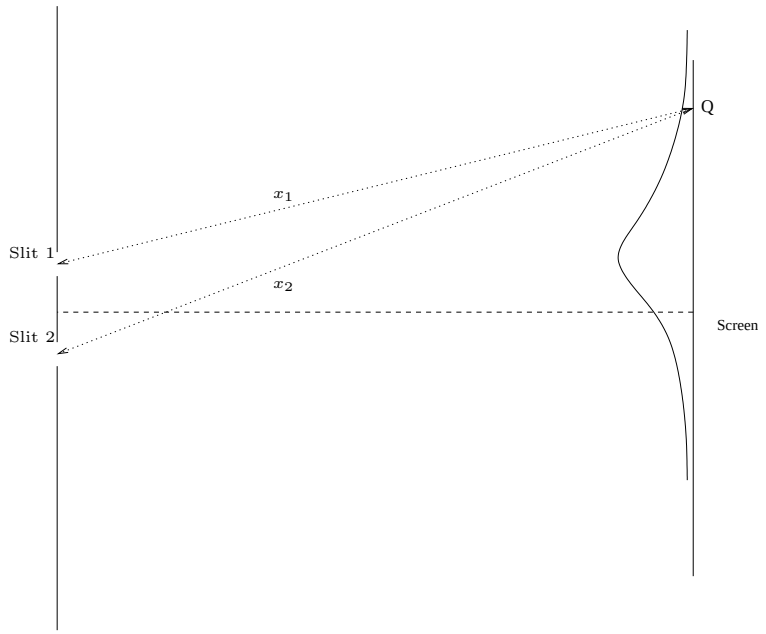


Figure 2.1: The two-slit experiment: one slit open

wave-particle duality in general, was largely responsible for the conclusion that a trajectory viewpoint would never be able to account for quantum phenomena. This view was certainly embraced by Bohr [20]. Because Bohr's complementarity, wave-particle duality, and the collapse of the wave function are such important aspects of the foundations of quantum theory, and because they are possibly best motivated by the two-slit experiment, it is worth giving a simplified discussion of the two-slit experiment here.

Suppose that the wave functions can be represented, simply, by travelling plane waves originating at the two slits: $\psi_1 = e^{i(kx_1 - \omega t)}$ and $\psi_2 = e^{i(kx_2 - \omega t)}$ where x_1 and x_2 represent the distances from the two slits to some given point Q on the screen; see Figure 2.1. Then if we write the total wave function as an equal superposition of ψ_1 and ψ_2, we have

$$\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2) \tag{2.1}$$

and to find the intensity of the pattern at Q, we find the probability

$$\begin{aligned} P = |\psi|^2 &= \frac{1}{2}|\psi_1 + \psi_2|^2 \\ &= \frac{1}{2}(\psi_1^* + \psi_2^*)(\psi_1 + \psi_2) \\ &= \frac{1}{2}|\psi_1|^2 + \frac{1}{2}|\psi_2|^2 + \frac{1}{2}\mathrm{Re}\{\psi_1^*\psi_2 + \psi_2^*\psi_1\}. \\ &= \frac{1}{2}|\psi_1|^2 + \frac{1}{2}|\psi_2|^2 + \cos k(x_2 - x_1). \end{aligned} \tag{2.2}$$

The cosine term represents the observed interference, which ultimately comes from the fact that $|\psi_1 + \psi_2|^2 \neq |\psi_1|^2 + |\psi_2|^2$. Of course, this choice of wave function is a simplification, but it yields an interference pattern such as the one observed. See [41] for a more complete discussion.

Suppose instead that we close one of the slits; this leaves $\psi = \psi_1$, for example, and the probability becomes $P = |\psi_1|^2$ and there is no interference. This is what we observe experimentally if we try to detect which slit the particle went through. If we assume that measuring the particle's position by measuring which slit it went through 'collapses' the superposition (2.1) to one or the other of its components, then we recover the experimentally observed result that as soon as the system is disturbed, the superposition is destroyed and the single-slit pattern is recovered. It is only when we leave the system alone that the particles seem to go through 'both slits at once,' interfering to give (2.1).

One could suggest that the particles are interfering with each other, leaving no mystery about single particles going through 'both slits at once'. However, this experiment has been done with only a single electron going through the slit system at any given time, and the interference pattern is still observed [85]. In other words, if we want to represent the individual quantum system, it seems that the superposition/collapse framework is required. Note that this kind of argument reappears in the case of the Stern-Gerlach experiment, in which a beam of atoms splits into two beams (spin up and spin down) no matter which way the apparatus is oriented.

These results are described well by the Copenhagen interpretation, as are many more; the 'collapse of the wave function' works as a way to predict the results of measurements. However, the collapse framework is not the only way to formally account for these results.

Indeed, the causal theory is able to duplicate the two-slit interference pattern. Fig. 2.2[1] shows Dewdney *et al.*'s [80] calculation of the trajectories; as one would expect from the continuity equation (1.5), the distribution of particles at the screen is the same as the standard quantum mechanical distribution, so the interference pattern is reproduced despite the fact that the particles are following well-defined trajectories, and are not behaving like waves. How is this possible?

The wave ψ is different when there are two slits open than when there is only one. As such, in the two-slit system, the wave guides the particle differently when both slits are open. The distribution ρ of particles on the screen duplicates the quantum distribution $|\psi|^2$, as it must according to the continuity equation– but the wave-like properties are evidence of the wave ψ. One might speculate that if the causal theory had been accepted as the standard one in the first place, experiments such as this one would have been taken as evidence that both a wave and particle really exist, rather than as evidence that there can be no classical-style understanding of quantum phenomena.

If one observes the particle at the slit system in an attempt to discover which slit it is going through, then one affects the wave function– according to the theory of measurement in both interpretations. In the causal interpretation, this means that the wave function splits into two non-overlapping packets with macroscopic separation, due to the coupling with the macroscopic apparatus. The particle must be in only one of the packets. That packet then evolves independently of the other, spatially separated, empty packet. The packet then looks just like ψ_1 (for the first slit) and the usual lack of interference pattern results. While the full theory of measurement will not be described here, this essentially means that the measurement process 'decouples' the two packets by coupling the particle position to

[1]Adapted from [18]

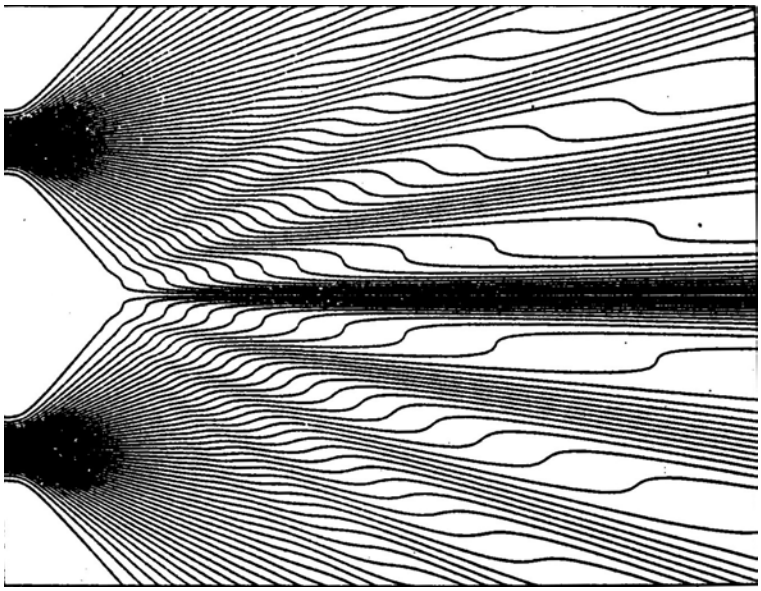


Figure 2.2: Trajectories for the two-slit experiment

a macroscopic measuring apparatus such as a pointer. For a more complete discussion of measurement in the causal interpretation, see [18, 61].

Note that the fact that the causal interpretation duplicates the results of quantum mechanics does not violate the no-hidden-variables theorem of Bell [10] because the causal program is not a local hidden variables theory; it is a nonlocal one. The wave ψ, for example, in the two slit experiment, must be different at slit 1 depending on whether or not slit 2 is open; the trajectories passing through the first slit depend nonlocally, in a 'spooky' way, on whether the second slit is open or not.

The perception that the 'only mystery' of quantum mechanics could not possibly be accounted for according to a classical trajectory paradigm is almost certainly responsible for a good part of the lack of interest in nonlocal hidden variables theories in general and in the causal program in specific. However, the results for the two-slit experiment, as well as the wealth of other calculations done by Dewdney and others (see, for example, [32, 31, 30, 80, 29]) show that it is possible to account for even the most unintuitive quantum experiments while holding to a classical understanding of what a particle is and what it does. The main

sacrifice that must be made is locality.

2.3 General Critiques

It is now generally accepted that the causal interpretation does indeed duplicate the statistical predictions of standard quantum mechanics. However, the fact that it is possible to do this does not automatically make it desirable in the eyes of the physics community. In this section we respond to the most common objections to the theory in general; these are, because they are so general, typically qualitative objections to the features of the causal theory. These objections are typically not credited to particular thinkers, but are common 'basic' objections on which more specific critiques of the theory are based. In the next section, some notable more specific objections to the theory will be addressed.

One of the most common and most fundamental objections to the causal interpretation is that its claims are fundamentally not observable. The centrality of the trajectories in the theory and the fact that it is based primarily on considerations of position mean that the trajectories of the particles being studied are the most basic entities described by the theory. However, the trajectories that it predicts are not (directly) observable due to the uncertainty principle– to observe a trajectory one must observe position and momentum or at least position as a function of time; since position and momentum are non-commuting operators, this would violate the uncertainty principle. Note, however, that the trajectories are not the *only* predictions of the theory; one can use the causal interpretation and still retain the ability to predict the standard probabilistic predictions of quantum theory.

Some objectors go further to say that because the trajectories themselves are not observable, the causal interpretation is nonphysical, or has no physical content. Note that this is a version of the positivist philosophical approach discussed in the previous chapter, due to the identification of physical meaning and content with what can be observed. As such, this version of this objection to the causal interpretation can be included in the positivist

approach to quantum mechanics in general; it was argued in the previous chapter that there are significant drawbacks of this approach.

The objection that the trajectories are not observable (and that they are therefore meaningless) is the main criticism of the causal interpretation given by physicists. However, there are advantages of a trajectory approach. As discussed in section 1.3, questions that are not allowable in the standard theory can be asked and perhaps answered in the causal theory. These include the question of what is the nature of 'reality' i.e. what does the quantum particle 'really' do, and more specific questions such as the question of tunnelling times, as well the nature of quantum transitions. The trajectory view also provides a clear way to approach the question of quantum chaos. Though unobservable, the trajectories do allow answers to questions that stem from a classical paradigm and which physicists seem unwilling to completely abandon.

A trajectory approach, or simply the more general realist approach of the causal interpretation, may also give rise to new questions that would not stem out of standard quantum theory. Part of the role of a theory is to help thinkers understand whatever parts of the world the theory describes, and to build new understandings by forming new hypotheses, which should ultimately be testable. So even if some hypotheses of a theory are not directly testable, the theory might spawn new testable questions. Because there is a role for the imagination in the formation of new hypotheses, it could be an advantage that the causal interpretation embodies a much less defeatist approach to new and imaginative questions based on the 'reality' of physical systems.

An example of this process is the work of Valentini on quantum disequilibrium [88]. In the causal program, it is generally assumed that the distribution of initial conditions is consistent with the quantum distribution

$$\rho(\mathbf{x}, 0) = |\psi(\mathbf{x}, 0)|^2 \tag{2.3}$$

which guarantees via the continuity equation (1.5) that the statistical predictions of standard quantum theory will be the averages over ensembles of trajectories. Bohm and Hiley [18], as well as Valentini [86, 87] have argued that under certain conditions, even if the system does not begin in an equilibrium distribution (by which they mean the $|\psi|^2$ distribution (2.3)), it will in time approach an equilibrium distribution in a coarse-grained sense.

Valentini has taken this notion further, to suppose that there might have been a time shortly after the formation of the universe when the *rules* of quantum theory held but when the distribution of matter had not yet 'relaxed' to equilibrium. Matter in a state of disequilibrium, i.e. matter that satisfies the laws of quantum mechanics except for (2.3) can be shown to violate the uncertainty principle and the no-signalling rule [86, 87]. This hypothesis is in theory testable in that there might be 'relic' disequilibrium particles left over from very early times; these particles would not obey the usual quantum mechanical relationships. Perhaps, for example, they would not give the usual multi-slit interference pattern if they were incident on a set of parallel slits. Valentini's work will be discussed with further in Section 2.5.2.

For the purposes of responding to criticisms of the causal interpretation, it is sufficient to point out that the trajectory approach of the causal program allows the distinction between the quantum distribution $\rho = |\psi|^2$ and the governing rules of quantum mechanics such as the Schrödinger, Pauli or Dirac equations, or the Klein-Gordon equation. This distinction allows the formulation of new, possibly testable hypotheses, though the trajectories themselves are not directly observable.

The objection that because the trajectories are unobservable there is no point in thinking about the interpretation, and it should not be taken seriously as a contending interpretation of quantum mechanics usually relies on the assumption that unobservable things are 'not physical' (the positivist statement), and that things that are 'not physical' can contain no physical content.

As argued in the previous chapter, the statement that 'unobservable things are not phys-

ical' is in itself not observable, and thus it itself implies that it should not be used in constructing a physical theory (any more than any other unobservable statements or entities). Also, irrational numbers are in some sense unobservable, at least directly, as are complex numbers. This does not prevent us from using them as a tool for understanding observable processes, for attributing a functional role to them in our physical theory, as some thinkers have done with the causal theory's trajectories. (See for example [91, 35, 22] for examples motivated by quantum chemistry, and [97, 96, 95, 94] for examples from quantum chaos and dynamical systems.) Scientists typically do not claim that theories that make use of complex or irrational numbers at a fundamental level are 'unphysical' because the tools used are not directly observable.

The argument that something 'unphysical' has no 'physical content' can also be criticized. One could argue that this theory is an example of one which, though it contains elements that are not 'physical' in a directly observable sense, has content in its interpretation, its explanation of quantum phenomena which were not explained (at least ontologically) before, and its approaches to problems in the existing theory such as the ones discussed in the previous chapter. The notion of 'physical content' must surely include observation, prediction, interpretation, understanding, and explanatory power, and should not be limited to observation alone. It is worth noting that the wave function itself is not observable, though the associated 'cloud of probability' is typically used to answer the question of why there is no radiation emitted from atoms in their ground state [61]. Thus, while officially there is no existence accorded to the unobservable wave function in the standard interpretation, since its attributes are taken to explain various experimental facts (including wave-particle duality), it plays an essential role despite its 'unphysical' nature.

Having accepted these arguments, physicists might still ask how, if one is unable to test the theory, one would know whether one is doing something meaningful or not– would the theory not be subject to the scientific method? This comment presupposes that the only way to do something worthwhile or meaningful in science is to do something that is directly

testable through experiment.

The question of testability is of great importance, and in studying the causal interpretation, every effort should be made to ensure that something in the end will be testable– this does not mean that all thinking should result in something that is directly testable at the moment. Because this objection has some merit, in this thesis we will not only study quantum trajectories but discuss the approach to 'quantum equilibrium' via relaxation, and suggest other areas in which the theory could lead to new physics in a standard sense.

We also note that many areas of mathematics are considered worthwhile not through their testability but through their substantive interest and connection to their field within mathematics. In physics, much research is done in areas that are far from testable at the moment (such as string theory, the study of highly theoretical spacetime solutions to Einstein's equations, etc.). Contributing to greater or even different understanding can be useful, as can examining closely the implications of our theories in a variety of observational and interpretational contexts. As with Valentini's work, theoretical results might be testable, where the original tenets of the theory are not *directly* testable.

One could argue that if a process of thought helps a researcher to model a physical system or set of systems in a new and more clear way (as is the case with irrational numbers) then it is a useful enterprise, especially if the new model can lead to questions and understandings that were not available in the old model. Furthermore, though consensus is that the causal interpretation is not experimentally distinguishable from standard quantum mechanics, we do not have a satisfactory theory of quantum measurement, nor a full list of quantities that we will *ever* desire or be able to measure, so it is not clear (at the axiomatic level) that the theory is not observably different from standard quantum mechanics. It does not seem reasonable to reject an interpretation on the grounds of its non-observability in the absence of a well-established, coherent theory of measurement. The work of Valentini [88] and Leavens [68, 74, 67, 66] give examples of the ways in which observable results can emerge from the process of examining quantum phenomena via the causal interpretation.

Even at this point, the physicist who believes in the standard theory might well object that when the standard theory 'does all a theory is supposed to do', what point is there in learning and using a new theory? This is, in a sense, a milder version of the above objection– even if one accepted it is acceptable to use the causal interpretation, one still might not have any particular motivation for doing so.

This objection is typically voiced by physicists who feel that all a physical theory needs to do is successfully predict measurement outcomes for experimental setups. That this is all a theory needs to do is a philosophical assertion not accepted by all. One might, for example, like a theory to be explanatory about the measurements it describes, give rise to a realistic kind of understanding about the systems it describes, give rise to new questions that bring in new experimental contexts, have the possibility of being testable, and extend current theory into new regimes (in this case the classical scale, relativistic velocities). See [26] for a discussion of these and other questions of what a theory is expected to do and why. Standard quantum theory does some of these. The causal theory also does some of them, neither interpretation being perfect. The advantages of the causal interpretation as outlined in Section 1.3 are appealing to a number of physicists and there is growing motivation within the physics community to work on problems in the foundations of quantum mechanics.

One last general objection, commonly voiced, is that the theory is so explicitly nonlocal. Einstein called such nonlocality 'spooky' action-at-a-distance; the nonlocality seems unphysical, and some people think that the causal interpretation cannot be a 'true' description of reality for that reason, and that the interpretation could never be consistent with relativity.

Bell comments in [9] that the standard theory is equally nonlocal in that all observations where both theories ask well-posed questions are the same. Therefore in some sense they contain the same 'amount' of nonlocality. However in the causal interpretation this is explicitly stated. This facilitates the examination of nonlocality and entanglement. Furthermore the causal interpretation provides, through the quantum potential and the existence of the wave in configuration space, a format for a better *explanation* of quantum nonlocality than

is provided in standard quantum mechanics.

With regards to relativity, Peter Holland and others are working on the problem of developing a relativistic version of the causal interpretation. [62, 60, 59] Certainly, there are ways to ascribe trajectories under the Dirac equation, so the theory is somewhat applicable there. It should be noted that standard quantum theory is also not fully consistent with relativity; if the causal theory is to agree with the standard one, this problem is likely to surface in the causal theory as well. Current research seems to indicate that the problem of a relativistic theory is about as difficult in the causal theory as in the standard theory [60].

In summary, the main general criticisms of the causal theory have been that: the trajectories are not observable and that therefore the theory has no physical content beyond the content of standard quantum mechanics, there is no meaning to unobservable quantities and they should not be considered real, the theory does not add anything new even if it is a viable alternative, and the nonlocality in the theory is unintuitive and 'spooky'. We have responded to these concerns by arguing that observable consequences could emerge from the theory indirectly, and that the positivist assertion that only observable things should be present in axiomatic statements of theories is not always tenable in the absence of a theory of measurement. We have also argued that the causal theory does add to standard quantum theory and that there are various insights that can be gained from its examination. The nonlocality in the causal theory is present in a different, less explicit, form in the standard theory; the standard theory is thus equally 'spooky'.

2.4 Specific Critiques

There are a number of more specific criticisms of the causal interpretation that are based on more detailed implications of the theory such as the computation of specific trajectories. In this section we respond to some of these. This section is intended to demonstrate that there are responses to such critiques and to give a few examples; it is not intended as to give a

complete and comprehensive list of all such objections, nor to respond to them. The ones chosen here, namely the 'surrealistic' accusation of Englert, Scully, Sussman and Walter [39], hereafter referred to as Englert *et al.*, and the work of Ghose [45, 44], are fairly well-known examples of criticisms of the causal theory.

2.4.1 An Analysis of the Englert-Scully Scheme

Englert *et al.*'s group found [39] that the Bohm trajectories for the double slit experiment were 'surrealistic', by which they meant 'physically unintuitive'. This is a serious charge for the causal theory especially since one of its advertised features is its return to a classical framework with intelligible results for individual systems. It is therefore worth investigating the charge further. While the we argue that the argument of Englert *et al.* is flawed, their symmetry considerations are fairly general, showing properties of the causal trajectories for a variety of possible experiments.

Englert *et al.* first consider a two-slit experiment and write

$$\psi = \psi_< + \psi_>, \tag{2.4}$$

where $\psi_<$ is the contribution to the overall wave function from the lower slit, and $\psi_>$ is the contribution from the upper slit. Then adding amplitudes yields $P = |\psi|^2 = |\psi_< + \psi_>|^2$, which recovers the usual interference pattern. They consider the particle to be incident parallel to the x-axis, so that the position of the slits is symmetric in z. Thus, the particle travels in the x direction and the z axis is an axis of symmetry. They treat the slit width as negligible, and take the two slits to be at positions $z = z_0$ and $z = -z_0$ on the z axis.

Now, writing the continuity equation for the causal theory (1.5) as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0, \tag{2.5}$$

where $\rho = R^2$, we can identify the density current $\mathbf{j} = \rho\mathbf{v}$ as

$$\mathbf{j} = \frac{R^2 \nabla S}{m}, \tag{2.6}$$

where $\mathbf{v}$ is the velocity (see (1.8)). We assume that the particle does not have spin, for the sake of comparison with Englert *et al.*'s results which are based on the original formulation of the causal theory. Now, note that

$$\psi^* \nabla \psi = R e^{-iS/\hbar} \left(\frac{i}{\hbar} R e^{iS/\hbar} \nabla S + e^{iS/\hbar} \nabla R \right) \tag{2.7}$$

so that

$$\psi^* \frac{\hbar}{i} \nabla \psi = R^2 \nabla S + \frac{\hbar}{i} R \nabla R \tag{2.8}$$

and we have

$$\mathbf{j} = \frac{1}{m} \mathrm{Re}\{\psi^* \frac{\hbar}{i} \nabla \psi\}. \tag{2.9}$$

This means, for example, that we can find the x component of the velocity by computing $\frac{1}{m}\mathrm{Re}\{\psi^* \frac{\hbar}{i} \frac{\partial \psi}{\partial x}\}$. As Englert *et al.* imply, we have

$$j_z = \frac{1}{m} \mathrm{Re} \left\{ (\psi_<^* + \psi_>^*) \frac{\hbar}{i} (\frac{\partial \psi_<}{\partial z} + \frac{\partial \psi_>}{\partial z}) \right\} \tag{2.10}$$

so that

$$\begin{aligned} j_z(-z_0) &= \frac{1}{m} \mathrm{Re} \left\{ (\psi_<^*(-z_0) + \psi_>^*(-z_0)) \frac{\hbar}{i} (\frac{\partial \psi_<(-z_0)}{\partial z} + \frac{\partial \psi_>(-z_0)}{\partial z}) \right\} \\ &= \frac{1}{m} \mathrm{Re} \left\{ (\psi_<^*(z_0) + \psi_>^*(z_0)) \frac{\hbar}{i} (-\frac{\partial \psi_<(z_0)}{\partial z} - \frac{\partial \psi_>(z_0)}{\partial z}) \right\} \\ &= -j_z(z_0). \end{aligned} \tag{2.11}$$

Therefore, j_z is an odd function and $j_z(0) = 0$, so that the trajectories do not cross the z axis. Note that this analysis does use the stated assumption the slit width is negligible,

because the z coordinates are taken to be $\pm z_0$. For now, let us accept this assumption without knowledge of how sensitive the system is to its violation.

Englert *et al.* claim that there exist one-bit which-way detectors that record whether or not an atom has passed through them without significantly altering the wave function. Suppose that we place such detectors just in front of the slits; then the wave function (they argue) becomes not (2.4) but

$$|\psi\rangle = |\psi_{>}\rangle \left|\begin{matrix}\text{yes}\\ \text{no}\end{matrix}\right\rangle + |\psi_{<}\rangle \left|\begin{matrix}\text{no}\\ \text{yes}\end{matrix}\right\rangle, \tag{2.12}$$

where the yes-no wave functions represent the detectors, and we see that there is now a correlation between the original atom and the detectors. The interference pattern is destroyed when the which-way information is available, but Englert *et al.* argue that the symmetry properties of the trajectories are preserved, so that it remains the case that there are no trajectories that cross the z axis.

Suppose now that the upper detector gives a 'yes' result, meaning that the probability distribution on the screen becomes $P = |\psi_{>}|^2$. This distribution does not vanish for $z < 0$, but by (2.11) there are no trajectories taking the particle from the top slit to the bottom half of the screen. Therefore, the atom can be observed at two points which are not connected by any trajectory determined by the causal theory, and the trajectories the theory predicts are physically unintuitive.

One could object that at the detector a process occurs which renders $\psi_{<}$ irrelevant, and therefore that the original symmetric trajectories are no longer the correct trajectories predicted by the causal theory. However, the authors anticipate this and state that this process would require some kind of macroscopic interaction that is not present in the which-way detectors and that may not be present until the information is 'read off', possibly after the atom hits the screen [39]. They claim that the problem remains.

Their argument contains several flaws. First, suppose that they are correct in saying that the symmetry properties of the trajectories are preserved when the detectors are added. If we

represent the wave function as the function given in (2.12), then we are explicitly considering a quantum superposition of two states, where in one of the states the atom goes through the top detector and the top slit, and in the other state the atom goes through the bottom slit and detector. However, representing this as a quantum superposition is contrary to the assumption that one *or* the other detectors fires. If we assume that one or the other detectors has fired by the time the atom goes through the slit system, then the wave function (2.12) should actually be written not as a quantum superposition, but as a statistical mixture, where we have classical probabilities of one half for each of the two distinct possibilities. This statistical mixture is quite a different beast, and one must be careful not to confuse it with the quantum superposition. In other words, in the standard interpretation there is a contradiction between writing the wave function as (2.12) and assuming that one of the detectors has fired. Once this has happened, whether the detector is macroscopic or not, the quantum potential will be altered and the symmetry of the trajectories will be broken. In order to examine this situation using the causal interpretation, one would need to represent the which-way detectors somehow, and include them in the process; they would affect the wave function and the quantum potential.

The representation of the wave function (2.12) is not valid unless we wish to discuss a situation in which the whole system, including the detectors, is in a superposition of the two components. This would imply that the detectors (which Englert *et al.* argue are one-bit) are in a superposition state of having fired and not having fired. While one might be able to do this in such a way as to retain the symmetry of the trajectories, it would also retain the additivity of probability amplitudes and possibly even the original interference pattern.

Dürr, Fusseder, Goldstein and Zanghi [33] reply to Englert *et al.*'s paper. They argue that in the standard interpretation, there is no meaning to the question of which slit a particle 'really' went through; thus the fact that the particle can be observed on the lower portion of the screen and that later, the 'which-way' information can be read off as $|\text{yes}\rangle$ is not readily interpretable. They argue that if one is going to use notions like the path of the

particle, one must use a theoretical framework in which such notions have meaning. While the causal framework does this, standard quantum theory does not, so that comparing the causal trajectory to the 'real' path of the particle (as predicted by the standard theory or as observed) is logically unclear. In orthodox quantum theory, they argue, the use of one bit detectors cannot resolve the problem that the concept of which slit the atom went through has no meaning. It is the causal theory's trajectory that gives it meaning.

In their reply, Englert *et al.* comment that "standard quantum theory has already clarified the significance of Schrödinger's wave function as a tool used by theoreticians to arrive at probabilistic predictions" and comment that it is dangerous to attribute more meaning than this to the wave function. In fact, they eventually conclude that "the state vector ψ serves the sole purpose of summarizing concisely our knowledge...; it enables us to make correct predictions... and a state reduction must be performed whenever we wish to account for newly acquired information about the system" [40]. The 'state reduction' is another way to refer to the collapse of the wave function.

Englert *et at* argue that their framework for discussing path detection is based on the local interaction of the photon with the one bit or which-way detector. However this still seems to assume a classical ontology, that there is a particle and that it follows a path and interacts with a detector; this does not seem to resolve Dürr's point about this contradiction with orthodox quantum theory. Englert *et al.* conclude with a quote of Aharonov: "Bohm's pathbreaking hidden variable theory of 1952 is often accused of artificiality and inelegance, and doubtless it is guilty of both" [1]. This is reminiscent of Bell's comment that no one could find a criticism of the causal theory more specific than 'metaphysical' [12]; it could surely be argued that the Copenhagen interpretation and the idea that the best physics can do is produce a theoretical tool for evaluating probabilities using wave function collapse is equally inelegant and artificial, and metaphysical.

Dürr *et al.* also report an experiment with the controversial 'which way' detectors, in which the detectors destroy the interference pattern as expected but where the 'back

action' of path detection does not affect the momentum of the atom enough to explain this destruction through the usual argument that the acquisition of spatial information causes an increase in uncertainty in momentum which then destroys the interference [34]. Instead they conclude that correlations between the detector and the atom are responsible. In other words, it is of value to consider mechanisms for the destruction of the interference pattern that do not rely on the uncertainty principle; both Dürr's group and Scully's group have discussed this problem. Scully's group seems to conclude that asking too many questions about what is happening in individual systems is not a valid procedure [40].

2.4.2 The argument of Ghose

Phartha Ghose has given several objections to the causal theory, claiming that it is not consistent with standard quantum theory. We will address one of these claims here, given in [45]. Ghose claims that in a two-slit experiment with pairs of particles (each presumed to be going through one of the slits), there is an inconsistency between the de Broglie-Bohm prediction for the probability of joint detection and the standard quantum mechanical prediction of the same quantity.

Ghose's argument goes as follows. Label the two slits A and B, and let the particle positions be given as $(x_i(t), y_i(t))$ where $i = 1, 2$, refers to the particles. The axis of symmetry in the slit system is the y-axis ($x = 0$); the particles travel in the y direction. The eventual detection will be at a screen a distance L from the slit system. Ghose assumes that the screen is sufficiently far from the slits that the waves can be assumed to be plane waves.

Assuming that the pairs of particles are bosons, their symmetric wave function can be written

$$\psi = \frac{1}{\sqrt{2}}\big(\psi_A(x_1, y_1, t)\psi_B(x_2, y_2, t) + \psi_A(x_2, y_2, t)\psi_B(x_1, y_1, t)\big),$$

where ψ_A refers to the wave function due to the first slit and ψ_B refers to that due to the second slit. This wave function is thus analagous to that in (2.4).

As in the slit experiment analysed by Englert *et al.*, this system has a symmetry property such that trajectories cannot cross the y-axis. This is because

$$\psi_A(x_1, y_1, t) = \psi_B(-x_1, y_1, t) \tag{2.13}$$

$$\psi_A(x_2, y_2, t) = \psi_B(-x_2, y_2, t) \tag{2.14}$$

and the wave function is symmetric under reflection in the plane of symmetry. This induces the relation between the velocities:

$$\begin{aligned} v_x(1)(x_1, x_2, y_2, t) &= -v_x(1)(x_1, x_2, y_2, t) \\ v_x(2)(x_1, x_2, y_2, t) &= -v_x(2)(x_1, x_2, y_2, t) \end{aligned} \tag{2.15}$$

Because of the symmetry, the velocities are zero on the axis of symmetry and trajectories cannot cross the axis.

However, Ghose does not take the same direction as Englert *et al.* Instead he argues that translation invariance in the region of the plane near the screen means that the quantity

$$\frac{d}{dt}(\dot{x_1} + \dot{x_2})$$

vanishes, so that

$$x_1(t) + x_2(t) = x_1(0) + x_2(0).$$

Hence, if $x_1(0)+x_2(0) = 0$ then the trajectories will be symmetric about the axis of symmetry.

Ghose then considers an experiment in which many pairs of particles are incident on the screen after coming through the slits as described above, and in which there are detectors at points x_1 and x_2 on the screen. They arrive at times t_i, and the probability of joint detection

is given by

$$\begin{aligned} P_{12} &= \lim_{n\to\infty} \sum_{i=0}^{n} \int dx_i \int dx_2 |\psi|^2 \delta((x_1) - x_1(t_i))\delta((x_2) - x_2(t_i))\delta((x_1(t_i) + x_2(t_i)) \\ &= \lim_{n\to\infty} \sum_{i=0}^{n} P(x_1(t_i), -x_1(t_i)) = 1, \end{aligned} \tag{2.16}$$

which Ghose states does not equal the standard quantum probability of joint detection. The reason given for this is that the trajectories somehow make the particles distinguishable, where in standard quantum theory they are indistinguishable. However Ghose does not explicitly state the standard quantum joint probability.

Louis Marchildon replied to Ghose's argument in [71] and [72]. He argued that it is not reasonable to assume a plane wave, which would imply that the translation invariance assumed by Ghose is not in fact a property of the system. Using spherical waves rather than plane waves, he derives the explicit form

$$\frac{d}{dt}(\dot{x_1} + \dot{x_2}) = \frac{\hbar k}{mL}(x_1 + x_2)$$

which does not vanish. The rest of Ghose's argument then does not follow.

However, it might seem that if the same wave function were chosen in the standard theory as in the causal theory, be it a plane wave or a spherical wave emanating from each slit, some kind of Ghose-type argument might still imply a discrepancy. We argue here that this is not the case.

In (2.16), the presence of the term $\delta((x_1(t_i) + x_2(t_i))$ in the integrand amounts to an assumption that $x_1(t_i) + x_2(t_i) = 0$. In Ghose's framework this is the same as assuming that $x_1(0) + x_2(0) = 0$, which is an approximation of very narrow slits. However, no matter how narrow the slits are, this is still a very special sub-ensemble of the initial distribution. In the causal theory, agreement with standard quantum theory *only* holds if the ensemble of initial positions is distributed according to $\rho = |\psi|^2$. Otherwise, very significant deviations

from standard quantum theory can result [86, 87].

To see this, one could consider the less well-motivated sub-ensemble consisting only of particles going through the top slit in a single-particle two-slit experiment such as that described in the previous section. In this case, all trajectories arrive at the top portion of the slit, clearly in violation of the standard interference pattern. The sub-ensemble chosen by Ghose has the same problem, though Ghose chose a more easily motivated sub-ensemble.

Even if Marchildon's argument that $x_1(t_i) + x_2(t_i) \neq x_1(0) + x_2(0)$ is taken into account, and it is only assumed that

$$x_1(t_i) + x_2(t_i) = 0, \tag{2.17}$$

then (2.17) is still a subensemble of the total system described by the causal theory, and therefore the predictions do not have to agree with the predictions of standard quantum theory.

Ghose responds to Marchildon's arguments in [44], choosing a more reasonable wave function, and arguing more generally that the causal theory is incompatible with the standard theory when the causal system is not ergodic. This is an interesting claim. However, he uses the same kind of sub-ensemble in this more recent work as in his earlier proof, and it can therefore be criticized on the same grounds. Furthermore, Marchildon has again responded, this time numerically, showing that the causal theory reproduces the results of standard quantum theory [73]. This hot debate will no doubt continue. The subject of ergodicity will be discussed again in Section 8.3.

In general, the supposed contradictions between the causal theory and the standard theory must be based in applications of the theories in slightly different ways, or on choices of sub-ensembles such as the one above, or on situations in which one or the other theory does not have clearly well-defined meaning (as Dürr *et al.* argued was the case when Englert *et al.* discussed which slit the particle 'really went through' under the standard interpretation). The result that because of the continuity equation, the distribution of final positions $\rho(t)$ in

the causal theory will always be given by

$$\rho(t) = |\psi(t)|^2$$

whenever

$$\rho(0) = |\psi(0)|^2$$

is not violated by a clever choice of wave function or slit symmetry.

2.5 A Review of Other Literature

2.5.1 Observer-Independent Theories

The literature on the causal interpretation is a subset of the literature about alternative interpretations/theories of quantum mechanics. There are several notable interpretations, which tend to focus on the desire for a quantum theory that does not depend on observers, or presuppose a classical scale. It is instructive, in order to put the causal theory in its proper context and present a review of the literature on the theory, to present a summary of the notable observer-independent interpretations. This subsection will also serve the purpose of presenting reasons for our choice of the causal interpretation over one of these other contenders.

One prominent observer-independent theory, known as the decoherent histories formulation, is primarily the work of Gell-Mann and Hartle [42]. In their interpretation, the 'environment' around a system essentially plays the role of the observer in the Copenhagen interpretation. In addition, one speaks of the probabilities of different histories actually happening; this is to be distinguished from the Copenhagen interpretation which yields only probabilities for measurement results and does not claim to represent what happens in the absence of measurements. To assign these probabilities to different histories, Gell-Mann and Hartle use projection operators. Suppose, for example, that there is a sequence of events

which can be represented with a sequence of projection operators E_i, $i = 1, ..n$. Then the probability for that sequence of events is given by:

$$P(h) = \langle E(h)\psi | E(h)\psi \rangle \,,$$

where $E(h) = E_n \ldots E_2 E_1$ [48]. However, completely 'fine-grained' histories cannot be assigned probabilities, for this would not be consistent with the usual result that not all quantities can be simultaneously known. Thus, the decoherent histories theory does not describe complete trajectories, but it *is* a realist theory. The basis for the decoherent histories formulation is therefore deeply dependent on the criteria by which decoherent histories are chosen. In fact, several such criteria have been explored [18, 42, 48], but it is not a simple matter to discover such criteria that are guaranteed never to assign probabilities to too many different histories, involving incompatible quantities.

In discussing the decoherent histories formulation, Bohm and Hiley point out that Gell-Mann and Hartle wish to create a quantum cosmology, and therefore their theory deals with nothing less than the wave function of the universe itself [18]. One of the possible criteria for decoherence, among other aspects of the theory, depends explicitly on this wave function [18]. While this, as well as the increasingly complex and decreasingly intuitive mathematics needed to define and describe decoherence, are drawbacks of the interpretation, both Bohm and Hiley, and Goldstein [18, 48, 47], point out that decoherent histories do provide an observer independent version of quantum theory, consistent with experimental results, in which the classical world can be seen to emerge without having been presupposed.

An approach to quantum theory that essentially limits the range of wave functions and that thereby avoids certain problems with the standard interpretation was proposed by Ghirardi, Rimini and Weber [43], and is known as 'spontaneous localization'. This theory preserves the Hilbert space formulation of quantum mechanics, while introducing localizing factors into the wave function. Specifically, the new wave function of the n^{th} particle is

written

$$\psi'(x, r_1, ..., r_n, t) = \frac{f(x - r_n)\psi(r_1, ..., r_n, t)}{R_n(x)},$$

where the function f is some suitable localizing function such as a gaussian $f(x) = Ae^{-\frac{x^2}{2\alpha^2}}$ and where $|R_n(x)|^2$ gives the probability distribution of the centre, x. The r_i are the particle coordinates. The constant α is to be a new constant of nature, and since each of the n particles is being localized in this way, the overall localization will increase with the number of particles. The range of the wave function, then, will be reduced with time and will be approximately α after a characteristic time τ/N for some τ, which is also to be a new constant of nature.

The main advantage of this theory is that it gives a consistent account of measurement without presupposing a classical level from which measurements are made [43, 18]. At the macroscopic stage, spontaneous localization shows that the wave functions for large systems are localized enough that interference effects do not occur, while they may still occur for quantum (few-particle) systems [43]. When a measurement is made, the localization is such that the system 'collapses' to a definite result and no Schrödinger cat-like paradox can result. Bohm and Hiley comment that while this theory looks promising, it has all the nonlocality of the standard interpretation, and it involves a certain number of seemingly arbitrary assumptions [18]. It does, however, preserve the Hilbert space formulation, which the causal theory does not emphasize, and which could be considered an advantage.

Perhaps less radical on the surface, but perhaps more important and more widely accepted by physicists, is Leslie Ballentine's statistical interpretation of quantum mechanics [7, 8], which was introduced briefly in Chapter 1. Ballentine argues that the wave function cannot represent an individual system, but rather, represents a statistical ensemble of similar systems. This avoids many problems with the standard theory, particularly the collapse of the wave function. In a statistical ensemble, the meaning of probabilities of measurements is clear: a certain portion of the ensemble will yield a particular measurement in correspondence to the predicted probability.

However, Ballentine goes beyond this reinterpretation. In the discussion of measurement in his book [8], he replaces the standard notion of measurement with a more general one which fails to require that a system be left in an eigenstate of the observable corresponding to the quantity that was measured. Suppose that the system being measured is originally in state $|r\rangle$, and the measuring apparatus is originally in a state $|0, m\rangle$ where m refers to incidental features of the apparatus which are not involved in the measurement. To each $|r\rangle$ there should correspond an α_r which will appear in the state of the apparatus if the system being measured is in state $|r\rangle$. Thus, the usual requirement for measurement can be written

$$U\,|r\rangle \otimes |0, m\rangle = |r\rangle \otimes |\alpha_r, m'\rangle$$

for some measurement operator U. However, Ballentine argues that this is not necessary. Why should the measurement leave the eigenstate $|r\rangle$ as it is? He argues instead that what is minimally necessary for measurement is simply that there exist a unique correspondence between r and α, so that the measurement process can be written

$$U\,|r\rangle \otimes |0, m\rangle = \sum_{r',m'} u_{r,m}^{r',m'}\,|r'\rangle \otimes |\alpha_r, m'\rangle\,,$$

with the restriction that U be unitary.

However, this leads to a puzzling macroscopic superposition in the following way. Suppose that we define

$$\sum_{r',m'} u_{r,m}^{r',m'}\,|r'\rangle \otimes |\alpha_r, m'\rangle = |\alpha_r\rangle\,.$$

This is in part a state of the measuring apparatus, which has macroscopic properties. However, linearity of U implies that if

$$|\psi\rangle = \sum_r c_r\,|r\rangle$$

then

$$U\left|\psi\right\rangle \otimes \left|0,m\right\rangle = \sum_r c_r \left|\alpha_r\right\rangle$$

which is a superposition of macroscopically distinguishable states! Ballentine argues that if a statistical interpretation of the wave function is chosen, this superposition is not a problem as the different possibilities can represent different systems. The superposition is, however, a problem if the mathematics is to represent a single system.

While Ballentine has presented a strong argument for the interpretation of $|\psi\rangle$ as representing a statistical ensemble, he points out that "the Statistical Interpretation considers a particle to always be at some position in space, each position being realized with relative frequency $|\psi(r)|^2$ in an ensemble of similarly prepared experiments" [7]. The statistical interpretation thus is not a positivist theory like standard quantum mechanics; it is a realist theory. The causal program takes this notion further, using the wave function as a generating function to find classical particle trajectories for individual systems.

2.5.2 Literature on the de Broglie-Bohm Causal Theory

The seminal paper on the causal theory was presented by Bohm in 1952 [17]; in this paper Bohm endorsed a version of de Broglie's pilot wave theory of 1927 [28]. Bohm's paper presented the causal theory, and showed that it is a hidden variables theory that recovers all the results of standard quantum theory, a feat which due to the proofs of von Neumann and others was believed to be impossible [90]. It was the original version of the causal theory, as introduced in the previous chapter, and it can be considered to be a hidden variables theory in that the initial conditions are extra 'variables' which, once specified, allow the path of the particle to be deterministically calculated. While de Broglie first conceived of the theory, he abandoned the idea after Pauli objected, at the 1927 Solvay Congress, that the model could not coherently be applied to two-body scattering processes [78].

It was not until Bohm addressed these concerns in his 1952 paper that the causal theory

became accepted as a possible interpretation of quantum mechanics. For the first two decades after 1952, there was not much interest in the theory. Since that time, however, the physics community has had increasing interest partly because of the explicit role of nonlocality in the theory via the quantum potential and the propagation of ψ in configuration space, and the recent experimental interest in nonlocality ([5, 4]). The theory's more satisfying foundations are also a source of appeal.

The recent book of Bohm and Hiley represents the most recent and most complete work by Bohm himself on the matter [18]. Bohm and Hiley introduce the interpretation, and extend the one-particle version to many-body systems. They proceed to examine the question of measurement, treating measurement as a process that does not presuppose a separate, classical scale, and that is not fundamentally reliant on the consciousness or presence of the observer. They also consider the question of nonlocality and show how their causal interpretation and the quantum potential are related to the EPR paradox [37] and Bell's inequalities; they examine the quantum-classical correspondence from the point of view of the theory.

Bohm and Hiley discuss several extensions of the theory; these include the role of statistics and stochastic processes, the Pauli equation, and possible relativistic extensions. While various authors have argued that because the causal formulation recovers the predictions of conventional quantum mechanics, there is nothing new in it, Bohm and Hiley propose extensions to the theory which may deviate from current theory in regimes where the current theory breaks down ([18] pp. 271-296). The book by Bohm and Hiley is one of the clearest introductions to the causal interpretation of quantum theory, and is widely cited in the literature.

However, during the time between the 1952 publication of the theory and the writing of [18], proponents of the theory believed that one reason for the lack of interest from the physics community was the lack of a more lengthy technical examination. This was provided by Holland [61]; his book examines the causal theory in considerable detail. Holland starts

with the relationship between the causal interpretation and classical Hamilton-Jacobi theory; he studies simple applications of the causal interpretation to standard introductory quantum mechanics problems such as simple potentials, tunnelling and interference. He discusses the quantum-classical correspondence, many-body systems, the theory of measurement; in short, all of the required subjects in order to supply the physics community with a good reference on the causal interpretation. Peter Holland is a proponent of the theory and argues that it can yield important insights into quantum processes.

Since that time, Peter Holland has continued to build on Bohm's work, particularly in terms of the search for a way to make the causal theory Lorentz covariant. He has, for example, given an application of the theory to n-body entangled spin-half systems under the Pauli equation, interpreting all of the degrees of freedom in the system via Euclidean tensors [59]. He has also given much thought to the question of uniqueness of trajectories in this kind of causal framework; see for example [62], in which he gives the spin term discussed in the previous chapter and discusses the relationship of uniqueness to Lorentz invariance.

Aside from the theory's own proponents, various physicists have made comments about the potential of the causal theory. J. S. Bell was one of these; he comments that "it is very instructive... it applies to the world at large, not just to idealized laboratory procedures" and that "the de Broglie-Bohm theory is sharp where the usual one is fuzzy and general where the usual one is special" [11]. From Bell's perspective, it is a merit of the theory to bring out quantum nonlocality explicitly and force the physics community to examine the matter. Bell also points out that even Pauli, Rosenfeld and Heisenberg "could produce no more devastating criticism of [the theory] than to brand it 'metaphysical' and 'ideological' " [9]. Bell argues that the theory merits attention, at the very least to play the role of a contrast to the usual interpretation.

Among the earlier and more important results in the causal interpretation is the result of Philippidis, Dewdney and Hiley [80]. They calculated the trajectories predicted by the causal theory for the two-slit experiment, as discussed above, and found that the results agreed

with the usual interference pattern. The same group has completed numerous calculations including spin-dependent trajectories for the Stern-Gerlach experiment and barrier traversal problems (see [32, 31, 30, 29]). This growing body of particular examples, showing that the trajectories really do make intuitive sense in particular problems, has been an important part of the literature on the causal theory. It is, however, by no means all that can be said about the theory.

There has been considerably more interest in the causal program in recent years than in the two decades following Bohm's 1952 paper. For example, Berndl and others [13] have built more mathematical foundations of the theory; they argue that while the causal interpretation solves some of the problems associated with standard quantum theory, it is necessary to show global existence of the particle motion, or solutions to (1.8), in order to interpret (1.5) as the continuity equation in a global sense. They consider approaches to the problem, and derive some criteria for global existence.

Appleby has done more specific work, including an examination of the trajectories for the free particle, focusing on the classical limit [3]. Appleby shows that a necessary and sufficient condition for there to be minimal deviation from classical trajectories in the motion of a free particle is that the state be a narrowly localised wave packet. Appleby also discusses various interpretations of the trajectories. One can, for example, view them as statistical aggregates of individual processes, so that when the velocity is zero it means that the sum of the velocities of the individual trajectories is zero [3]. Appleby has also examined the question of the classical limit in the causal theory in the context of quantum Brownian motion, where it is found that if the system is initially in an approximate energy eigenstate, then the causal trajectory has a tendency to approach the classical trajectory on longer time scales. This requires taking into account the role of the environment in producing the classical limit. Appleby has also examined the question of when a system in contact with a heat bath will behave approximately classically under the causal interpretation [2].

Nogami, Toyama and van Dijk [76] have examined the causal description of a decaying

quantum system. They found that there were deviations from the usual exponential law for very small and very large times. The decay process in the causal version is slower in the beginning than the usual model would suggest. They conclude that while the statistical predictions of quantum theory are also the statistical predictions in the causal framework, the potential to ask questions about individual events offered by the causal view is of value.

Spiller *et al.* [83] agree with this statement; they have examined the trajectories for the one dimensional square potential barrier, in view of finding the tunnelling times predicted by the causal framework. While standard quantum mechanics predicts probabilities that tunnelling will be observed, it does not predict how long the particle will spend in the classically forbidden region [68, 74]. While Spiller *et al.* use an idealized (plane wave) wave function to calculate trajectories analytically, they compare their result to the corresponding result for a Gaussian wave packet. These calculations have been performed both by Spiller *et al.* and by Dewdney and Hiley [30], who give a detailed analysis. These authors conclude that one can indeed think of quantum theory as ensemble of individual processes; one does not need to assume that individual processes are unanalysable, and that furthermore, this results in the predictions of quantities like tunnelling times which are not accessible in the standard framework.

The issue of tunnelling times has been examined in considerable detail by Leavens [68, 74, 67, 66]. He argues that the causal theory gives unambiguous results for tunnelling times, where the standard theory does not; furthermore these tunnelling times are in theory observable. Because there is no good agreement on what the predictions of the standard theory would be, it is not clear that these observations would test the causal theory in comparison to the standard one, but it would at least be possible to verify or refute the predictions of the theory, subject to the uncertainty principle. However, Leavens has concluded that in practice, for the wide range of tunnelling problems he considered, the times would be of the order of $10^{-15}s$, and therefore are not measurable at the moment [66].

Sprung and Wu have a slightly different approach [97, 96, 95, 94]. They ask more general

questions about the causal theory's trajectories in terms of flow properties, looking at collections of trajectories as a flow. They have considered the properties of the flow near nodal points where $\psi = 0$, which they refer to as quantum vortices, as well as on vortices arising in the transport of electrons through a quantum wire [95, 96]. More recently they have studied the relationship between the trajectories and quantum chaos; this is an interesting area of research in that the causal framework gives the opportunity to examine conditions under which quantum systems exhibit classically chaotic trajectories. They argue that the quantum vortex is the main factor driving chaotic motion [97].

The work of Antony Valentini, mentioned in the previous section, adds an interesting new dimension to the causal interpretation. Valentini argues that the rules of evolution of physical systems, including the Schrödinger, Pauli and Dirac equations, might be as they are in the causal interpretation but that the distribution assumption

$$\rho = |\psi|^2$$

might not be fundamental, but instead it might be an 'equilibrium' distribution from which deviation is theoretically possible.

This is not without precedent. Bohm and Hiley argued in their book that if a system did not begin in the quantum $|\psi|^2$ distribution, then it would naturally evolve toward that distribution in time, in a coarse-grained sense. While the fine-grained distribution would never be $|\psi|^2$, if one divided the configuration space into bins and averaged over those coarse-grained bins, the distribution would always come to look like $|\psi|^2$ in time [18].

Valentini has given a quantum analogy to the classical H-theorem [86], in which he shows that a function analogous to H will always decrease with time; furthermore he gives an expression for the characteristic relaxation time τ over which a system will approach quantum equilibrium (see Section 8.3 for further discussion). This, Valentini argues, presents the possibility of new physics based on the idea that there might somewhere be particles which

are not currently in quantum equilibrium. Perhaps these would be relic particles remaining from the creation of the universe, for example. He has shown that such disequilibrium systems, though they would obey the Schrödinger equation or other quantum mechanical equations, would violate uncertainty the no-signalling rule and other predictions of quantum mechanics [89, 86, 87].

Basil Hiley, coauthor of Bohm and Hiley [18], has continued to build upon Bohm's ideas, though his research is not limited to quantum theory. Hiley has also replied in detail to various criticisms of the causal theory. For example, with regard to the surrealistic accusation of Englert *et al.*, he argues in [55] that the trajectories can provide deeper insight into quantum processes, and agrees with Dürr that Englert *et al.* refer to the causal theory giving a 'wrong' answer to the question of which slit the trajectories 'really' go through, where in the standard theory there question of which slit the particle 'really' goes through has no meaning. Hiley, in [55], also replied to a criticism of Griffiths [51] that the causal theory contradicts the consistent histories approach.

Hiley's group (including Oliver Cohen, Owen Maroney, David Robson, Melvin Brown, Robert Callaghan, Milan Glendza, Arleta Griffor, Ryo Morikawa, Lindon Neil and Graham Yendall) is focusing on the idea of wholeness, as evidenced by the interconnected, nonlocal nature of quantum systems shown by the quantum potential, and as applied to large-scale interconnected structures such as space-time. Their goal, in part, has been to develop a mathematical description suitable for non-reductionist theories; this is built upon non-commuting algebras. See [56, 57, 58].

In addition to such theoretical work, the causal theory has recently been playing a significant role in the practical calculations of chemical physics and quantum chemistry: to name only a few references, in quantum tunnelling dynamics [15], nonadiabatic transitions [22], reactive scattering [98], dissociation dynamics [91] and hybrid classical/quantum schemes to study complex systems [35].

The literature on the causal theory has to some extent focused on the debate about

whether the theory is worth considering. What consensus there is seems to say that it is; furthermore, recent interest in nonlocality and the experimental contradictions to Bell's inequalities inspire continued interest in the causal theory and its explanatory framework [5, 4]. In so far as the theory has been examined, there is a focus on the computation of trajectories and on the debate about whether these trajectories are realistic and on what they mean. Researchers such as Holland, Valentini and Hiley are developing the theory and its implications beyond the question of what trajectories look like. However, even in the area of trajectory calculation, the literature is far from complete in its examination.

In the next chapters, we will build on the literature on the causal theory's trajectories with the application of the theory to the eigenstates of the Schrödinger equation. However, we will argue in Chapters 7 and 8 that the application to hydrogen has implications beyond showing that the causal theory's trajectories are intuitive and consistent.

Chapter 3

Eigenstates of the Schrödinger equation

3.1 Introduction

In the previous chapters, we have argued that there is merit in considering the causal theory. We begin our considerations with some calculations showing that the theory can be applied coherently to some simple systems, which should be simple enough to give clearly intelligible, interpretable results, but physically meaningful enough that the coherent application of the causal theory is significant.

We saw in Chapter 1, for example, that the momentum of the stationary wave

$$\psi = e^{ikx}$$

was $\hbar k$ as expected. However, this is not necessarily a convincing application of the causal theory, because the wave function is not normalized, and is used primarily as a simplification.

The causal theory was explored by Bohm and others, and the original theory was developed by Holland extensively in his book [61]. However, the spin term as given in (1.16) was not included in most of these earlier examinations of the theory's applications. Although the

additional term is divergence-free and thus there is no change to the continuity equation, it is by no means guaranteed that the new momentum equation will yield 'intuitively satisfying' trajectories. It would a disadvantage to the theory if it did not, for its intuitive appeal is considered one of its primary virtues.

The original statement of the causal theory, without the additional spin-dependent term given in (1.16), gave the somewhat puzzling result that the momentum of the electron in any s-state of hydrogen will be zero– it will be zero in any real eigenstate of any system. However, this is no longer the case if the additional term is taken into account. This, in addition to the reasons for further exploration of the theory given in the two previous chapters, motivates us to apply the theory to the hydrogen atom, and compute the electron trajectories taking the spin dependence into account.

Consider an electron in the $1s$ ground eigenstate of hydrogen,

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}, \tag{3.1}$$

where $a = \hbar^2/(m_e e^2)$ is the Bohr radius.[1] We assume that the electron is in a definite spin eigenstate: Without loss of generality, let its spin vector be given by $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$. Holland [61] stated that the trajectory is a circle about the z axis, with angular frequency

$$\frac{d\phi}{dt} = \frac{\hbar}{m_e a r}. \tag{3.2}$$

All points on a sphere of radius r orbit the z axis at the same angular velocity. If $r = a$, the angular frequency is on the order of 10^{16} s^{-1}. However, the trajectories for other eigenstates are not given in [61].

In the general case, because the momentum equation (1.16) now involves spin, a full description of the electron in the atom – provided by an appropriate wavefunction – will

[1]For the purpose of avoiding confusion with the quantum number m, we shall denote the mass of the electron as m_e.

have to involve both spatial as well as spin information. Let us denote this "full" wavefunction of the electron by $\Psi(\mathbf{x}, \mathbf{s}, t)$, where $\mathbf{s}$ denotes appropriate spin coordinates. Since the hamiltonian describing the evolution of Ψ is the simple spin-independent hydrogen atom hamiltonian $\hat{H}_0$, we may write Ψ as the tensor product

$$\Psi = \psi(\mathbf{x}, t)\zeta(\mathbf{s}) \tag{3.3}$$

where $\psi(\mathbf{x}, t)$ is a solution of the time-dependent Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}_0\psi, \tag{3.4}$$

and $\zeta(\mathbf{s})$ is an eigenfunction of the (commuting) spin operators $\hat{S}^2$ and $\hat{S}_z$, with $\hat{S}^2\zeta = \frac{3}{4}\hbar\zeta$ and $\hat{S}_z\zeta = \frac{1}{2}\hbar\zeta$. Thus ζ defines the "alpha" or "spin up" state corresponding to the spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$. With this simplification, the remainder of the discussion can focus on the evolution of the spatial portion of the wavefunction $\psi(\mathbf{x}, t)$. Given an initial position $\mathbf{x}_0$ of the electron, and its wave function, (1.16) will determine the initial momentum $\mathbf{p}_0$, and the full trajectory can be computed.

3.2 Eigenstate Trajectories

3.2.1 A Qualitative Analysis

There is considerable information that can be gained from a qualitative analysis of (1.16), as it applies to the Schrödinger eigenstate wave functions, without doing any specific computations. We shall present this analysis in this section, before moving on in the next section to compute several specific trajectories.

We consider an electron with spin vector $\mathbf{s}$ that begins in a hydrogenic eigenstate, i.e., $\psi(\mathbf{x}, 0) = \psi_{nlm}(\mathbf{x})$. Here, ψ_{nlm} are the standard energy-angular momentum eigenstates which are eigenstate of the energy, the orbital angular momentum L and the z-component of the

orbital angular momentum, L_z. They are given by

$$\psi_{nlm} = N_{nlm} e^{-r/na} \big(\frac{2r}{na}\big)^l L^{2l+1}_{n-l-1}(2r/na) Y^m_l(\theta, \phi), \tag{3.5}$$

where the L^{2l+1}_{n-l-1} are the associated Laguerre polynomials, and the $Y^m_l(\theta, \phi)$ are the spherical harmonics. For the moment, the form of the Laguerre polynomials is not relevant; the spherical harmonics are given by

$$\begin{aligned} Y_{\ell m}(\theta, \phi) &= \frac{1}{\sqrt{2\pi}} P_{\ell m}(\cos\theta) e^{im\phi} \\ P_{\ell m}(x) &= \sqrt{\frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}}\frac{1}{2^\ell \ell!}(1-x^2)^{m/2}\frac{d^{\ell+m}}{dx^{(\ell+m)}}(x^2-1)^\ell, \quad m \geq 0 \\ P_{\ell,-m}(x) &= (-1)^m P_{\ell m}(x), \quad m < 0. \end{aligned} \tag{3.6}$$

We use coordinates in which ϕ is the angle measured counter-clockwise from the positive x axis, θ is the angle measured down from the positive z axis and r is the radius. These wave functions will also be represented by

$$\psi_{nlm} = N_{nlm} R_{n\ell}(r) Y^m_l(\theta, \phi),$$

where the $R_{n\ell}(r)$ represent the radial functions.

The wave function may be written

$$\psi_{nlm} = N_{n\ell m} f(r) P_{\ell m}(\cos\theta) e^{im\phi}, \tag{3.7}$$

where $N_{n\ell m}$ is a normalization constant, and the time-dependent wave function is given by

$$\psi(\mathbf{x}, t) = N_{n\ell m} f(r) P_{\ell m}(\cos\theta) e^{im\phi} e^{-iE_n t/\hbar}. \tag{3.8}$$

The function $f(r)$ is

$$f(r) = e^{-r/na}\big(\frac{2r}{na}\big)^l L^{2l+1}_{n-l-1}(2r/na).$$

From (3.8), we see that when $m = 0$, $\nabla S = 0$, and otherwise $\nabla S = (\hbar m/r\sin\theta)\hat{\phi}$. The original momentum that the causal theory would predict from (1.8) is either 0 or a constant in the ϕ direction. The original formulation of the causal theory would thus have predicted that in some states the electron is stationary and that in others, it circles about the z axis. Note that when $\nabla S \neq 0$, it points in the $\hat{\phi}$ direction, and thus is perpendicular to the direction of the spin. The total momentum computed from (1.16) is given by

$$\mathbf{p} = \nabla \log\rho \times \mathbf{s} + \frac{\hbar m}{r\sin\theta}\hat{e}_\phi. \tag{3.9}$$

Some simple qualitative information about the electron trajectories is readily found from examining the extra term. First, the vector $\nabla \log\rho$ points in the direction of the steepest increase in $\log\rho$, hence in $\rho = |\psi|^2$. Because of the cross product, the additional momentum vector is perpendicular to this direction, so that its contribution to the motion is along level surfaces of $|\psi|^2$. The additional momentum is also perpendicular to the direction of the spin, assumed to lie along the z axis in this discussion. This implies that the additional term does not change the fact that z is constant along trajectories.

In the $1s$ state, $\nabla S = 0$ and the momentum is due to the $\nabla \log\rho \times \mathbf{s}$ term. The wave function is a function of r only, so that surfaces on which ψ is constant are spheres. Since the spin is assumed to be in the z direction, the fact that $\nabla \log\rho \times \mathbf{s}$ is perpendicular to the spin implies that z is constant. The intersections of planes of constant z and spheres (with constant r) are circles about the z axis. Thus, the additional momentum term $\nabla \log\rho \times \mathbf{s}$ yields a circular trajectory about the z axis. This is in contrast to the trajectory which would result from ∇S alone for the ground state, namely that the momentum is identically zero. While this qualitative analysis gives the shape of the trajectory, the angular velocity of this orbit cannot be determined from this analysis.

For the $2s$ case, with quantum numbers $(n, l, m) = (2, 0, 0)$, the wavefunction is given by

$$\psi_{200} = \frac{1}{\sqrt{32\pi a^3}}(1 - \frac{r}{2a})e^{-r/2a}. \tag{3.10}$$

Like the ground state wave function, this wave function has $\nabla S = 0$ so that the entire trajectory is determined by the properties of the spin-dependent extra term $\nabla \log \rho \times \mathbf{s}$. The level surfaces of ψ_{200} are spheres whose intersection with planes of constant z are circles about the z axis.

In the $2p_0$ case, $(n, l, m) = (2, 1, 0)$, the wavefunction is given by

$$\psi_{210} = \frac{1}{\sqrt{32\pi a^5}} r e^{-r/2a} \cos\theta. \tag{3.11}$$

The condition that both $|\psi|^2$ and z be constant can be written

$$|\psi_{210}|^2 = \frac{1}{32\pi a^5} e^{-r/a} (r\cos\theta)^2 = \frac{1}{32\pi a^5} e^{-r/a}(C) = \text{constant},$$

which can be satisfied only if both r and θ are constant, once again yielding circular orbits about the z axis.

In the other $2p$ cases, $(n, l, m) = (2, 1, \pm 1)$, the wavefunctions are given by

$$\psi_{21(\pm 1)} = \mp \frac{1}{\sqrt{32\pi a^5}} r e^{-r/2a} \sin\theta e^{\pm i\phi}. \tag{3.12}$$

We know that ∇S gives a contribution to the momentum only in the $\hat{\phi}$ direction. This implies that it does not affect $|\psi|^2$, which remains constant. The condition $\rho = |\psi|^2 = \text{constant}$ yields a relation $r = r(\theta)$ defined implicitly by

$$\sin\theta = \frac{K}{r} e^{r/2a}, \tag{3.13}$$

where K is a constant. Since $z = r\cos\theta$ is also constant, it follows that both r and θ are

constants of motion so that the spin term implies circular motion about the z-axis. Because $m \neq 0$, this momentum must be added to the momentum given by ∇S, also in the $\hat{e}_\phi$ direction; the total momentum is in the $\hat{e}_\phi$ direction and the trajectories are again circles about the z axis.

We can generalize this qualitative analysis to apply to all of the eigenstates given by (3.5). The part of the momentum resulting from ∇S will not affect the fact that $|\psi|^2$ is constant, because $|\psi|^2$ never depends on ϕ. The condition that the momentum be perpendicular to the spin vector means that motion is constrained to a plane of constant z, so that $z = r\cos\theta$ is constant. Furthermore, because $|\psi|^2$ is constant, from (3.7) we have

$$f^2(r)P^2_{\ell m}(\cos\theta) = K = \text{constant} \tag{3.14}$$

as well. Inserting $r\cos\theta = C$ and rearranging gives

$$f^2\big(\frac{C}{\cos\theta}\big) = \frac{K}{P^2_{\ell m}(\cos\theta)}. \tag{3.15}$$

However, this relationship is not satisfied identically by the functions $f(r)$ and $P_{\ell m}(\cos\theta)$; the only way for it to be true in general is if both r and θ are constants of motion. This yields circular motion about the z axis, as anticipated, for all eigenstates given by (3.5).

3.2.2 A More Detailed Dynamical Description of the Trajectories

Though the above analysis shows the shape of the trajectories for the relevant eigenstates, it has limitations. The time-dependence in particular is not available by such methods. At this point, the periodicity of the behaviour is not even guaranteed, for the electron could in theory follow a complicated path along the circular trajectory. It is therefore desirable to extract quantitative information such as the angular velocity $d\phi/dt$ of the circular orbits. We first analyze the differential equations of motion defined by (3.9).

The gradient term from (3.9) is given by

$$\nabla \log \rho = \nabla \log \psi^* \psi = 2\mathrm{Re}\left(\frac{(\nabla\psi)\psi^*}{\psi\psi^*}\right). \tag{3.16}$$

For real wavefunctions, this simplifies to

$$\nabla \log \rho = 2\frac{\nabla\psi}{\psi}. \tag{3.17}$$

In spherical polar coordinates (r, θ, ϕ), the spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$ is given by

$$\mathbf{s} = \frac{\hbar}{2}(\cos\theta\hat{r} - \sin\theta\hat{\theta}). \tag{3.18}$$

It is convenient to compute the cross product in the (right-handed) spherical polar coordinate system:

$$\mathbf{A} \times \mathbf{B} = \begin{vmatrix} \hat{\theta} & \hat{\phi} & \hat{r} \\ A_\theta & A_\phi & A_r \\ B_\theta & B_\phi & B_r \end{vmatrix}. \tag{3.19}$$

For the $1s$ ground state defined in (3.1), $\nabla\psi = -\frac{1}{a}\psi\hat{r}$. Thus

$$\mathbf{p} = \frac{\hbar}{a}\sin\theta\hat{\phi}. \tag{3.20}$$

Since $p_r = p_\theta = 0$, it follows that r and θ are constant, implying that z is constant, i.e. circular orbits about the z-axis. Holland's result in (3.2) follows.

For the $2s$ wavefunction defined in(3.10),

$$\frac{\nabla\psi_{200}}{\psi_{200}} = -\frac{1}{2a}\left[\frac{1}{1-\frac{r}{2a}} + 1\right]\hat{r}, \tag{3.21}$$

so that

$$\mathbf{p} = -\frac{\hbar}{2a}\sin\theta\left[\frac{1}{1-\frac{r}{2a}} + 1\right]\hat{\phi}. \tag{3.22}$$

Once again r and θ are constant. From the relation $d\phi/dt = p_\phi/mr\sin\theta$, we have

$$\frac{d\phi}{dt} = -\frac{\hbar}{2m_e ar}\left[\frac{1}{\frac{r}{2a}-1} - 1\right]. \tag{3.23}$$

Note that the pole at $r = 2a$ coincides with the zero of the $2s$ wavefunction, implying that the probability of finding the electron at $r = 2a$ is zero. Also note that (i) $\dot{\phi} > 0$ for $0 < r < 2a$, (ii) $\dot{\phi} < 0$ for $2a < r < 3a$, (iii) $\dot{\phi} = 0$ for $r = 3a$ and (iv) $\dot{\phi} > 0$ for $r > 3a$. For $r = a$, the angular velocity $\dot{\phi}$ is equal to that of the $1s$ ground state.

For the $2p_0$ state defined in (3.11),

$$\frac{\nabla\psi_{210}}{\psi_{210}} = \frac{1}{r}(1 - \frac{r}{2a})\hat{r} - \frac{\sin\theta}{r\cos\theta}\hat{\theta}. \tag{3.24}$$

From (3.9),

$$\mathbf{p} = \frac{\hbar\sin\theta}{2a}\hat{\phi}, \tag{3.25}$$

implying that

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e ar}. \tag{3.26}$$

This is one-half the angular velocity for the $1s$ ground state.

For the $2p$ states with $m = \pm 1$, whose wave functions are given in (3.12), the spherical symmetry has been lost and we find for $m = 1$ that

$$\mathbf{p} = -\frac{\hbar}{r}\left[\sin\theta(1 - \frac{r}{2a}) + \frac{\cos^2\theta}{\sin\theta} - \frac{1}{\sin\theta}\right]\hat{\phi}. \tag{3.27}$$

Here, the last term in the brackets is the term from the original ∇S momentum, which must be added because the wave function is not real. The angular rate of revolution is given by

$$\frac{d\phi}{dt} = \frac{p_\phi}{m_e r\sin\theta} = \frac{\hbar}{2m_e ar}. \tag{3.28}$$

For each of the hydrogen eigenstates studied above, the trajectories are circular orbits

about the z axis with *constant* rates of angular revolution. The fact that it is the z axis that is the axis of symmetry is due to the assumed orientation of the electron spin vector $\mathbf{s}$.

However, the eigenstates as given are not the only possible eigenstates; in the cases where there is degeneracy, for example, various linear combinations can be formed. In these cases, the trajectories will not always be circles about the z axis; in fact, there can be considerable complexity.

3.2.3 The $2p_x$ and $2p_y$ Real Eigenstates

We now examine the causal trajectories for the real hydrogen wavefunctions [69],

$$\begin{aligned} \psi_{2p_x} &= Nre^{-r/2a}\sin\theta\cos\phi \\ \psi_{2p_y} &= Nre^{-r/2a}\sin\theta\sin\phi, \end{aligned} \tag{3.29}$$

where $N = 1/\sqrt{32\pi a^5}$. The probability distributions associated with these wavefunctions are the familiar orbitals used in descriptions of organic chemical bonding [69]. It is therefore of interest to find the Bohm trajectories for these wave functions.

The ψ_{2p_x} and ψ_{2p_y} wavefunctions are obtained by appropriate linear combinations of the energetically degenerate eigenfunctions $\psi_{21(\pm1)}$ of (3.12). As such, they are also eigenfunctions of the hydrogen atom hamiltonian $\hat{H}_0$ with energy E_2; they are also eigenstates of L^2. However, they are not eigenstates of L_z, so we cannot expect the same rotation about the z axis that we have seen in the previous eigenstates.

Because the wave functions are real, $\nabla S = 0$. The cross product of (3.9) has components in all three variables, resulting in a system of three coupled ordinary differential equations which must be integrated to find the trajectories.

The system of ordinary differential equations associated with the ψ_{2p_x} wavefunction is

given by

$$\begin{aligned}
\frac{dr}{dt} &= -\frac{\hbar}{mr}\tan\phi \\
\frac{d\theta}{dt} &= -\frac{\hbar}{mr^2}\cot\theta\tan\phi \\
\frac{d\phi}{dt} &= -\frac{\hbar}{mr^2}(1-\frac{r}{2a}+\cot^2\theta).
\end{aligned} \tag{3.30}$$

From the first two differential equations, we have

$$\frac{dr}{d\theta} = r\tan\theta, \tag{3.31}$$

which is easily integrated to give $z = r\cos\theta = C$, in agreement with our earlier analysis. It also follows from (3.30) that r and θ are constant when $\phi = 0$ or π. If $\theta = \pi/2$ as well, then $\dot{\phi} = 0$ for $r = 2a$, implying the existence of two equilibrium points at $(x, y, z) = (2a, 0, 0)$ and $(-2a, 0, 0)$. At these points, the electron is stationary. In fact, these are two particular cases of an infinity of equilibrium points that are given by the conditions $\phi = 0, \pi$ (the xz plane) and

$$1 - \frac{r}{2a} + \cot^2\theta = 0. \tag{3.32}$$

By virtue of the above relation and (3.27), the equilibrium points of this system lie on the two curves defined by (3.32) in the xz plane as well as their reflections about the z axis. Each of these points corresponds to the points of highest and lowest "elevation" (from the horizontal xy plane) of the familiar dumb-belled level surfaces $\rho = \psi^2 = C$ of the orbital. At all of these points, the electron is stationary.

The system of equations in (3.30) may be integrated numerically. To do this, it is useful to introduce the dimensionless variables $\xi = r/a$ and $\tau = \omega_0 t$, where

$$\omega_0 = \frac{E_2 - E_1}{\hbar} = \frac{3\hbar}{8ma^2} \tag{3.33}$$

is the angular frequency associated with the $n = 1$ to $n = 2$ transition in the hydrogen atom

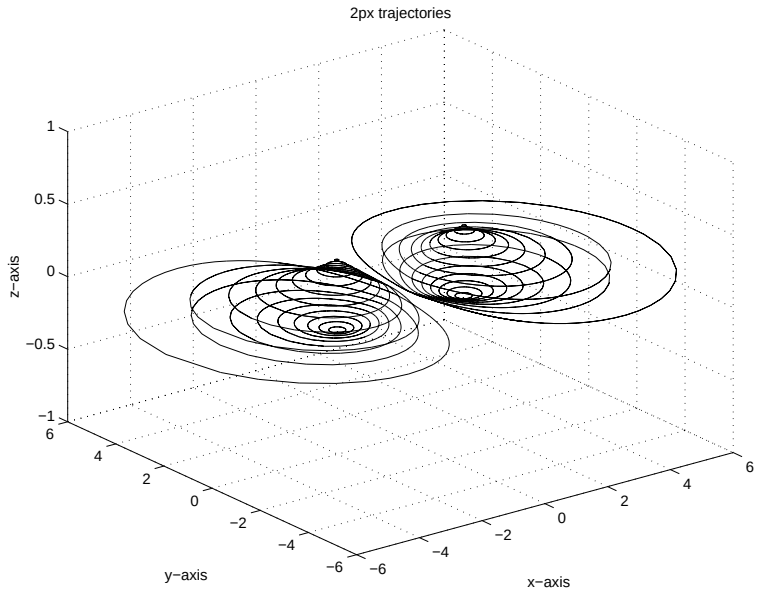


Figure 3.1: Spin-dependent Bohm trajectories for the $2p_x$ hydrogen eigenstate

($\omega_0 \approx 1.549 \times 10^{16}$ s^{-1}). The scaled equations become

$$\begin{aligned}
\frac{d\xi}{d\tau} &= -\frac{8}{3\xi}\tan\phi \\
\frac{d\theta}{d\tau} &= -\frac{8}{3\xi^2}\cot\theta\tan\phi \\
\frac{d\phi}{d\tau} &= -\frac{8}{3\xi^2}(1-\frac{\xi}{2}+\cot^2\theta).
\end{aligned} \tag{3.34}$$

Figure 1 shows the numerically integrated trajectories for several initial conditions in the xz plane. Note that there is a good qualitative agreement between these trajectories and the orbital shapes of the $2p_x$ state as depicted in textbook contour plots [69]. (No orbits cross the yz plane since it is a nodal surface.) The numerical results confirm that motion is periodic. The angular frequency is observed to be on the order of ω_0, 10^{15}. These periodic orbits are stable in the sense of Lyapunov; two trajectories with nearby initial conditions remain near each other.

The nondimensional and numerical analysis of the $2p_y$ case proceeds in a similar fashion. The resulting system of differential equations represents a rotation of the system in (3.30)

by an angle of $\pi/2$ in ϕ.

To summarize this section, we have shown that the spin-dependent trajectories for the ground and first excited states of the hydrogen atom are stable periodic orbits. There are no exceptional orbits that deviate from this regularity. For some of the $2p$ states, these orbits include families of stationary points that have zero Lebesgue measure in $\mathbf{R}^3$. These results are intuitively more acceptable than the original prediction of the causal theory that *all* trajectories associated with some eigenstates are stationary.

3.3 Concluding Remarks

The first set of applications of the causal theory has shown that the theory gives reasonably intuitive results when applied to a simple but physically reasonable system. The trajectories of the electron about the hydrogen atom in all eigenstates of the energy, orbital angular momentum and z-component of the orbital angular momentum have been shown to be circles about the z axis, and the angular rates of revolution have been found explicitly for the $n = 1$ and $n = 2$ eigenstates. The rates of revolution are constants, implying that motion is periodic, and is fairly simple; the electrons do not reverse direction, but proceed in an orderly fashion around the circular trajectories. Table 3.1 summarizes the results of the computation of angular rotation rates, for future reference.

In addition, it is an achievement for this periodicity to appear again in the $2p_x$ and $2p_y$ eigenstates. We knew beforehand that the *density* of the trajectories would be as it is in standard quantum mechanics, so long as the initial conditions were chosen with a $|\psi|^2$ distribution. This does not, however, imply that the orbits follow the qualitative shape of the well-known orbital wave function densities. The additional result that the trajectories are as shown in Fig. 1 is new, as is the periodicity of motion on those trajectories.

The results given in this chapter are the first step in developing the causal theory as applied to the hydrogen atom, when the spin is taken into account. However, the spin has

Quantum Number n, ℓ, m	**Rotation rate** $d\phi/dt$
$1, 0, 0$	$\frac{\hbar}{m_e a r}$
$2, 0, 0$	$\frac{\hbar}{2m_e a r}(\frac{1}{1-\frac{r}{2a}} + 1)$
$2, 1, 0$	$\frac{\hbar}{2m_e a r}$
$2, 1, \pm 1$	$\frac{\pm\hbar}{2m_e a r}$

Table 3.1: Angular rates of revolution for Schrödinger eigenstates

been taken into account only in the simplest possibly way, as we have assumed that the spin is constant. In the next chapter, the spin is taken into account further, when the trajectories for the electron in eigenstates of the hydrogen atom are found for the Pauli equation.

Chapter 4

Eigenstates of the Pauli Equation

4.1 Introduction

While the spin term certainly changed the nature of the causal theory's application to atomic systems even within the context of the Schrödinger equation, the Schrödinger equation does not constitute a full inclusion of spin, because it is assumed that the spin remains constant (see (3.3) and the following discussion). Thus, in order to more fully take the spin into account, the next logical step is to examine the causal theory under the Pauli equation. The Pauli equation is the non-relativistic limit of the Dirac equation, and includes the spin via its description of the wave function not as a single function but as a two-component spinor.

Under the assumptions of the previous chapter, it was seen that the trajectories for the electron in the hydrogen atom under the Schrödinger equation are circles about the z axis. Here, we will see that for the most closely comparable eigenstates of the Pauli equation, the results of the causal theory are very similar and are in agreement in the relevant limiting cases.

The Pauli equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m_e}(-i\hbar\nabla + e\mathbf{A})^2\psi + \frac{e\hbar}{2m_e}\boldsymbol{\sigma}\cdot\mathbf{B}\psi - eV\psi \tag{4.1}$$

describes the time evolution of the wave function ψ, where ψ is a two-component wave function (or Pauli spinor), and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the three 2×2 Pauli matrices. Note that, following Bohm and Hiley [18], we have used units in which $c = 1$, and recall that we denote the magnitude of the electric charge by e. (4.1) is obtained from the relativistic Dirac equation by taking the non-relativistic limit, in which the two smaller components of the 4-component Dirac wave function are neglected; the Pauli equation thus describes the evolution of the two large components [14].

In the case of the hydrogen atom, the Pauli equation reads

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_e}\nabla^2\psi - \frac{e^2}{r}\psi. \tag{4.2}$$

This is obtained from (4.1) by setting the magnetic field $\mathbf{B}$ and the vector potential $\mathbf{A}$ equal to zero, and setting the (scalar) potential V to be the Coulomb potential $V = e/r$, where e is the electric charge. Equation (4.2) gives rise to the current [54, 52]

$$\mathbf{j} = \mathbf{j}_A + \mathbf{j}_B = \frac{\hbar}{2m_e i}(\psi^\dagger\nabla\psi - \psi\nabla\psi^\dagger) + \frac{\hbar}{2m}\nabla \times (\psi^\dagger\sigma\psi). \tag{4.3}$$

The first term $\mathbf{j}_A$ is referred to as the Schrödinger current because one can write the term ∇S as

$$\nabla S = \frac{\hbar}{2m_e}(\psi^\dagger\nabla\psi - \psi\nabla\psi^\dagger)$$

and ∇S was the original momentum term for the causal theory under the Schrödinger equation. The second term $\mathbf{j}_B$ is the spin-dependent term, which reduces to $\nabla \log\rho \times \mathbf{s}$ if the system is in an eigenstate of the spin operator. In this case (4.3) reduces to (1.16). The velocity is obtained from the current by the relation

$$\mathbf{v} = \frac{\mathbf{j}}{\rho} \tag{4.4}$$

where $\rho = \psi^\dagger\psi$; this is the generalization of the original causal formulation to the fully

spin-dependent, but non-relativistic, case. (For further discussion, see [18]).

To show that $\mathbf{j}_B$ reduces to $\nabla \log \rho \times \mathbf{s}$ in the case that the particle is in an eigenstate of s_z, we must relate $\frac{\hbar}{2m}\nabla \times (\psi^\dagger \sigma \psi)$ to $\nabla \log \rho \times \mathbf{s}$. We do this in the case that

$$\psi = \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix},$$

in other words we assume that the wave function is an eigenfunction of s_z in the 'up' direction. Computing $(\psi^\dagger \sigma \psi)$ gives

$$(\psi^\dagger \sigma \psi)_x = 0 = (\psi^\dagger \sigma \psi)_y, \qquad (\psi^\dagger \sigma \psi)_z = |\psi_1|^2 = \rho.$$

Taking the curl gives

$$\nabla \times (\psi^\dagger \sigma \psi) = \frac{\partial \rho}{\partial y}\hat{e}_x + \frac{\partial \rho}{\partial x}\hat{e}_y.$$

Now, when $\mathbf{s} = \frac{\hbar}{2}\hat{e}_z$, we have

$$\nabla \rho \times \mathbf{s} = \frac{\hbar}{2}\left(\frac{\partial \rho}{\partial y}\hat{e}_x + \frac{\partial \rho}{\partial x}\hat{e}_y\right).$$

Thus,

$$\mathbf{j}_B = \frac{\hbar}{2m}\nabla \times (\psi^\dagger \sigma \psi) = \frac{1}{m}\nabla \rho \times \mathbf{s}.$$

The last term corresponds to a velocity

$$\mathbf{v}_B = \frac{\mathbf{j}_B}{\rho} = \frac{1}{m}\frac{\nabla \rho \times \mathbf{s}}{\rho}$$

which corresponds to the momentum term

$$\mathbf{p}_B = \nabla \log \rho \times \mathbf{s},$$

in agreement with (1.16). Holland's argument that this term is necessary in the Schrödinger theory is based on this derivation (see [62, 54, 52, 53]) and on Holland's argument that while the original Schrödinger momentum

$$\mathbf{p} = \nabla S$$

is not unique, the Dirac current (see Chapter 5) is unique, and the non-relativistic limit ultimately requires the addition of $\nabla \log \rho \times \mathbf{s}$ to the momentum [62]. As we shall see, if this term were not used in the Schrödinger context, there could be no agreement between the Pauli trajectories and the Schrödinger ones.

Thus, the extra term in (1.16) which was not included in the original formulation of the causal theory does not need to be added to the momentum here, as it is implicitly already present in the dependence of the current on the spin. Therefore, the work that was done on the Pauli equation by Bohm and others [19, 18] is relevant. Indeed, Bohm showed that the trajectories, with a suitable choice of eigenfunction, are again circles about the z axis. However, this result did not agree with the Schrödinger results at that time for the Pauli eigenstates that also happen to be spin eigenstates, because the Schrödinger momentum for those states was identically zero. This could potentially have been a worrying fact about the causal theory, as the theory's intuitive appeal is one of its claimed advantages. The notion that the Pauli equation would give a different trajectory for the electron than the Schrödinger equation for the ground ($1s$) state, for example, is not intuitively appealing.

In this chapter we examine the application of (4.3) to the hydrogen atom eigenstates, which are two-component solutions to the Pauli equation. While it was known before this work was done that the trajectories would be circles about the z-axis, we apply the causal theory to hydrogen eigenstates and fully compute the rates of revolution, so that they may be compared in relevant cases to the results of the previous chapter. However, the choice of eigenstates is not as clear as it was in the Schrödinger case, where we assumed a spin eigenstate and chose the usual energy eigenfunctions spin-independent wave functions. Therefore, it is worth briefly discussing which eigenstates shall be chosen, and why.

In the case of the Schrödinger equation for hydrogen, it is usually assumed that spin interactions are negligible so that the wave function can be written as a product of spatial- and spin-dependent terms (see (3.3)):

$$\Psi = \psi(\mathbf{r}, t)\zeta(\mathbf{s}). \tag{4.5}$$

As is well known, the spatial hydrogenic energy Schrödinger eigenfunctions,

$$\psi_{n,\ell,m}(r, \theta, \phi) = R_{n,\ell}(r)Y_{\ell m}(\theta, \phi), \tag{4.6}$$

which are solutions to the (spinless) time-independent Schrödinger equation, are also simultaneous eigenstates of the orbital angular momentum operator L^2, with eigenvalues $\hbar^2\ell(\ell+1)$, and the operator L_z, with eigenvalues $\hbar m$. These are the familiar eigenfunctions which were discussed in the previous chapter.

Under the Pauli and Dirac equations, rather than taking eigenfunctions of the hamiltonian and L^2, the total orbital angular momentum operator, one considers eigenfunctions of the hamiltonian and M^2, the total angular momentum operator. This is because the orbital and spin angular momenta combine– they are no longer independent and it is not generally true that L^2 commutes with H. For both the Pauli and Dirac equations, each component of M, the total angular momentum operator, commutes with the Hamiltonian H, implying that M^2 commutes with H as well. For this reason, it is conventional to choose eigenstates of H, M^2 and M_z, with eigenvalues E_n, $\hbar^2 j(j + \frac{1}{2})$ and $\hbar m$, respectively.

In the Pauli case, considered in this chapter, it also happens that the orbital angular momentum operator L^2 commutes with the hamiltonian. Thus, we are free to choose eigenstates which are eigenstates of L^2 with eigenvalue $\hbar^2\ell(\ell + 1)$, as well as M^2. These will be the eigenstates chosen here; note that the z direction is 'singled out' because the eigenstates are chosen to be eigenstates of M_z, though the spin is no longer assumed to be constant. The eigenstates are thus characterized by quantum numbers $n, \ell, j,$ and m, corresponding

to the operators $H, L^2, M^2 \text{and} M_z$, with corresponding eigenvalues E, $\hbar^2\ell(\ell+1)$, $\hbar^2 j(j+\frac{1}{2})$ and $\hbar m$ respectively.

Finally, in the following discussions, the time-dependent phase factor $e^{-iE_nt/\hbar}$ that accompanies the eigenfunctions in the solution of the time-dependent Pauli and Dirac equations will be ignored since it contributes nothing to the associated currents.

The relevant eigenfunctions are given by [14]

$$\psi_{n,\ell,j=\ell+\frac{1}{2},m} = \frac{1}{\sqrt{2\ell+1}} R_{n\ell}(r) \begin{pmatrix} \sqrt{\ell+m+\frac{1}{2}}\ Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\ -\sqrt{\ell-m+\frac{1}{2}}\ Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix} \tag{4.7}$$

and

$$\psi_{n,\ell,j=\ell-\frac{1}{2},m} = \frac{1}{\sqrt{2\ell+1}} R_{n\ell}(r) \begin{pmatrix} \sqrt{\ell-m+\frac{1}{2}}\ Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\ell+m+\frac{1}{2}}\ Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}. \tag{4.8}$$

Here, $R_{n\ell}(r)$ are the usual radial wavefunctions for the hydrogen atom, and $Y_{\ell,m\pm\frac{1}{2}}(\theta,\phi)$ are the usual spherical harmonics.[1] We use polar coordinates in which r is the radius, ϕ is the angle measured counterclockwise from the $x-$axis and θ is the angle measured down from the z-axis.

The eigenfunctions given in (4.7) and (4.8) can be classified as follows: For each n, we have possible ℓ values of $\ell = 0, 1, ..., n-1$. For each ℓ value, m can assume the values $m = -\ell + 1/2, -\ell + 3/2, ..., \ell - 1/2$ (or $m = -j, ..j$), and for each of these there are two possibilities given by $j = \ell + 1/2$ and $j = \ell - 1/2$; hence the form of (4.7) and (4.8). See [14] for a discussion of these constraints.

[1] These are as given in (3.6). We use this convention for the relevant functions for consistency with [14]:

$$Y_{\ell m}(\theta,\phi) = \frac{1}{\sqrt{2\pi}} P_{\ell m}(\cos\theta) e^{im\phi}$$
$$P_{\ell m}(x) = \sqrt{\frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}}\frac{1}{2^\ell \ell!}(1-x^2)^{m/2}\frac{d^{\ell+m}}{dx^{(\ell+m)}}(x^2-1)^\ell, \quad m \geq 0$$
$$P_{\ell,-m}(x) = (-1)^m P_{\ell m}(x), \quad m < 0.$$

In the next section, we derive some general results for the trajectories of the electron in these eigenstates. In the following section, the first few trajectories are computed explicitly for the sake of comparison to the Schrödinger case presented in the previous chapter.

4.2 General Hydrogen Eigenstates

As noted above, the wave functions given in (4.7) and (4.8) are eigenfunctions of L^2 (the orbital angular momentum), with eigenvalue $\ell(\ell+1)$, M^2 (the total angular momentum) with eigenvalue $j(j+1)$, and M_z (the z-component of the total angular momentum) with eigenvalue m. They are *not* in general eigenstates of s_z, the spin in the z- direction. However, some of these states, namely the ones in which one component of the spinor vanishes, *are* eigenstates of s_z. We will refer to these states as 'spin eigenstates'. For these states, we expect that the rate of angular rotation will agree with the rate found in the previous chapter, using the Schrödinger equation and assuming that all the states were spin eigenstates. In other cases, where neither component of the spinor vanishes, there is no particular reason to expect that the trajectories will agree with the Schrödinger trajectories.

Examining (4.3) and (4.4), we write the two contributions to the velocity as follows:

$$\mathbf{v}_a = \frac{\mathbf{j}_a}{\rho} = \frac{\hbar}{2m_e i}\frac{(\psi^\dagger\nabla\psi - \psi\nabla\psi^\dagger)}{\psi^\dagger\psi} = \frac{\hbar}{m_e}\frac{\mathrm{Im}(\psi^\dagger\nabla\psi)}{\psi^\dagger\psi} \tag{4.9}$$

and

$$\mathbf{v}_b = \frac{\mathbf{j}_b}{\rho} = \frac{\hbar}{2m_e}\frac{\nabla\times\mathbf{s}}{\psi^\dagger\psi} \tag{4.10}$$

where $\mathbf{s} = \psi^\dagger\sigma\psi$ is the 'spin vector', and m_e is the mass of the electron. The problem of finding trajectories for the above hydrogen eigenstates is now expressed as the problem of computing $\mathbf{v}_a$ and $\mathbf{v}_b$ for the wave functions given in (4.7) and (4.8).

We first examine the term $\mathbf{v}_a$, resulting from the Schrödinger current. Writing

$$\psi = \frac{1}{\sqrt{2\ell+1}} R_{n\ell}(r) \begin{pmatrix} v_1(\theta,\phi) \\ v_2(\theta,\phi) \end{pmatrix},$$

the term $\mathrm{Im}\{\psi^\dagger \nabla\psi\}$ can be shown to be

$$\mathrm{Im}\{\psi^\dagger\nabla\psi\} = \frac{1}{2\ell+1}\mathrm{Im}\big\{R_{n\ell}R'_{n\ell}(|v_1|^2+|v_2|^2)\hat{e}_r + \frac{1}{r}R^2_{n\ell}(v_1^*\frac{\partial v_1}{\partial\theta} + v_2^*\frac{\partial v_2}{\partial\theta})\hat{e}_\theta + \frac{1}{r\sin\theta}R^2_{n\ell}(v_1^*\frac{\partial v_1}{\partial\phi} + v_2^*\frac{\partial v_2}{\partial\phi})\hat{e}_\phi\big\}. \quad (4.11)$$

The only nonzero imaginary term comes from the $\hat{e}_\phi$ component:

$$v_k^*\frac{\partial v_k}{\partial\phi} = i(m \pm \frac{1}{2})|v_k|^2, \quad k = 1,2$$

so that

$$\mathrm{Im}(\psi^\dagger\nabla\psi) = \frac{1}{(2\ell+1)r\sin\theta}R^2_{n\ell}\Big((m-\frac{1}{2})|v_1|^2 + (m+\frac{1}{2})|v_2|^2\Big)\hat{e}_\phi.$$

Now,

$$\psi^\dagger\psi = \rho = \frac{1}{2\ell+1}R^2_{n\ell}(|v_1|^2+|v_2|^2)$$

which, from (4.9), gives

$$\mathbf{v}_a = \frac{\hbar}{m_e r\sin\theta}\Big(m + \frac{1}{2}(\frac{|v_2|^2-|v_1|^2}{|v_1|^2+|v_2|^2})\Big)\hat{e}_\phi. \quad (4.12)$$

Thus in all of the states, the first term $\mathbf{v}_a$ gives motion only in the $\hat{e}_\phi$ direction, yielding circular motion about the z-axis. Recall that in the Schrödinger case, where it was assumed that the system remained in an eigenstate of s_z, this part of the current was zero for real eigenstates (see (3.8) and (3.9)). Here, however, it is possible for the Schrödinger current $\mathbf{j}_a$ to contribute to the momentum even when the wave function is real.

It remains to compute $\mathbf{j}_b$ and the corresponding velocity $\mathbf{v}_b$, with reference to (4.10). To

do this, we first find the three components of $\psi^\dagger\sigma\psi$:

$$\psi^\dagger\sigma\psi = \frac{1}{2\ell+1}R_{n\ell}(r)^2\Big(2\mathrm{Re}\{v_1^* v_2\}, 2\mathrm{Im}\{v_1^* v_2\}, |v_1|^2 - |v_2|^2\Big). \tag{4.13}$$

Now, from the form of the wave functions (4.7) and (4.8), we have

$$2\mathrm{Re}(v_1^* v_2) = 2c_1c_2N_1N_2P_\ell^{m-\frac{1}{2}}(\theta)P_\ell^{m+\frac{1}{2}}(\theta)\cos\phi$$

and

$$2\mathrm{Im}(v_1^* v_2) = 2c_1c_2N_1N_2P_\ell^{m-\frac{1}{2}}(\theta)P_\ell^{m+\frac{1}{2}}(\theta)\sin\phi$$

where the c_i are given in (4.7) and (4.8) and the N_i are the normalization constants of the relevant spherical harmonics. For simplicity of notation, define

$$a = c_1N_1P_\ell^{m-\frac{1}{2}}(\theta), \quad b = c_2N_2P_\ell^{m+\frac{1}{2}}(\theta). \tag{4.14}$$

Thus, if we write (4.13) $\psi^\dagger\sigma\psi = \frac{1}{2\ell+1}R_{n\ell}^2(r)\mathbf{w}$, the vector $\mathbf{w}$ can be written in Cartesian form as

$$(w_x, w_y, w_z) = (2ab\cos\phi, 2ab\sin\phi, a^2 - b^2). \tag{4.15}$$

Now, if we were to write $\mathbf{w}$ in polar form, in terms of polar coordinates r_s, θ_s and ϕ_s, we would write

$$\begin{aligned} w_x &= r_s\sin\theta_s\cos\phi_s \\ w_y &= r_s\sin\theta_s\sin\phi_s \\ w_z &= r_s\cos\theta_s \end{aligned} \tag{4.16}$$

where the orientation of the spin vector $\mathbf{s} = \psi^\dagger\sigma\psi$ is given by the angles θ_s and ϕ_s. (See also [14] for further treatment of the spin vector.) Comparing with (4.15), we might write

$r_s = a^2 + b^2$, $\phi_s = \phi$ and compute θ_s in terms of θ with the relations

$$\cos\theta_s = \frac{a^2 - b^2}{a^2 + b^2}, \qquad \sin\theta_s = \frac{2ab}{a^2 + b^2}. \tag{4.17}$$

However, this is only consistent with the definition of spherical coordinates if $2ab \geq 0$, because θ_s is restricted to the interval $[0, \pi]$. When this condition is not met, instead of (4.17), the polar coordinates for $\mathbf{w}$ are given by $r_s = a^2 + b^2$, $\phi_s = \phi + \pi$ and

$$\cos\theta_s = \frac{a^2 - b^2}{a^2 + b^2}, \qquad \sin\theta_s = \frac{|2ab|}{a^2 + b^2} = -\frac{2ab}{a^2 + b^2}.$$

In both cases, we can write $\phi_s = \phi$, so that $\mathbf{w}$ (and hence $\mathbf{s}$) is in a plane containing $\mathbf{r}$ (the position vector) and the z axis. Therefore, we can write $\mathbf{s}$ as a combination of $\hat{e}_r$ and $\hat{e}_\theta$, which are unit vectors in the common plane of $\mathbf{s}$ and $\mathbf{r}$. In both cases, we find that the following holds: Rewriting in polar coordinates (where $\hat{e}_r$, $\hat{e}_\theta$ and $\hat{e}_\phi$ are the polar unit vectors taken from the position of the electron),

$$\mathbf{s} = \Big(s\cos\theta(\frac{a^2 - b^2}{a^2 + b^2}) + s\sin\theta(\frac{2ab}{a^2 + b^2})\Big)\hat{e}_r - \Big(s\sin\theta(\frac{a^2 - b^2}{a^2 + b^2}) - s\cos\theta(\frac{2ab}{a^2 + b^2})\Big)\hat{e}_\theta \tag{4.18}$$

where $s = \psi^\dagger\psi$. We therefore write $\mathbf{s} = s_r\hat{e}_r + s_\theta\hat{e}_\theta$ with

$$\begin{aligned} s_r &= s\cos\theta(\frac{a^2 - b^2}{a^2 + b^2}) + s\sin\theta(\frac{2ab}{a^2 + b^2}) \\ s_\theta &= -s\sin\theta(\frac{a^2 - b^2}{a^2 + b^2}) + s\cos\theta(\frac{2ab}{a^2 + b^2}). \end{aligned} \tag{4.19}$$

For a derivation of this statement, see the Appendix of this chapter.

Now that we have an expression for the vector $\mathbf{s}$, to compute $\mathbf{v}_b$ from (4.10) it remains

to find $\nabla \times \mathbf{s}$. In polar coordinates we can write (for a general vector $\mathbf{s}$)

$$\nabla \times \mathbf{s} = \frac{1}{r\sin\theta}\Big(\cos\theta s_\phi + \sin\theta\frac{\partial s_\phi}{\partial\theta} - \frac{\partial s_\theta}{\partial\phi}\Big)\hat{e}_r + \frac{1}{r\sin\theta}\Big(\frac{\partial s_r}{\partial\phi} - \sin\theta s_\phi - r\sin\theta\frac{\partial s_\phi}{\partial r}\Big)\hat{e}_\theta + \frac{1}{r}\Big(s_\theta + r\frac{\partial s_\theta}{\partial r} - \frac{\partial s_r}{\partial\theta}\Big)\hat{e}_\phi. \quad (4.20)$$

Now, since $\mathbf{s}$ has the form (4.18), and a and b are given by (4.14), s_ϕ, $\frac{\partial s_\theta}{\partial\phi}$ and $\frac{\partial s_\phi}{\partial r}$ vanish. The above cross product then has only an $\hat{e}_\phi$ component, given by

$$\nabla \times \mathbf{s} = \frac{1}{r}\Big(s_\theta + r\frac{\partial s_\theta}{\partial r} - \frac{\partial s_r}{\partial\theta}\Big)\hat{e}_\phi \quad (4.21)$$

so that

$$\mathbf{v}_b = \frac{\hbar}{2m_e}\frac{\nabla\times\mathbf{s}}{\psi^\dagger\psi} = \frac{\hbar}{2m_e r s}\Big(s_\theta + r\frac{\partial s_\theta}{\partial r} - \frac{\partial s_r}{\partial\theta}\Big)\hat{e}_\phi. \quad (4.22)$$

In other words, as for $\mathbf{v}_a$, the contribution to the velocity from $\mathbf{v}_b$ is again only in the ϕ direction. Adding the two contributions yields a total velocity in the $\hat{e}_\phi$ direction

$$\mathbf{v} = \mathbf{v}_a + \mathbf{v}_b = \frac{\hbar}{m_e r\sin\theta}\Big(m + \frac{1}{2}\big(\frac{|v_2|^2 - |v_1|^2}{|v_1|^2 + |v_2|^2}\big)\Big)\hat{e}_\phi + \frac{\hbar}{2m_e r s}\Big(s_\theta + r\frac{\partial s_\theta}{\partial r} - \frac{\partial s_r}{\partial\theta}\Big)\hat{e}_\phi. \quad (4.23)$$

This concludes the proof that *all motion for all eigenstates of the form* (4.7) *and* (4.8) *consists of circular revolution about the z-axis.* Thus, r and θ are constants of motion.

Furthermore, from (4.14), we know that the quantities a and b do not depend on ϕ. Since r and θ are constants of motion, a and b are constants of motion as well, so that (with reference to (4.19)) the components s_r and s_θ are constant in time. However, that due to the fact that ϕ changes, the vectors $\hat{e}_r$, $\hat{e}_\theta$ and $\hat{e}_\phi$ are themselves time-dependent so the spin vector is not constant, while its components in spherical coordinates are. We now see that the total velocity in the $\hat{e}_\phi$ direction, from (4.23), depends on r, θ, and $s = \psi^\dagger\psi$. The only way that this could depend on ϕ, and therefore not be constant in time, is if s depended on

ϕ. But this is not the case.

Recalling the form of the wave functions from (4.7) and (4.8), it is clear that $s = \psi^\dagger \psi$ for $j = \ell + \frac{1}{2}$ will be of the form

$$s = C_1 R_{n\ell}(r)^2 \big(N_1^2 (P_{\ell(m-\frac{1}{2})}(\cos\theta))^2 + N_2^2 (P_{\ell(m+\frac{1}{2})}(\cos\theta))^2 \big) \tag{4.24}$$

where C_1, N_1 and N_2 are the various normalization constants. The above is a function of r and θ only, because the ϕ dependence in the wave function only occurs in the oscillatory exponentials. Thus, the magnitude of the wave function is also a constant of motion. The same holds for the case $j = \ell - \frac{1}{2}$.

This means that *all* terms in (4.23) are constants of motion. Therefore, the angular velocity will be constant, and will depend on r and θ. The problem of explicitly finding the trajectories has been considerably simplified to the problem of computing the angular rates of revolution.

It will be useful in what follows to understand the relationship between the velocities for positive and negative (corresponding) values of m. Recall that for $j = \ell + \frac{1}{2}$,

$$\psi_{n,\ell,j=l+\frac{1}{2},m} = \frac{1}{\sqrt{2\ell+1}} R_{n\ell}(r) \begin{pmatrix} \sqrt{\ell+m+\frac{1}{2}}\; Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\ -\sqrt{\ell-m+\frac{1}{2}}\; Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

and

$$Y_{\ell m} = \frac{1}{\sqrt{2\pi}} P_{\ell m} e^{im\phi}, \quad P_{\ell,-m}(x) = (-1)^m P_{\ell m}(x).$$

Also, from the derivation above, the spin vector $\mathbf{s}$ is proportional to

$$\mathbf{w} = (2\mathrm{Re}\{v_1^* v_2\}, 2\mathrm{Im}\{v_1^* v_2\}, |v_1|^2 - |v_2|^2).$$

When m is replaced by $-m$, we have (denoting the new term with a superscript $^{(-)}$ and the

old with $^{(+)}$)

$$v_1^{(-)} = \sqrt{l-m+\tfrac{1}{2}} Y_{l,-m-\frac{1}{2}} = \sqrt{l-m+\tfrac{1}{2}} \frac{1}{\sqrt{2\pi}} (-1)^{m+\frac{1}{2}} P_{l,m+\frac{1}{2}} e^{i(-m-\frac{1}{2})\phi} = v_2^{*(+)}.$$

Similarly,

$$\begin{aligned} v_2^{(-)} &= -\sqrt{l+m+\tfrac{1}{2}} \frac{1}{\sqrt{2\pi}} P_{l,-m+\frac{1}{2}} e^{i(-m+\frac{1}{2})\phi} \\ &= -\sqrt{l+m+\tfrac{1}{2}} \frac{1}{\sqrt{2\pi}} (-1)^{m-\frac{1}{2}} P_{l,m-\frac{1}{2}} e^{-i(m-\frac{1}{2})\phi} = -v_1^{*(+)}. \end{aligned}$$

Therefore,

$$(|v_1|^2 - |v_2|^2)^{(-)} = -(|v_1|^2 - |v_2|^2)^{(+)},$$

and furthermore,

$$(v_1^* v_2)^{(-)} = v_2^{(+)}(-v_1^{*(+)}) = (-v_1^* v_2)^{(+)}.$$

This implies that all three components of $\mathbf{w}$ change sign when m is replaced with $-m$ (and the other eigenvalues are left constant), so that the vector $\mathbf{s} = \frac{1}{2l+1} R_{nl}^2(r)\mathbf{w}$ changes sign. Hence

$$\mathbf{v}_a^{(-)} = \frac{\hbar}{m_e r \sin\theta} \Big(m + \frac{1}{2} \big(\frac{(|v_2|^2 - |v_1|^2)^{(-)}}{(|v_1|^2 + |v_2|^2} \big)^{(-)} \big) \Big) \hat{e}_\phi = -\mathbf{v}_a^{(+)}$$

and

$$\mathbf{v}_b^{(-)} = \frac{\hbar}{2m_e} \frac{\nabla \times \mathbf{s}^{(-)}}{\psi^\dagger \psi} = -\mathbf{v}_b^{(+)}.$$

Thus, both $\mathbf{v}_a$ and $\mathbf{v}_b$ change sign when m changes sign, so that the overall velocity simply changes direction. A similar proof holds for the case $j = \ell - \frac{1}{2}$. This simplifies the computation of the rates of revolution; the task at hand is now to compute only the rates of revolution for positive m. These rates of revolution determine the trajectories for each eigenstate, while the fixed values of r and θ are determined by the initial conditions.

4.3 Trajectories for $n = 1$ and $n = 2$ Eigenstates

In this section we compute the rate of ϕ revolution explicitly for the first few hydrogen eigenstates. Note that the rate of revolution $d\phi/dt$ is related to the speed v in the $\hat{e}_\phi$ direction by the relationship

$$\frac{d\phi}{dt} = \frac{v}{r\sin\theta}. \tag{4.25}$$

In each case, we compute $\mathbf{v}_a$, then write $s = \psi^\dagger\psi$ explicitly, and find s_r and s_θ from (4.19), to ultimately compute $\mathbf{v}_b$ and hence the total velocity.

4.3.1 n=1

For the ground state, we have from (4.7) that

$$\psi_{1,0,\frac{1}{2},\frac{1}{2}} = R_{10}(r)\begin{pmatrix} Y_{00} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$\psi_{1,0,\frac{1}{2},-\frac{1}{2}} = R_{10}(r)\begin{pmatrix} 0 \\ Y_{00} \end{pmatrix} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Note that one component of the spinor is zero and $m = \frac{1}{2}$, so the contribution to the velocity from $\mathbf{v}_a$ vanishes, and the only contribution is from $\mathbf{v}_b$. Now,

$$s = \psi^\dagger\psi = \frac{1}{\pi a^3} e^{-2r/a}$$

so that

$$\frac{\partial s}{\partial \theta} = 0.$$

When $m = \frac{1}{2}$, we find $s_r = s\cos\theta$ and $s_\theta = -s\sin\theta$, which yields

$$\nabla \times \mathbf{s} = -\frac{\partial s}{\partial r}\sin\theta = \frac{1}{\pi a^3}(\frac{2}{a}) e^{-2r/a}\sin\theta$$

so that

$$\mathbf{v}_b = \frac{\hbar}{2m_e s}\nabla \times \mathbf{s} = \frac{\hbar}{m_e a}\sin\theta \hat{e}_\phi.$$

Therefore

$$\frac{d\phi}{dt} = \pm\frac{\hbar}{m_e a r}, \quad m = \pm\frac{1}{2}. \tag{4.26}$$

This is in agreement with the result for the ground state ϕ revolution given in [61] and in the previous chapter.

4.3.2 n=2

In the $n = 2$ case, we can have either $\ell = 0$ or $\ell = 1$; in the first of these we are restricted to $j = \frac{1}{2}$, $m = \pm\frac{1}{2}$, and in the second, there is the additional possibility of $j = \frac{3}{2}$, for which m can take on the values $\pm\frac{3}{2}, \pm\frac{1}{2}$.

$\ell = 0$

The two $\ell = 0$ wave functions are given by

$$\psi_{2,0,\frac{1}{2},\frac{1}{2}} = R_{20}(r)\begin{pmatrix} Y_{00} \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_{2,0,\frac{1}{2},-\frac{1}{2}} = R_{20}(r)\begin{pmatrix} 0 \\ Y_{00} \end{pmatrix} \tag{4.27}$$

where

$$R_{20} = 2\big(\frac{1}{2a}\big)^{3/2}\big(1 - \frac{r}{2a}\big)e^{-r/2a}, \quad Y_{00} = \frac{1}{\sqrt{4\pi}}.$$

In both cases the contribution to the velocity from the Schrödinger current term ($\mathbf{v}_a$) vanishes. We then have

$$s = \psi^\dagger\psi = \frac{1}{16\pi^2 a^3}\Big(1 - \frac{r}{2a}\Big)^2 e^{-r/a}.$$

Again, in the case $m = \frac{1}{2}$, we find that $s_r = s\cos\theta$ and $s_\theta = -s\sin\theta$. Since s is a function of r only, $\nabla \times \mathbf{s}$ reduces to

$$\nabla \times \mathbf{s} = -\sin\theta\frac{ds}{dr} = -\frac{1}{4\pi a^4}\Big(1 - \frac{r}{2a}\Big)e^{-r/a}\Big(2 - \frac{r}{2a}\Big)$$

so that

$$\mathbf{v}_b = \frac{\hbar}{2m_e a}\frac{\nabla \times \mathbf{s}}{s} = \frac{\hbar}{2m_e}\sin\theta\Big(\frac{2-\frac{r}{2a}}{1-\frac{r}{2a}}\Big),$$

which yields

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e a r}\Big(\frac{1}{1-\frac{r}{2a}}+1\Big) \implies \frac{d\phi}{dt} = \pm\frac{\hbar}{2m_e a r}\Big(\frac{1}{1-\frac{r}{2a}}+1\Big), \quad m = \pm\frac{1}{2}. \tag{4.28}$$

This agrees with the result for the $2s$ ϕ revolution given in the previous chapter (see Table 3.1).

$\boldsymbol{\ell = 1}$

There are six cases for which $l = 1$; two for $j = \frac{1}{2}$ and four for $j = \frac{3}{2}$. They are given by

$$\psi_{2,1,\frac{1}{2},\frac{1}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix} Y_{10} \\ \sqrt{2}Y_{11}\end{pmatrix}$$

$$\psi_{2,1,\frac{1}{2},-\frac{1}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix} \sqrt{2}Y_{11} \\ Y_{10}\end{pmatrix}$$

$$\psi_{2,1,\frac{3}{2},\frac{1}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix} \sqrt{2}Y_{10} \\ -Y_{11}\end{pmatrix}$$

$$\psi_{2,1,\frac{3}{2},-\frac{1}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix} Y_{11} \\ \sqrt{2}Y_{10}\end{pmatrix}$$

$$\psi_{2,1,\frac{3}{2},\frac{3}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix} \sqrt{3}Y_{11} \\ 0\end{pmatrix}$$

$$\psi_{2,1,\frac{3}{2},-\frac{3}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix} 0 \\ -\sqrt{3}Y_{11}\end{pmatrix}$$

The relevant radial and spherical functions are

$$R_{21}(r) = \frac{1}{\sqrt{3}}\big(\frac{1}{2a}\big)^{3/2}\big(\frac{r}{a}\big)e^{-r/2a}, \quad Y_{10} = \big(\frac{3}{4\pi}\big)^{1/2}\cos\theta, \quad Y_{11} = \big(\frac{3}{8\pi}\big)^{1/2}\sin\theta e^{i\phi}.$$

1). $\mathbf{j = \frac{3}{2}}$, $\mathbf{m = \pm\frac{3}{2}}$

This is another case for which the computation of the velocity is simplified by the fact that

one component of the wave function vanishes. From the above we have

$$\psi_{2,1,\frac{3}{2},\frac{3}{2}} = \frac{1}{\sqrt{3}} R_{21}(r) \begin{pmatrix} \sqrt{3}Y_{11} \\ 0 \end{pmatrix}$$

and

$$\psi_{2,1,\frac{3}{2},-\frac{3}{2}} = \frac{1}{\sqrt{3}} R_{21}(r) \begin{pmatrix} 0 \\ -\sqrt{3}Y_{11} \end{pmatrix}$$

Although one component vanishes, $\mathbf{v}_a$ does not vanish; from (4.12) we find

$$\mathbf{v}_a = \pm \frac{\hbar}{m_e r^2 \sin^2\theta} \hat{e}_\phi.$$

To find $\mathbf{v}_b$, we find

$$s = \psi^\dagger \psi = \frac{1}{32\pi a^5} r^2 e^{-r/a} \big(\frac{3}{8\pi}\big) \sin^2\theta$$

which gives

$$\frac{\partial s}{\partial r} = \frac{1}{32\pi a^5} \big(\frac{3}{8\pi}\big) \Big(2r - \frac{r^2}{a}\Big) e^{-r/a} \sin^2\theta$$

and

$$\frac{\partial s}{\partial \theta} = \frac{1}{32\pi a^5} \big(\frac{3}{8\pi}\big) r^2 e^{-r/a} 2 \sin\theta\cos\theta.$$

Now, for positive m, we find

$$\nabla \times \mathbf{s} = -\frac{\partial s}{\partial r} \sin\theta - \frac{1}{r} \frac{\partial s}{\partial \theta} \cos\theta.$$

Substituting the above derivatives and dividing by s gives

$$\mathbf{v}_b = \frac{\hbar}{2m_e} \frac{\nabla \times \mathbf{s}}{s} = -\frac{\hbar}{m_e r} \Big(\sin\theta \big(1 - \frac{r}{2a}\big) + \frac{\cos^2\theta}{\sin\theta} \Big) \hat{e}_\phi.$$

Simplifying, and adding the $\mathbf{v}_a$ and $\mathbf{v}_b$ components together yields

$$\frac{d\phi}{dt} = \pm \frac{\hbar}{2m_e a r}, \quad m = \pm \frac{1}{2}. \tag{4.29}$$

These results are also consistent with the rate of revolution given in Table 3.1.

2). $\mathbf{j} = \frac{1}{2}$, $\mathbf{m} = \pm\frac{1}{2}$

Now the wave function is no longer a spin eigenstate and neither component vanishes, so now both $\mathbf{v}_a$ and $\mathbf{v}_b$ will contribute to the velocity. We have

$$\psi_{2,1,\frac{1}{2},\frac{1}{2}} = \frac{1}{\sqrt{3}} R_{21}(r) \begin{pmatrix} Y_{10} \\ \sqrt{2}Y_{11} \end{pmatrix} \quad \text{and} \quad \psi_{2,1,\frac{1}{2},-\frac{1}{2}} = \frac{1}{\sqrt{3}} R_{21}(r) \begin{pmatrix} \sqrt{2}Y_{11} \\ Y_{10} \end{pmatrix}.$$

Now, from (4.12),

$$\mathbf{v}_a = \frac{\hbar}{m_e r \sin\theta} \Big(\pm \frac{1}{2} \mp \frac{1}{2} \cos 2\theta \Big) \hat{e}_\phi = \pm \frac{\hbar}{m_e r \sin\theta} \hat{e}_\phi.$$

which in turn gives

$$\Big(\frac{d\phi}{dt}\Big)_a = \pm \frac{\hbar}{m_e r^2}. \tag{4.30}$$

It remains to compute the ϕ revolution from the $\mathbf{v}_b$ term (4.10). Note that

$$s = s(r) = \frac{1}{128\pi^2 a^5} r^2 e^{-r/a}.$$

For $m = \frac{1}{2}$, we have $s_r = s\cos\theta$ and $s_\theta = s\sin\theta$. Now,

$$\nabla \times \mathbf{s} = \frac{1}{r} \Big(2s \sin\theta + 2s \big(1 - \frac{r}{2a}\big) \sin\theta \Big) \hat{e}_\phi \tag{4.31}$$

so that

$$\mathbf{v}_b = \frac{\hbar}{2m_e} \frac{\nabla \times \mathbf{s}}{s} = \frac{\hbar}{m_e r} \sin\theta (2 - \frac{r}{2a}), \tag{4.32}$$

and

$$\big(\frac{d\phi}{dt}\big)_b = \frac{\hbar}{m_e r^2} (2 - \frac{r}{2a}).$$

Adding the $\mathbf{v}_a$ and $\mathbf{v}_b$ terms together now gives a final trajectory described by

$$\frac{d\phi}{dt} = \pm\frac{\hbar}{m_e r^2}(3 - \frac{r}{2a}), \qquad m = \pm\frac{1}{2}. \tag{4.33}$$

For this state, there is no eigenstate in the Schrödinger case with which to compare the rate of revolution. However, the result given in (4.33) is interesting in another sense: it predicts the existence of an equilibrium surface defined by $r = 6a$. On this sphere, the rate of revolution $d\phi/dt$ is zero, and because r and θ are constants of motion, the particle is stationary. Inside this sphere, the rotation is in the counter-clockwise direction, and outside it, the rotation is clockwise. The existence of this equilibrium surface brings up the question of what keeps the electron stationary; the causal theory's answer is that the quantum potential exactly balances the classical potential when $r = 6a$, and the particle thus remains stationary. Note, though, that since the sphere $r = 6a$ is a set of zero measure in $\mathbb{R}^3$, the probability of finding the particle there is zero.

3). $\mathbf{j = \frac{3}{2}}$, $\mathbf{m = \pm\frac{1}{2}}$

The remaining case $j = \frac{3}{2}$, $m = \pm\frac{1}{2}$ has the wave functions

$$\psi_{2,1,\frac{3}{2},\frac{1}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix}\sqrt{2}Y_{10}\\ -Y_{11}\end{pmatrix} \quad \text{and} \quad \psi_{2,1,\frac{3}{2},-\frac{1}{2}} = \frac{1}{\sqrt{3}}R_{21}(r)\begin{pmatrix}Y_{11}\\ \sqrt{2}Y_{10}\end{pmatrix}.$$

The component $\mathbf{v}_a$ of the velocity for $m = \pm\frac{1}{2}$ is given by

$$\mathbf{v}_a = \frac{\hbar}{m_e r\sin\theta}\Big(\pm\frac{1}{2} \pm (\frac{1}{2})\frac{\sin^2\theta - 4\cos^2\theta}{\sin^2\theta + 4\cos^2\theta}\Big) \tag{4.34}$$

which simplifies to

$$\mathbf{v}_a = \pm\frac{\hbar}{m_e r\sin\theta}\Big(\frac{1}{4\cos^2\theta + \sin^2\theta}\Big). \tag{4.35}$$

In the $m = \frac{1}{2}$ case we have the following:

$$\frac{a^2 - b^2}{a^2 + b^2} = \frac{4\cos^2\theta - \sin^2\theta}{4\cos^2\theta + \sin^2\theta}, \qquad \frac{2ab}{a^2 + b^2} = \frac{-4\sin\theta\cos\theta}{4\cos^2\theta + \sin^2\theta}.$$

To simplify the notation, define

$$D(\theta) = 4\cos^2\theta + \sin^2\theta.$$

Furthermore,

$$\begin{aligned} s = \psi^\dagger\psi &= \frac{1}{3}R_{21}^2(2|Y_{10}|^2 + |Y_{11}|^2) \\ &= \frac{1}{3}(\frac{1}{32\pi a^5})r^2e^{-r/a}\big(\frac{3}{2}\pi\cos^2\theta + \frac{3}{8}\pi\sin^2\theta\big) \\ &= R(r)D(\theta) \end{aligned} \tag{4.36}$$

where

$$R(r) \equiv \frac{1}{256a^5}r^2e^{-r/a}.$$

This will simplify the expression for $\mathbf{v}_b$. Now we can find the components of the spin vector from (4.19):

$$\begin{aligned} s_\theta &= -RD\sin\theta\frac{(4\cos^2\theta - \sin^2\theta)}{D} + RD\cos\theta\frac{(-4\sin\theta\cos\theta)}{D} \\ &= -R(8\cos^2\theta\sin\theta - \sin^3\theta) \end{aligned} \tag{4.37}$$

and similarly,

$$s_r = R(4\cos^3\theta - 5\cos\theta\sin^2\theta). \tag{4.38}$$

The use of $R(r)$ and $D(\theta)$ allows $\mathbf{v}_b$ to be computed easily from (4.22) which upon substitu-

tion of the above quantities becomes

$$\mathbf{v}_b = \frac{\hbar}{2m_e r D}\Big(-(8\cos^2\theta\sin\theta - \sin^3\theta) - (2 - \frac{r}{a})(8\cos^2\theta\sin\theta - \sin^3\theta) \\ - \frac{d}{d\theta}(4\cos^3\theta - 5\cos\theta\sin^2\theta)\Big). \quad (4.39)$$

Taking the necessary derivative and simplifying gives

$$\mathbf{v}_b = -\frac{\hbar}{2m_e r D}\sin\theta\Big(2 - \frac{8r}{a}\cos^2\theta + \frac{r}{a}\sin^2\theta\Big)\hat{e}_\phi. \quad (4.40)$$

The corresponding rate of change of ϕ is

$$\big(\frac{d\phi}{dt}\big)_b = -\frac{\hbar}{2m_e r^2 D}\Big(2 - \frac{8r}{a}\cos^2\theta + \frac{r}{a}\sin^2\theta\Big).$$

Adding this to (4.35) and expanding the denominator term D gives a total rate of revolution of

$$\frac{d\phi}{dt} = \pm\frac{\hbar}{2m_e r a}\Big(\frac{8\cos^2\theta - \sin^2\theta}{4\cos^2\theta + \sin^2\theta}\Big), \quad m = \pm\frac{1}{2}. \quad (4.41)$$

The denominator never vanishes, as both $\cos^2\theta$ and $\sin^2\theta$ are at least zero and are not zero at the same point. However, as in the previous case, there is an equilibrium surface on which $d\phi/dt$ vanishes. This equilibrium occurs for $\theta = \alpha$, where α is a solution to

$$8\cos^2\alpha = \sin^2\alpha.$$

Together with the constraint that $\alpha \in [0, \pi]$, this gives two solutions

$$\alpha = \arctan(2\sqrt{2}) \quad \text{and} \quad \alpha' = \pi - \arctan(2\sqrt{2}).$$

These solutions make physical sense in that the surface defined by a constant value of θ is a cone in the three-dimensional space. The fact that both α and $\pi - \alpha$ are solutions means

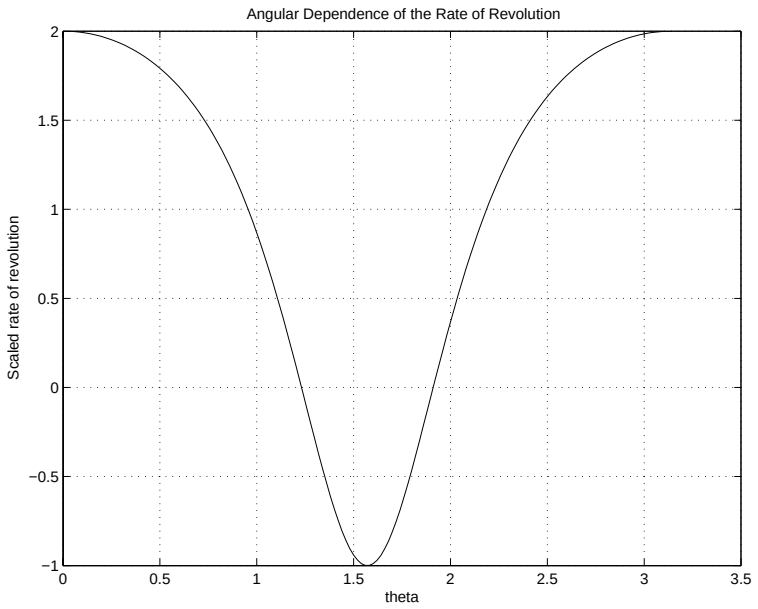


Figure 4.1: The dependence of $d\phi/dt$ on the angle θ

that both the top and bottom halves of this cone make up the equilibrium surface. When $\theta < \alpha$ or $\theta > \pi - \alpha$, the rotation is in the counterclockwise direction. Otherwise, the rotation is clockwise. And as in the previous case, the equilibrium surface itself is of measure zero, so that the probability of finding the particle there is infinitesimal. A plot of the θ dependence of $d\phi/dt$ (for constant r) is shown in Figure 4.1. There is again no analogous Schrödinger case with which we can compare the rate of revolution.

This concludes our calculation of specific rates of revolution for Pauli hydrogen eigenstates.

4.4 Concluding Remarks

We have developed general features of the de Broglie-Bohm trajectories for hydrogen eigenstates based on the Pauli equation. For the eigenstates chosen, which are eigenstates of the hamiltonian H, the orbital angular momentum L^2, the total angular momentum M^2, and the z component of the total angular momentum, M_z, the motion of the electron is confined

Quantum Number n, ℓ, j, m	**Rotation rate** $d\phi/dt$
$1, 0, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{m_e a r}$
$2, 0, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{2m_e a r}(\frac{1}{1-\frac{r}{2a}}+1)$
$2, 1, \frac{3}{2}, \pm\frac{3}{2}$	$\pm\frac{\hbar}{2m_e a r}$
$2, 1, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{m_e r^2}(3-\frac{r}{2a})$
$2, 1, \frac{3}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{2m_e r a}\frac{8\cos^2\theta-\sin^2\theta}{4\cos^2\theta+\sin^2\theta}$

Table 4.1: Angular rates of revolution for Pauli eigenstates

to circular motion about the z axis (z is constant), characterized by the angular velocity $d\phi/dt$. This is true in general for eigenstates of these operators. We have also computed the rates or angular revolution for the $n = 1$ and $n = 2$ hydrogen eigenstates, and given a general procedure for the computation for other eigenstates. It is interesting to note that while the equation for the velocity

$$\mathbf{v} = \frac{\mathbf{j}}{\rho}$$

is easy to state, and the expression for the current (4.3) is easy to write down, the actual computation of the trajectories in the causal theory can be quite complicated even for eigenstates, which are in general much simpler than combinations of eigenstates. Table 4.1 summarizes the results of the calculations.

In the cases where the Pauli eigenstates are also eigenstates of the s_z spin operator, our results agree with the computations of the trajectories using the Schrödinger eigenstates of the previous chapter. Because of the complicated nature of the trajectory calculations, this fact was by no means obvious from the outset. It is a nice result, however, in that the theory would not be as intuitively appealing if this kind of agreement were not to be found.

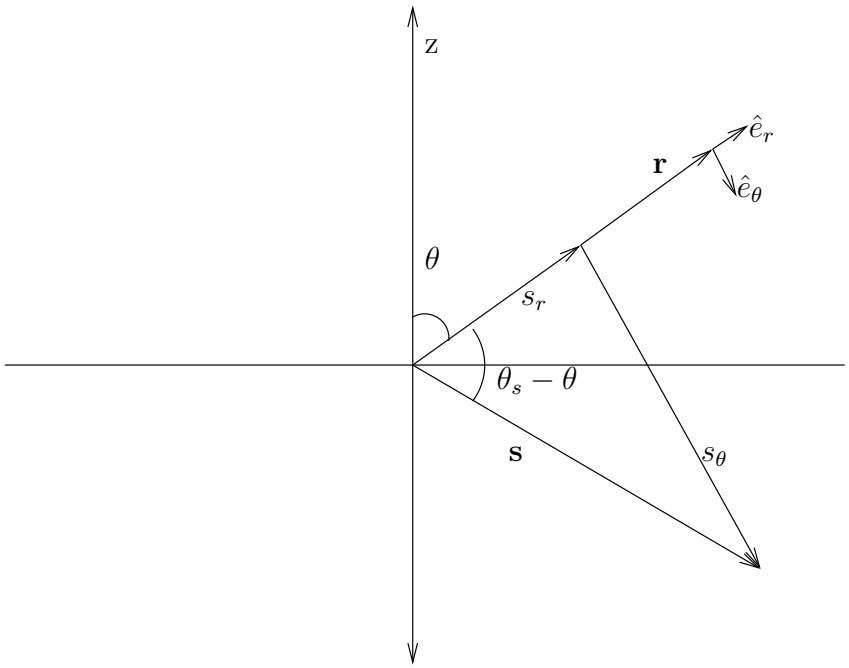


Figure 4.2: Components of the spin vector for $2ab \geq 0$

4.5 Appendix

First we show the required relation (4.19) in the case $2ab \geq 0$. Write (with $\hat{e}_r$ and $\hat{e}_\theta$ defined by the position vector)

$$\begin{aligned} \mathbf{s} &= s_r \hat{e}_r + s_\theta \hat{e}_\theta \\ &= s\cos(\theta - \theta_s)\hat{e}_r - s\sin(\theta - \theta_s)\hat{e}_\theta, \end{aligned} \tag{4.42}$$

as can be seen from Fig. 4.2, where

$$s = |\mathbf{s}| = |\psi^\dagger \sigma \psi| = \psi^\dagger \psi = \rho. \tag{4.43}$$

Recall from (4.17) that in the case $2ab \geq 0$,

$$\cos\theta_s = \frac{a^2 - b^2}{a^2 + b^2}, \qquad \sin\theta_s = \frac{2ab}{a^2 + b^2}. \tag{4.44}$$

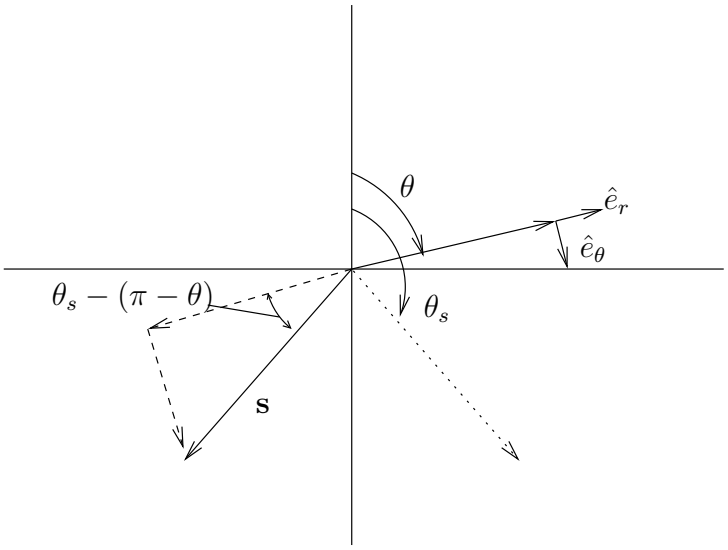


Figure 4.3: Components of the spin vector for $2ab < 0$

The expression in (4.42) can be expanded out directly to give the required relation (4.18),

$$\begin{aligned}\mathbf{s} &= (s\cos\theta\cos\theta_s + s\sin\theta\sin\theta_s)\hat{e}_r - (s\sin\theta\cos\theta_s - s\cos\theta\sin\theta_s)\hat{e}_\theta \\ &= \Big(s\cos\theta(\frac{a^2-b^2}{a^2+b^2}) + s\sin\theta(\frac{2ab}{a^2+b^2})\Big)\hat{e}_r - \Big(s\sin\theta(\frac{a^2-b^2}{a^2+b^2}) - s\cos\theta(\frac{2ab}{a^2+b^2})\Big)\hat{e}_\theta.\end{aligned} \tag{4.45}$$

Now, in the case $2ab < 0$, we must define (instead of (4.17))

$$\cos\theta_s = \frac{a^2-b^2}{a^2+b^2}, \qquad \sin\theta_s = \frac{-2ab}{a^2+b^2}. \tag{4.46}$$

because otherwise the resulting θ_s is not within $[0, \pi]$. In this case, referring to Fig. 4.3,

$$\begin{aligned}s_r &= -s\cos(\theta_s - (\pi - \theta)) = s\cos(\theta_s + \theta) \\ s_\theta &= s\sin(\theta_s - (\pi - \theta)) = -s\sin(\theta_s + \theta).\end{aligned} \tag{4.47}$$

where as indicated, $\theta_s \in [0, \pi]$, and $\phi_s = \phi + \pi$ gives the required reflection about the z axis. From (4.47) and (4.46), we have

$$
\begin{aligned}
\mathbf{s} &= (s\cos\theta\cos\theta_s - s\sin\theta\sin\theta_s)\hat{e}_r - (s\sin\theta\cos\theta_s + s\cos\theta\sin\theta_s)\hat{e}_\theta \\
&= \Big(s\cos\theta(\frac{a^2-b^2}{a^2+b^2}) - s\sin\theta(\frac{-2ab}{a^2+b^2})\Big)\hat{e}_r - \Big(s\sin\theta(\frac{a^2-b^2}{a^2+b^2}) + s\cos\theta(\frac{-2ab}{a^2+b^2})\Big)\hat{e}_\theta \\
&= \Big(s\cos\theta(\frac{a^2-b^2}{a^2+b^2}) + s\sin\theta(\frac{2ab}{a^2+b^2})\Big)\hat{e}_r - \Big(s\sin\theta(\frac{a^2-b^2}{a^2+b^2}) - s\cos\theta(\frac{2ab}{a^2+b^2})\Big)\hat{e}_\theta,
\end{aligned}
\tag{4.48}
$$

which is again the required relation (4.18). Therefore, we can write for either case

$$
\begin{aligned}
s_r &= s\cos\theta(\frac{a^2-b^2}{a^2+b^2}) + s\sin\theta(\frac{2ab}{a^2+b^2}) \\
s_\theta &= -s\sin\theta(\frac{a^2-b^2}{a^2+b^2}) + s\cos\theta(\frac{2ab}{a^2+b^2}),
\end{aligned}
\tag{4.49}
$$

as was given in (4.19).

Chapter 5

Eigenstates of the Dirac Equation

5.1 Introduction

The Dirac equation

$$i\hbar\frac{\partial}{\partial t}\psi = (-e\phi + \beta E_o + \boldsymbol{\alpha}\cdot(c\mathbf{p} + e\mathbf{A}))\psi \tag{5.1}$$

where the hamiltonian H is given by

$$H = -e\phi + \beta E_o + \boldsymbol{\alpha}\cdot(c\mathbf{p} + e\mathbf{A})$$

forms the basis of a relativistic description of the hydrogen atom and is known to account for such phenomena as the fine structure splitting, whereas the Schrödinger equation does not. The Pauli equation might be seen as lying 'in between' the Dirac and Schrödinger equations, as it is non-relativistic but does account for spin. As was seen in the previous chapter, the causal trajectories for the electron of the hydrogen atom are qualitatively similar for the Pauli and Schrödinger equations; all trajectories in the eigenstates we examined take the form of circles about the z axis with various constant rates of revolution, which depend on the wave function and on the initial conditions.

Recall that the goal of examining these trajectories in detail was to answer the question

of whether the causal theory gives a satisfactory picture of the hydrogen atom in terms of trajectories. It has now been seen that there is considerable consistency between the results for the Schrödinger and Pauli equations; qualitatively the trajectories are the same, and furthermore, the rates of revolution determined from the Pauli equation agree with the rates of revolution from the Schrödinger equation in the cases where one would expect such agreement, namely where the Pauli eigenstates also happen to be eigenstates of the spin in the z direction. It remains now to examine the trajectories for the hydrogen atom using the Dirac equation and examine the degree of consistency with the results given in the previous two chapters. This is the task of the present chapter.

To do this, we must choose the 'relevant' eigenstates, or those which are most related to the eigenstates chosen in the previous two chapters. In the Schrödinger case, our eigenstates were eigenstates of the hamiltonian H, the orbital angular momentum L^2 and the z component of the orbital angular momentum, L_z. In the Pauli case, we chose eigenstates of the hamiltonian H, the orbital angular momentum L^2, the total angular momentum M^2 and the z component of the total angular momentum, M_z.

This choice of eigenstates is no longer possible in the Dirac case, because L^2 no longer commutes with the hamiltonian. We are restricted, therefore, to eigenstates of H, M^2 and M_z. However, there is one further subtlety. Although the orbital angular momentum does not commute with the hamiltonian in the Dirac case, it can be shown that eigenstates can be found for which

$$\mathbf{L}^2\psi = \hbar^2\ell(\ell+1)\psi + \hbar^2 w, \tag{5.2}$$

where the spinor w is negligible. (Its large components actually vanish.) That is to say, ℓ is 'almost' a good quantum number [14]. Hence for both the Dirac and Pauli cases considered in this thesis, eigenstates are presented in terms of quantum numbers n, ℓ, j and m for purposes of comparison, even though ℓ is not strictly a good quantum number in the Dirac case. This is also useful in the computation of the Dirac eigenstates (see [14]), because one can make use of the fact that we already know the form of the two large components of the eigenfunctions–

it turns out that their form is the same as the form of the Pauli eigenfunctions from (4.7) and (4.8), with a different radial function. Because the Dirac eigenfunctions are thus built upon the (approximately correct) Pauli eigenfunctions, it is useful to present them in terms of the quantum number ℓ.

Recall that the way the causal theory ascribes a trajectory to particles can be generalized to the Pauli and Dirac equations using the relationship

$$\mathbf{p} = \frac{\mathbf{j}}{\rho}$$

where $\mathbf{j}$ is the current, and $\rho = \psi^\dagger \psi$. In the Pauli case, this gave rise to the velocity in (4.3). In the Dirac case, the current is given by

$$\mathbf{j} = c\psi^\dagger \boldsymbol{\alpha} \psi = (j_x, j_y, j_z) \tag{5.3}$$

where $\boldsymbol{\alpha}$ are the 4x4 Dirac matrices, given by

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$$

and the $\boldsymbol{\sigma}$ are the Pauli matrices. The wave function ψ is now a 4-component vector function found by solving the Dirac equation for the hydrogen potential, finding eigenstates of the relevant operators as discussed above. We will not repeat this process here, but will simply refer to its results.

The relevant hydrogen eigenstate wave functions are given in [14]; written in four com-

ponents, they are for $j = \ell + \frac{1}{2}$:

$$\begin{aligned}
\psi_1 &= g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}}Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\
\psi_2 &= -g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}}Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \\
\psi_3 &= -if(r)\sqrt{\frac{\ell - m + \frac{3}{2}}{2\ell + 3}}Y_{\ell+1,m-\frac{1}{2}}(\theta,\phi) \\
\psi_4 &= -if(r)\sqrt{\frac{\ell + m + \frac{3}{2}}{2\ell + 3}}Y_{\ell+1,m+\frac{1}{2}}(\theta,\phi)
\end{aligned} \tag{5.4}$$

and for $j = \ell - \frac{1}{2}$ they are

$$\begin{aligned}
\psi_1 &= g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}}Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\
\psi_2 &= g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}}Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \\
\psi_3 &= -if(r)\sqrt{\frac{\ell + m - \frac{1}{2}}{2\ell - 1}}Y_{\ell-1,m-\frac{1}{2}}(\theta,\phi) \\
\psi_4 &= if(r)\sqrt{\frac{\ell - m - \frac{1}{2}}{2\ell - 1}}Y_{\ell-1,m+\frac{1}{2}}(\theta,\phi).
\end{aligned} \tag{5.5}$$

The $Y_{\ell,m}$ are the usual spherical harmonics[1] and $f(r)$ and $g(r)$ are the normalized radial Dirac eigenfunctions (see [14] p. 69).

[1]Recall that in our spherical coordinates θ is measured down from the positive z axis and ϕ is measured clockwise from the x axis. Recall also that we use the following convention for the relevant functions:

$$\begin{aligned}
Y_{\ell m}(\theta,\phi) &= \frac{1}{\sqrt{2\pi}}P_{\ell m}(\cos\theta)e^{im\phi} \\
P_{\ell m}(x) &= \sqrt{\frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}}\frac{1}{2^\ell \ell!}(1-x^2)^{m/2}\frac{d^{\ell+m}}{dx^{(\ell+m)}}(x^2-1)^\ell, \quad m \geq 0 \\
P_{\ell,-m}(x) &= (-1)^m P_{\ell m}(x), \quad m < 0.
\end{aligned}$$

5.2 Trajectories for Generic Hydrogen Eigenstates

In this section, we study the causal theory's trajectories for general hydrogen eigenstates, showing features common to all of the states. In the next section, we proceed to compute the non-relativistic limits of the $n = 1$ and $n = 2$ states, for the purpose of comparing them to our earlier results from the Pauli and Schrödinger equations.

The components of the current (5.3) become, in terms of the components of the wave function,

$$\begin{aligned}
\frac{1}{c}j_x &= 2\mathrm{Re}\{\psi_1^\dagger\psi_4\} + 2\mathrm{Re}\{\psi_2^\dagger\psi_3\} \\
\frac{1}{c}j_y &= 2\mathrm{Im}\{\psi_1^\dagger\psi_4\} - 2\mathrm{Im}\{\psi_2^\dagger\psi_3\} \\
\frac{1}{c}j_z &= 2\mathrm{Re}\{\psi_1^\dagger\psi_3\} - 2\mathrm{Re}\{\psi_2^\dagger\psi_4\}.
\end{aligned} \tag{5.6}$$

The task is to compute these components and use them to find the momentum of the electron, which in turn will determine the trajectory. Applying (5.6) to hydrogen, we compute the components using the wave functions given in (5.4) and (5.5); beginning with the z component, we find that in the $j = \ell + \frac{1}{2}$ case,

$$\psi_1^\dagger\psi_3 = -if(r)g(r)\sqrt{\frac{\ell+m+\frac{1}{2}}{2\ell+1}}\sqrt{\frac{\ell-m+\frac{3}{2}}{2\ell+3}}Y_{\ell,m-\frac{1}{2}}(\theta,\phi)^*Y_{\ell+1,m-\frac{1}{2}}(\theta,\phi)$$

and

$$\psi_2^\dagger\psi_4 = if(r)g(r)\sqrt{\frac{\ell-m+\frac{1}{2}}{2\ell+1}}\sqrt{\frac{\ell+m+\frac{3}{2}}{2\ell+3}}Y_{\ell,m+\frac{1}{2}}(\theta,\phi)^*Y_{\ell+1,m+\frac{1}{2}}(\theta,\phi).$$

Because the complex parts of the spherical harmonics are in the ϕ exponentials– i.e.

$$e^{-i(m-1/2)\phi}e^{i(m-1/2)\phi} = e^{-i(m+1/2)\phi}e^{i(m+1/2)\phi} = 1,$$

both $\psi_1^\dagger\psi_3$ and $\psi_2^\dagger\psi_4$ are imaginary. From (5.6), we see that the z component of the current contains only the real parts of these expression, and thus there is thus no contribution to j_z

in the $j = \ell + \frac{1}{2}$ case. The $j = \ell - \frac{1}{2}$ case is very similar, and again j_z is identically zero. This shows that in general, motion is constrained to planes of constant z. While this is a simple result, it applies to all hydrogen eigenstates of the form (5.4) and (5.5), and is therefore of general interest. It is also the first indication that the eigenfunctions in (5.4) and (5.5) will yield trajectories consistent with those obtained in previous chapters.

First considering the $j = \ell + \frac{1}{2}$ case, we find the other components of the current similarly:

$$\frac{1}{c} j_x = 2 \sin\phi f(r) g(r) \left(\sqrt{\tfrac{\ell+m+\frac{1}{2}}{2\ell+1}} \sqrt{\tfrac{\ell+m+\frac{3}{2}}{2\ell-1}} P_{\ell,m-\frac{1}{2}} P_{\ell+1,m+\frac{1}{2}} + \sqrt{\tfrac{\ell-m+\frac{1}{2}}{2\ell+1}} \sqrt{\tfrac{\ell-m+\frac{3}{2}}{2\ell+3}} P_{\ell,m+\frac{1}{2}} P_{\ell+1,m-\frac{1}{2}} \right) \tag{5.7}$$

and we define $F(\cos\theta)$ to be the quantity in brackets so that

$$\frac{1}{c} j_x = 2 \sin\phi f(r) g(r) F(\cos\theta).$$

Because of their similarity in form, j_y also contains $F(\cos\theta)$;

$$\frac{1}{c} j_y = -2 \cos\phi f(r) g(r) F(\cos\theta).$$

Thus, the motion of the electron in the plane of constant z is given by the differential equations

$$\begin{aligned} \dot{x} &= \frac{j_x}{\psi^\dagger \psi} = \frac{2c f(r) g(r) F(\cos\theta) \sin\phi}{\psi^\dagger \psi} \\ \dot{y} &= \frac{j_y}{\psi^\dagger \psi} = \frac{-2c f(r) g(r) F(\cos\theta) \cos\phi}{\psi^\dagger \psi}. \end{aligned} \tag{5.8}$$

Now, noting that we can write $x = r \sin\theta \cos\phi$ and $y = r \sin\theta \sin\phi$, we have

$$x\dot{x} + y\dot{y} = 0 = \frac{d}{dt}(x^2 + y^2).$$

This shows that in the $j = \ell + \frac{1}{2}$ case, xy motion is circular about the z axis.

A similar proof holds for the $j = \ell - \frac{1}{2}$ case. For the sake of the computations in the next

section, the current terms for this case are

$$\begin{aligned}\frac{1}{c}j_x &= -2\sin\phi f(r)g(r)\left(\sqrt{\tfrac{\ell-m+\frac{1}{2}}{2\ell+1}}\sqrt{\tfrac{\ell-m-\frac{1}{2}}{2\ell-1}}P_{\ell,m-\frac{1}{2}}P_{\ell-1,m+\frac{1}{2}} + \sqrt{\tfrac{\ell+m+\frac{1}{2}}{2\ell+1}}\sqrt{\tfrac{\ell+m-\frac{1}{2}}{2\ell-1}}P_{\ell,m+\frac{1}{2}}P_{\ell-1,m-\frac{1}{2}}\right) \\ &= -2\sin\phi f(r)g(r)G(\cos\theta)\end{aligned} \tag{5.9}$$

where we have defined $G(\cos\theta)$ as the term in brackets in the line above, and

$$\frac{1}{c}j_y = 2\cos\phi f(r)g(r)G(\cos\theta). \tag{5.10}$$

This is similar to the $j = \ell + \frac{1}{2}$ case, but we have a new function $G(\cos\theta)$ and a sign change. We obtain

$$\dot{x} = \frac{cJ_x}{\psi^\dagger\psi} = -\frac{2cf(r)g(r)G(\cos\theta)\sin\phi}{\psi^\dagger\psi}$$

and

$$\dot{y} = \frac{cJ_x}{\psi^\dagger\psi} = \frac{2cf(r)g(r)G(\cos\theta)\cos\phi}{\psi^\dagger\psi}.$$

Again, $x\dot{x} + y\dot{y} = 0$ so that $\frac{d}{dt}(x^2+y^2) = 0$ and the motion is circular. Together with the result that the motion is always constrained to planes of constant z, this shows that in all the hydrogen eigenstates of the forms (5.4) and (5.5), the only possible electron trajectories are circles of constant elevation, rotating about the z axis.

Furthermore, as in the Pauli and Schrödinger cases presented previously, the current terms (and in fact also the momentum) depend only on r and θ, which are constant, and not on ϕ. The motion can therefore be completely characterized by the initial position and the rate of revolution $d\phi/dt$, which is a function of r and θ which are determined by the initial conditions and fixed thereafter. The rate of revolution can be computed from the current terms. This situation is by now familiar; indeed, this is the qualitative consistency we sought with the Schrödinger and Pauli cases.

As in the Pauli case, it is useful to show in general what happens when the sign of m

changes. With reference to (5.7), one can see that the quantity in brackets, $F(\cos\theta)$, changes sign when m changes from positive to negative. To see this, note that the coefficients of the two summands of $F(\cos\theta)$ are interchanged:

$$\sqrt{\frac{\ell+m+\frac{1}{2}}{2\ell+1}} \to \sqrt{\frac{\ell-m+\frac{1}{2}}{2\ell+1}} \tag{5.11}$$

and

$$\sqrt{\frac{\ell+m+\frac{3}{2}}{2\ell+1}} \to \sqrt{\frac{\ell-m+\frac{3}{2}}{2\ell+1}}. \tag{5.12}$$

Furthermore, when $m \to -m$, we have

$$P_{\ell,m-\frac{1}{2}} \to P_{\ell,-m-\frac{1}{2}} = P_{\ell,-(m+\frac{1}{2})} = (-1)^{m+\frac{1}{2}} P_{\ell,m+\frac{1}{2}}. \tag{5.13}$$

The polynomial products change as follows:

$$P_{\ell,m-\frac{1}{2}} P_{\ell+1,m+\frac{1}{2}} \to (-1)^{m+\frac{1}{2}} P_{\ell,m+\frac{1}{2}} (-1)^{m-\frac{1}{2}} P_{\ell+1,m-\frac{1}{2}} = (-1)^{2m} P_{\ell,m+\frac{1}{2}} P_{\ell+1,m-\frac{1}{2}}. \tag{5.14}$$

Since the m values are all half-integers, $2m$ is odd, and $(-1)^{2m} = -1$. This change happens in the other polynomial product as well. Together with the interchange of the coefficients, this means that when m is replaced with $-m$, $F(\cos\theta)$ simply changes sign overall. This is also the case with $G(\cos\theta)$, as can be easily verified.

Thus, the angular rotation simply changes direction, but maintains the same functional form, for $m = \pm\frac{1}{2}$. This was also the case for the Pauli trajectories, which means that we have another early indication of consistency between the Pauli and Dirac cases. Indeed, if this overall sign change as $m \to -m$ did not occur, there would be no possibility of overall agreement with the Pauli trajectories. It was not, however, obvious at the outset of the Dirac equation calculations that this overall sign change would again appear.

In general, we find the angular rate of revolution from (5.8) using the relation

$$\dot{y} = (r \sin\theta \cos\phi)\dot{\phi}. \tag{5.15}$$

From (5.8), it follows that

$$\frac{d\phi}{dt} = -\frac{2cf(r)g(r)F(\cos\theta)}{\psi^\dagger\psi r \sin\theta\cos\phi} \tag{5.16}$$

in the case $j = \ell + \frac{1}{2}$. For the case $j = \ell - \frac{1}{2}$, we find

$$\frac{d\phi}{dt} = \frac{2cf(r)g(r)G(\cos\theta)}{\psi^\dagger\psi r \sin\theta\cos\phi}. \tag{5.17}$$

This allows the rate of revolution, and hence the whole trajectory, to be calculated for any of the wave functions given in (5.4) or (5.5).

We turn in the next section to some computations of these rates of revolution for the first few eigenstates, including their non-relativistic limits.

5.2.1 Angular Velocities for $n = 1$ and $n = 2$ Dirac Eigenstates

Although (5.16) and (5.17) are simple in appearance, the functions $f(r)$, $g(r)$ – and therefore $\psi^\dagger\psi$ – are quite complicated in form. Since we already know the qualitative motion, explicit computations of the rates of revolution for the general case, beyond the result given in (5.16), are not particularly enlightening.

However, it is enlightening to examine the nonrelativistic limits of (5.16) and compare the results to the values computed from the Pauli equation. Because the Pauli equation is non-relativistic, one would not expect agreement between the Dirac results in general and the Pauli results, but one would expect agreement in the non-relativistic limit. In what follows, we examine the nonrelativistic limits of (5.16) for the $n = 1$ and $n = 2$ eigenstates so that they may be compared to the results presented in Tables 3.1 and 4.1. Note that we compute only the positive m value since the angular velocity simply changes sign for negative m.

n=1

In the ground state, we have [14]

$$\begin{aligned} g(r) &= \left(\frac{2}{a}\right)^{3/2} \sqrt{\frac{1+\epsilon_1}{2\Gamma(2\gamma_1+1)}} e^{-\rho_1/2} \rho_1^{\gamma_1-1} \\ f(r) &= -\sqrt{\frac{1-\epsilon_1}{1+\epsilon_1}} g = -\delta g, \end{aligned} \tag{5.18}$$

where

$$\gamma_1 = \sqrt{1-\alpha^2}, \quad \rho_1 = 2r/a, \quad \epsilon_1 = \left(1+\frac{\alpha^2}{\gamma_1^2}\right)^{-1/2}, \quad \delta = \sqrt{\frac{1-\epsilon_1}{1+\epsilon_1}}, \tag{5.19}$$

α is the fine structure constant, $\alpha = \frac{e^2}{\hbar c}$ in cgs units, and a is the Bohr radius. Recall that a can be written $a = \frac{\hbar}{m_e e^2}$. These relations will be used to write the Dirac rotation rates in terms of a rather than α.

The ground state wave function is given by

$$\psi_1 = \frac{g}{\sqrt{4\pi}}, \quad \psi_2 = 0, \quad \psi_3 = -\frac{1}{\sqrt{4\pi}} if \cos\theta, \quad \psi_4 = -\frac{1}{\sqrt{4\pi}} if \sin\theta e^{i\phi}. \tag{5.20}$$

This gives

$$\rho = \psi^\dagger \psi = \frac{1}{4\pi}(1+\delta^2) g^2 \quad \text{and} \quad F(\cos\theta) = \frac{1}{4\pi}\sin\theta. \tag{5.21}$$

Substitution into (5.16) yields, after cancellation,

$$\frac{d\phi}{dt} = (\frac{2}{r})\frac{\delta c}{1+\delta^2}. \tag{5.22}$$

In the nonrelativistic limit, $c \to \infty$, which implies that $\alpha = e^2/\hbar c \to 0$ and $\gamma_1 \to 1$. Furthermore, this implies that $\epsilon_1 \to 1$ and $\delta \to 0$. In order to determine the behaviour of δc, we expand ϵ_1 as

$$\epsilon_1 \approx 1 - \frac{1}{2}(\frac{\alpha^2}{\gamma_1^2}) \tag{5.23}$$

so that

$$\frac{1-\epsilon_1}{1+\epsilon_1} \to \frac{1}{4}\alpha^2 \quad \text{as} \quad c \to \infty. \tag{5.24}$$

Therefore $\delta \to \frac{1}{2}\alpha$. Substitution into (5.22) yields

$$\frac{d\phi}{dt} \to \frac{1}{r}\alpha c = \frac{e^2}{r\hbar}, \tag{5.25}$$

which, when written in terms of the Bohr radius a, becomes

$$\frac{d\phi}{dt} = \frac{\hbar}{m_e a r}. \tag{5.26}$$

This is the now-familiar angular rotation rate for the ground state wave function. It agrees with the rate found for the Schrödinger and Pauli equations in earlier chapters, as it should.

n=2

Here, there are 4 cases. The quantum number ℓ can take the values 0 or 1. When $\ell = 1$, $j = \frac{3}{2}$ or $\frac{1}{2}$. When $j = \frac{3}{2}$, m can be either $\frac{3}{2}$ or $\frac{1}{2}$. We begin with $\ell = 0$.

1. $2S_{1/2}$ $(n = 2, \quad \ell = 0, \quad j = \frac{1}{2}, \quad m = \frac{1}{2})$

   As in the $1s$ case, we have the wave function

$$\psi_1 = \frac{g}{\sqrt{4\pi}}, \quad \psi_2 = 0, \quad \psi_3 = -\frac{1}{\sqrt{4\pi}} if \cos\theta, \quad \psi_4 = -\frac{1}{\sqrt{4\pi}} if \sin\theta e^{i\phi}, \tag{5.27}$$

   where the functions $f(r)$ and $g(r)$ are suitably modified for the $n = 2$ case. Again, their exact functional form is not relevant, but the relationship between f and g is important; here, rather than (5.19) we have

$$\rho_2 = \frac{2r}{N_2 a}, \quad N_2 = \sqrt{2(1+\gamma_1)}, \quad \epsilon_2 = \left(1 + (\frac{\alpha}{1+\gamma_1})^2\right)^{-1/2}, \quad \delta = \sqrt{\frac{1-\epsilon_2}{1+\epsilon_2}} A \tag{5.28}$$

and the number A is given by

$$A = \frac{(2\gamma_1 + 1)(N_2 + 2) - (N_2 + 1)\rho_2}{(2\gamma_1 + 1)N_2 - (N_2 + 1)\rho_2}. \tag{5.29}$$

After some cancellation, substitution of the wave function into (5.16) gives, as in (5.22),

$$\frac{d\phi}{dt} = (\frac{2}{r})\frac{\delta c}{1 + \delta^2}. \tag{5.30}$$

Once again, we examine how the quantities in (5.28) behave in the nonrelativistic limit $c \to \infty$. In this case,

$$\epsilon_2 \approx 1 - \frac{1}{2}(\frac{\alpha}{1 + \gamma_1})^2 \tag{5.31}$$

so that

$$\sqrt{\frac{1 - \epsilon_2}{1 + \epsilon_2}} \to \frac{\alpha}{4}. \tag{5.32}$$

As $\alpha \to 0$, $\gamma_1 \to 1$ by (5.28), and hence $N_2 \to 2$. Thus the limit of A in (5.28) is

$$A \to \frac{4 - \rho_2}{2 - \rho_2}. \tag{5.33}$$

This implies that

$$\delta c \to \alpha c \frac{4 - \rho_2}{4(2 - \rho_2)} \tag{5.34}$$

and (5.30) becomes

$$\frac{d\phi}{dt} = \frac{e^2(4 - \rho_2)}{2\hbar r(2 - \rho_2)}, \tag{5.35}$$

which can be rewritten, using (5.28) to relate ρ_2 to r, as

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e a r}\left(1 - \frac{1}{\frac{r}{2a} - 1}\right). \tag{5.36}$$

This is the angular rotation rate for the $2s$ Schrödinger state given in Chapter 3, and is also in agreement with the Pauli result of Table 4.1.

2. $2P_{3/2}$ $(n = 2, \quad \ell = 1, \quad j = \frac{3}{2}, \quad m = \frac{3}{2})$

In this case the wave function is given by

$$\psi_1 = \sqrt{\frac{3}{8\pi}} g \sin\theta e^{i\phi}, \quad \psi_2 = 0, \quad \psi_3 = -if\sqrt{\frac{3}{8\pi}} \cos\theta \sin\theta e^{i\phi}, \quad \psi_4 = -if\sqrt{\frac{3}{8\pi}} \sin^2\theta e^{3i\phi}. \tag{5.37}$$

The functions f and g, and the relationship between them, will be the same as in the above case, because only m has changed. However, we now have $\psi^\dagger\psi = \frac{3}{8\pi}\sin^2\theta g^2$ in the limit as $\delta \to 0$. Therefore, the expression corresponding to (5.22) is

$$\frac{d\phi}{dt} = \frac{-2c\delta}{r}. \tag{5.38}$$

Substitution of the nonrelativistic limiting expressions from the previous case yields

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e a r}. \tag{5.39}$$

This is the angular rotation rate for the $2p_1$ state given earlier in both Chapters 3 and 4.

3. $2P_{1/2}$ $(n = 2, \quad \ell = 1, \quad j = \frac{1}{2}, \quad m = \frac{1}{2})$

This case is similar to the previous one although the functional forms of f and g are different. We have

$$\psi_1 = \frac{1}{\sqrt{4\pi}} g \cos\theta, \quad \psi_2 = \frac{1}{\sqrt{4\pi}} g \sin\theta e^{i\phi}, \quad \psi_3 = -if\frac{1}{\sqrt{4\pi}}, \quad \psi_4 = 0 \tag{5.40}$$

and because $j = \ell - \frac{1}{2}$ here, rather than $\ell + \frac{1}{2}$, we now have a sign change (see (5.17), so that

$$\frac{d\phi}{dt} = -\left(\frac{2}{r}\right)\frac{\delta c}{1+\delta^2} \tag{5.41}$$

and most of the definitions of (5.28) remain the same. In this case, the term A is given

by

$$A = \frac{(2\gamma_1 + 1)N_2 - (N_2 - 1)\rho_2}{(2\gamma_1 + 1)(N_2 - 2) - (N_2 - 1)\rho_2}. \tag{5.42}$$

In the non-relativistic limit,

$$A \to \frac{6 - \rho_2}{-\rho_2} \tag{5.43}$$

so that

$$\frac{d\phi}{dt} = \frac{\hbar}{m_e r^2}\left(3 - \frac{r}{2a}\right). \tag{5.44}$$

In this case, no comparison can be made with any Schrödinger state. However, we do have agreement with the Pauli result for the corresponding state, given in Table 4.1, as expected.

4. $2P_{3/2}$ $(n = 2, \quad \ell = 1, \quad j = \frac{3}{2}, \quad m = \frac{1}{2})$

This case is somewhat different. Here, the wave function is

$$\begin{aligned} \psi_1 = \frac{1}{\sqrt{2\pi}} g\cos\theta, \quad \psi_2 = -\frac{1}{\sqrt{8\pi}} g\sin\theta e^{i\phi} \\ \psi_3 = -if\frac{1}{\sqrt{8\pi}}(3\cos^2\theta - 1), \quad \psi_4 = -if\sqrt{\frac{9}{8\pi}}\sin\theta\cos\theta e^{i\phi} \end{aligned} \tag{5.45}$$

and

$$\psi^\dagger\psi = \frac{1}{8\pi}(4\cos^2\theta + \sin^2\theta)g^2 + \frac{1}{8\pi}((3\cos^2\theta - 1)^2 + 3\sin^2\theta\cos^2\theta)f^2. \tag{5.46}$$

Furthermore, the function $F(cos\theta)$ becomes

$$F(cos\theta) = \frac{1}{8\pi}\sin\theta(8\cos^2\theta - \sin^2\theta). \tag{5.47}$$

Again, $f = -\delta g$, with

$$\delta = \sqrt{\frac{1 - \epsilon_3}{1 + \epsilon_3}}, \quad \epsilon_3 = \left(1 + \frac{\alpha^2}{\gamma_2^2}\right)^{-1/2}, \quad \gamma_2 = \sqrt{4 - \alpha^2} \tag{5.48}$$

and we find from (5.16) that

$$\frac{d\phi}{dt} = \frac{2\delta c(8\cos^2\theta - \sin^2\theta)}{r(4\cos^2\theta + \sin^2\theta)}. \tag{5.49}$$

As $c \to \infty$,

$$\epsilon_3 \approx 1 - \frac{1}{2}(\frac{\alpha}{2})^2 \tag{5.50}$$

so that $\delta c \to \frac{\alpha c}{4}$. After substituting and rewriting $\alpha = \frac{e^2}{\hbar c}$ and $a = \frac{\hbar}{m_e e^2}$, we obtain

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e ar}(\frac{8\cos^2\theta - \sin^2\theta}{4\cos^2\theta + \sin^2\theta}). \tag{5.51}$$

Once again, no comparison can be made with any Schrödinger state, but comparing to the Pauli result in Table 4.1, we see that there is agreement between the non-relativistic limit of the Dirac trajectory, computed here, and the Pauli trajectory computed in Chapter 4.

In each case presented above, the nonrelativistic limit of the Dirac angular velocity agrees with the corresponding Pauli result given in Table 4.1. We expect this, since the Pauli equation is the nonrelativistic limit of the Dirac equation. However, the results are not obvious, since the expressions in (5.3) and (4.3) for the Dirac and Pauli currents are quite different.

5.3 Concluding Remarks

In this chapter, we have determined the general features of de Broglie-Bohm trajectories for energy/total angular momentum eigenstates of the Dirac hamiltonian for hydrogen. In all cases, the electron, assumed to be in an eigenstate of M_z, the z-component of the total angular momentum, M, is confined to a plane of constant z-value and executes circular motion about the z-axis with a constant angular velocity $d\phi/dt$. As well, we have outlined

a procedure to compute these angular velocities for general eigenstates and have explicitly computed them for the $n = 1$ and $n = 2$ Dirac hydrogen eigenstates.

Our investigation of the agreement between the Schrödinger, Pauli and Dirac causal trajectories can now be completed. First, in the cases where the Pauli eigenstates are also eigenstates of the s_z operator, our results from the Pauli equation agree with earlier computations of the trajectories of corresponding Schrödinger eigenstates; this was seen at the end of the last chapter. However, the Pauli-Dirac agreement does not depend on whether the state is an eigenstate of any particular operator, as was the case in the Pauli-Schrödinger comparison, because our states are eigenstates of the same operators (except for L^2). Rather, the agreement depends on taking the non-relativistic limit. In this chapter, we showed that the nonrelativistic limits of the Dirac results agree with the Pauli results in all of the relevant eigenstates.

These trajectory computations, considering the Schrödinger, Pauli and Dirac equations, give a picture of the hydrogen eigenstates from the point of view of the causal theory. They show, in essence, that the de Broglie-Bohm causal picture can be applied coherently to the hydrogen atom, moving from the Schrödinger to the Pauli and ultimately to the Dirac equation. The expected and intuitive limiting agreements among the three equations are respected by the causal trajectories. The results of this chapter are also given in [25].

Of course, these results do not completely characterize the hydrogen atom. For example, one may wish to consider trajectories for Pauli or Dirac wave functions other than those considered in these chapters. For example, it may be interesting to examine trajectories for particular linear combinations of eigenstates, as indeed, we examined trajectories for the familiar Schrödinger $2p_x$ and $2p_y$ orbitals used in descriptions of chemical bonding in Chapter 3. The method of computing trajectories outlined in this and the previous chapter can be extended in a straightforward manner to treat such linear combinations in the Pauli and Dirac cases, although the computations themselves may well become quite complicated. One might not generally expect that the trajectories for other eigenstates would be circular,

nor that they would be circles about the z axis.

In addition to various constant linear combinations of eigenstates such as the $2px$ and $2py$ states described above, there are some interesting questions with physical relevance which can be examined using the causal theory, and which are relevant to extending the application of the causal theory to the hydrogen atom. One such problem is the question of transition; given the now fairly comprehensive characterization of stationary states trajectories, what would the trajectories look like for a transition between two eigenstates? It would be interesting to note whether one could see a clear progression between the behaviour of the trajectory in an 'initial' state, as characterized by the angular rate of revolution, and the behaviour in the new state after a transition has occurred. In the next chapter, we will examine this problem by finding trajectories associated with a time-varying linear combination of the $1s$ and $2p_0$ hydrogenic Schrödinger wave functions, using a hamiltonian that simulates an electronic transition induced by an oscillating electric field.

Chapter 6

A Transition in Hydrogen

6.1 Introduction

This thesis has so far been focused on the computation of electron trajectories for eigenstates of the hydrogen atom. As mentioned in the concluding remarks of the last chapter, the question of the transitions between two such eigenstates is a very natural extension of this work. The computation of trajectories during a transition is illuminating and will continue to build an impression of the intuitive way in which the causal theory describes the hydrogen atom.

Bohm himself introduced the idea of studying transitions in terms of the causal interpretation, examining the Franck-Hertz experiment and the photoelectric and Compton effects [18]. He attempted to show that the seemingly discontinuous and poorly defined transfers of energy and momentum in transitions could be accounted for in a continuous manner by means of the quantum potential that arises in the causal formalism. More recently in this vein, Dewdney and Lam [32] studied transitions of (spinless) particles in a one-dimensional infinite square well potential.

In this chapter we employ the causal theory to study the problem of a $1s$-$2p_0$ electronic transition in hydrogen induced by an oscillating (semiclassical) electromagnetic field, taking

the spin of the electron into account. This is done using the Schrödinger equation, rather than the Pauli or Dirac equations discussed in the previous chapters, essentially for reasons of simplicity. The resulting trajectories are therefore non-relativistic, and while the spin of the electron is taken into account via the extra term (see (1.16)), the Schrödinger equation carries the assumption that the electron remains in an eigenstate of the spin operator.

We examine solutions of the equation of motion (1.16) for an electron with spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$ (the "α" or "spin up" state) as it undergoes a transition from the $1s$ to $2p_0$ state in hydrogen due to the presence of an oscillating electric field. We may assume that the electron has constant spin vector since the hamiltonian describing the atom in the field (this hamiltonian will be given in the next section) is spin-independent. As was done in Chapter 3 in (3.3), the wavefunction of the electron $\Psi(\mathbf{x}, \mathbf{s}, t)$ may then be written as the tensor product $\psi(\mathbf{x}, t)\zeta(\mathbf{s})$ where $\zeta(\mathbf{s})$ is assumed to be an eigenfunction of the commuting spin operators $\hat{S}^2$ and $\hat{S}_z$, with $\hat{S}^2\zeta = \frac{3\hbar}{4}\zeta$ and $\hat{S}_z\zeta = \frac{\hbar}{2}\zeta$. As such, the remainder of our discussion may simply be focused on the evolution of the spatial portion of the wavefunction, $\psi(\mathbf{x}, t)$ according to (3.4).

In [23], as a precursor to this study, we examined the trajectories dictated by (1.16) for an electron with spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$ and spatial wavefunction that begins as a linear combination of $1s$ and $2p_0$ hydrogenic eigenfunctions:

$$\psi(\mathbf{x}, 0) = c_1\psi_{100}(\mathbf{x}) + c_2\psi_{210}(\mathbf{x}), \tag{6.1}$$

where $|c_1|^2 + |c_2|^2 = 1$. The time evolution of this wavefunction under the hydrogen atom hamiltonian is

$$\psi(\mathbf{x}, t) = c_1\psi_{100}(\mathbf{x})e^{-iE_1t/\hbar} + c_2\psi_{210}(\mathbf{x})e^{-iE_2t/\hbar}. \tag{6.2}$$

Many of the qualitative features of the $1s$-$2p_0$ transition problem studied below are captured by this model. As expected, however, the more detailed time evolution of the electron trajectories over these surfaces due to the oscillating field is missing. This time dependence

must be found by integrating the equations of motion which follow from (1.16).

6.2 Solution of the Transition Problem

Our model of the transition process assumes that a hydrogen atom in its ground ($n = 1$) state is subject to an oscillating electric field, which represents polarized radiation. The effects of the magnetic field in the radiation are neglected here. It will be assumed that the radiation is polarized so that the electric field is in the z direction. This semiclassical treatment is well-known and a hamiltonian similar to the one used here is frequently used in a perturbation approach to the problem of transition [49, 82]. Thus, the hamiltonian used to describe this transition will have the form $\hat{H} = \hat{H}_0 + \hat{H}'$, where $\hat{H}_0$ is the hydrogen atom hamiltonian and $\hat{H}'$ represents the radiation due to an oscillating electric field $\mathbf{E} = E_0 \cos(\omega t)\hat{e}_z$.

It can be shown that if ω is chosen to be sufficiently close to the $1s - 2p_0$ transition frequency,

$$\omega \approx \omega_0 = \frac{E_2 - E_1}{\hbar} \approx 1.549 \times 10^{16}\ \mathrm{s}^{-1}, \tag{6.3}$$

so that $\omega_0 - \omega \ll \omega_0 + \omega$, then the hamiltonian representing the semiclassical radiation, $\hat{H}' = -ezE_0 \cos \omega t$, is well approximated by

$$\hat{H}' = -\frac{1}{2} ezE_0 e^{-i\omega t}, \tag{6.4}$$

since the term $i(\omega + \omega_0)^{-1} \sin \omega t$ is negligible. This approximation is known as the rotating wave approximation. Here, e denotes the magnitude of the electric charge. See Appendix 6.5 for a derivation of the equivalence of our hamiltonian and the usual one. This approach allows the equations for the wavefunction coefficients to be solved exactly so that perturbation methods need not be employed. The closeness of ω to ω_0 also allows the transition probability to approach unity at various times rather than remaining small for all times.

Recall that the wave functions under the Schrödinger equation, given in (3.5), are

$$\psi_{nlm} = N_{nlm} e^{-r/na} \big(\frac{2r}{na}\big)^l L^{2l+1}_{n-l-1}(2r/na) Y^m_l(\theta, \phi), \tag{6.5}$$

where the L^{2l+1}_{n-l-1} are the associated Laguerre polynomials, and the $Y^m_l(\theta, \phi)$ are the spherical harmonics as given in (3.6). The probability of transition between two states $|\psi_1\rangle$ and $|\psi_2\rangle$ is related to the matrix element $\langle\psi_2| \hat{H}' |\psi_1\rangle$.

In the case of the hydrogen atom the only nonvanishing matrix element, assuming an $n = 1$ to $n = 2$ transition, with this semiclassical choice of hamiltonian, is between the ground state ψ_{100} and the $2p_0$ state ψ_{210}:

$$\begin{aligned} \langle\psi_{100}| \hat{H}' |\psi_{210}\rangle &= -\langle\psi_{100}| eE_0 r\cos\theta |\psi_{210}\rangle \frac{1}{2} e^{-i\omega t} \\ &= -\frac{64\sqrt{2}}{243} aeE_0 e^{-i\omega t}, \end{aligned} \tag{6.6}$$

where a is the Bohr radius. This, together with the fact that we will choose the frequency ω of our incoming radiation to be very near the frequency ω_0 of the $1-2$ transition, means that essentially only the $1s$-$2p_0$ transition will be stimulated.

Therefore, the time-dependent wavefunction can be written as a linear combination of the $|\psi_{100}\rangle$ and $|\psi_{210}\rangle$ wavefunctions:

$$\psi(t) = c_a(t)\psi_{100} e^{-iE_1 t/\hbar} + c_b(t)\psi_{210} e^{-iE_2 t/\hbar}. \tag{6.7}$$

Substitution into the Schrödinger equation yields the following equations for $c_a(t)$ and $c_b(t)$:

$$\begin{aligned} \dot{c_a} &= -\frac{i}{\hbar}\frac{V_{12}}{2} e^{-i(\omega_0-\omega)t} c_b, \\ \dot{c_b} &= -\frac{i}{\hbar}\frac{V_{12}}{2} e^{i(\omega_0-\omega)t} c_a, \end{aligned} \tag{6.8}$$

where

$$V_{12} = -\frac{128\sqrt{2}}{243} aeE_0.$$

These differential equations can be solved exactly to give

$$\begin{aligned} c_a(t) &= \frac{\sigma+\Omega}{2\sigma} e^{\frac{1}{2}i(\Omega-\sigma)t} + \frac{\sigma-\Omega}{2\sigma} e^{\frac{1}{2}i(\Omega+\sigma)t}, \\ c_b(t) &= \frac{\nu}{2\sigma} e^{\frac{1}{2}i(\Omega-\sigma)t} - \frac{\nu}{2\sigma} e^{\frac{1}{2}i(\Omega+\sigma)t}, \end{aligned} \tag{6.9}$$

where

$$\begin{aligned} \Omega &= \omega_0 - \omega, \\ \nu &= \frac{V_{12}}{\hbar}, \\ \sigma &= \sqrt{\Omega^2 + \nu^2}. \end{aligned} \tag{6.10}$$

The wavefunction $\psi(\mathbf{x}, t)$ may now be written explicitly as

$$\psi(\mathbf{x}, t) = \frac{1}{\sqrt{\pi a^3}} c_a(t) e^{-r/a} e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{32\pi a^5}} c_b(t) r e^{-r/2a} \cos\theta e^{-iE_2 t/\hbar}. \tag{6.11}$$

To compute the momentum according to (1.16), note that the first term ∇S has only $\hat{r}$ and $\hat{\theta}$ components. Since we are assuming a constant spin vector $\mathbf{s} = \frac{\hbar}{2}\hat{k}$, it follows that the vector $\nabla \log \rho \times \mathbf{s}$ points in the $\hat{\phi}$ direction.

Calculating ∇S from (6.11) yields

$$\begin{aligned} p_{\hat{r}} &= \frac{\hbar\nu\beta}{2\sigma} \frac{\cos\theta e^{-3r/2a}(1 + \frac{r}{2a})T(t)}{D(r,\theta,t)}, \\ p_{\hat{\theta}} &= \frac{\hbar\nu\beta}{2\sigma} \frac{\sin\theta e^{-3r/2a} T(t)}{D(r,\theta,t)}, \end{aligned} \tag{6.12}$$

where $\beta = 4\sqrt{2}a$ is the ratio of the normalizing factors of the two wavefunctions,

$$T(t) = -\cos\omega_0 t \sin\sigma t - \frac{\Omega}{\sigma}\sin\omega_0 t + \frac{\Omega}{\sigma}\cos\sigma t \sin\omega_0 t \tag{6.13}$$

and

$$D(r,\theta,t) = e^{-2r/a}\frac{1}{2\sigma^2}(\sigma^2+\Omega^2+\nu^2\cos\sigma t) + \beta^2 r^2 e^{-r/a}\cos^2\theta\frac{\nu^2}{2\sigma^2}(1-\cos\sigma t) \\ + \frac{\nu}{\sigma}\beta r e^{-\frac{3r}{2a}}\cos\theta(\frac{\Omega}{\sigma}\cos\omega_0 t - \frac{\Omega}{\sigma}\cos\sigma t\cos\omega_0 t - \sin\omega_0 t\sin\sigma t). \quad (6.14)$$

The denominator $D(r,\theta,t)$ in the above expressions is proportional to $|\psi(\mathbf{x},t)|^2$.

The second term in (1.16), $\nabla\log\rho\times\mathbf{s}$, can be computed in the (right-handed) spherical polar coordinate system with the relationship

$$\mathbf{A}\times\mathbf{B} = \begin{vmatrix} \hat{e}_\theta & \hat{e}_\phi & \hat{e}_r \\ A_\theta & A_\phi & A_r \\ B_\theta & B_\phi & B_r \end{vmatrix}. \quad (6.15)$$

Using the simplification

$$\nabla\log\rho = 2\mathrm{Re}\left(\frac{(\nabla\psi)\psi^*}{\psi^*\psi}\right),$$

we find the $\hat{\phi}$ component of the momentum to be

$$p_{\hat{\phi}} = \frac{\hbar\beta}{D}(-\chi_r\sin\theta - \chi_\theta\cos\theta), \quad (6.16)$$

where

$$\chi_r = \frac{1}{\beta a}|c_a|^2 e^{-2r/a} + \beta|c_b|^2\cos^2\theta e^{-r/a}r(1-\frac{r}{2a}) + \cos\theta e^{-3r/2a}(1-\frac{3r}{2a})T'(t),$$
$$\chi_\theta = -\beta|c_b|^2 e^{-r/a}\sin\theta\cos\theta r - e^{-3r/2a}\sin\theta\ T'(t)$$

and

$$T'(t) = \frac{\nu}{2\sigma}(\frac{\Omega}{\sigma}\cos\omega_0 t - \frac{\Omega}{\sigma}\cos\sigma t\cos\omega_0 t - \sin\sigma t\sin\omega_o t). \quad (6.17)$$

In summary, the three components of the momentum are given by (6.12) and (6.16). It

is worth noting again that the spin-dependent momentum term $\nabla \log \rho \times \mathbf{s}$ in (1.16) is responsible for the ϕ-momentum $p_{\hat{\phi}}$.

It is useful to rescale these equations by defining the following dimensionless variables:

$$\xi = \frac{r}{a}, \qquad \tau = \omega_0 t. \tag{6.18}$$

In these variables, (6.12) and (6.16) give rise to the following system of differential equations in ξ, θ, and ϕ as functions of τ:

$$\begin{aligned} \frac{d\xi}{d\tau} &= \frac{\nu}{3\sqrt{2}\sigma}\left(\cos\theta e^{-3\xi/2}(1+\frac{\xi}{2})\right)\frac{\tilde{T}(\tau)}{D} \\ \frac{d\theta}{d\tau} &= \frac{\nu}{3\sqrt{2}\sigma}\left(\sin\theta\frac{e^{-3\xi/2}}{\xi}\right)\frac{\tilde{T}(\tau)}{D} \\ \frac{d\phi}{d\tau} &= -\frac{\nu}{3\sqrt{2}\sigma\xi D}(\chi_r + \chi_\theta\cot\theta), \end{aligned} \tag{6.19}$$

where we have used the following relations:

$$\frac{d\phi}{d\tau} = \frac{p_\phi}{ma\omega_0\xi\sin\theta}$$

and

$$\frac{\hbar}{ma\omega_0} = \frac{8}{3}a.$$

Some important qualitative features of the solutions to these differential equations may be extracted. First note that the ξ and θ equations are independent of ϕ. From these two equations, we have

$$\frac{d\xi}{d\theta} = -\xi\left(1+\frac{\xi}{2}\right)\cot\theta, \tag{6.20}$$

which is obtained by dividing the first equation by the second. Note that where the denominator D is zero, the magnitude of the wave function $|\psi|^2$ is also zero, so there is zero probability of finding the particle in those regions. The resulting differential equation is

separable, and is easily solved to give

$$\xi = \frac{2}{A\sin\theta - 1}, \qquad A = \frac{2+\xi_0}{\xi_0 \sin\theta_0} > 1, \tag{6.21}$$

where $\xi_0 = \xi(0)$ and $\theta_0 = \theta(0)$. This relation defines a family of hyperbolae in vertical planes that contain the z-axis. (Note that the right hand side of (6.20) is determined by the functional forms of the $1s$ and $2p_0$ wavefunctions. Other allowable pairs of wavefunctions will yield different types of curves.) These hyperbolae thus define the relationship between r and θ on the trajectories. In the $x - z$ plane, these hyperbolae take the form

$$(A-1)x^2 - 4Ax + 4 = z^2, \tag{6.22}$$

where $x = \xi \sin\theta$ and $z = \xi\cos\theta$.

Each trajectory, i.e. each solution of (6.19), must therefore lie on a surface obtained by rotating one such hyperbola about the z-axis (see [23]). This rotation corresponds to the ϕ part of the evolution. Thus, any circle about the z axis is contained in one of the rotated hyperbolae, so the hyperbolae contain the eigenstate trajectories. This characterization of the space in terms of invariant hyperboloids on which the trajectories lie has been obtained without any time-dependent integration of the differential equations determining the trajectories. The time-dependent behaviour of the trajectories lying on these invariant sets must be determined numerically.

6.3 Numerical Results

At this stage, while the invariant surfaces discovered in the previous section are interesting, it is not yet clear how the causal theory describes a transition between the ground state and the $2p_0$ state. It would be nice if it were possible to clearly characterize the transition in terms of properties of the motion, showing that at the beginning of the process, the motion

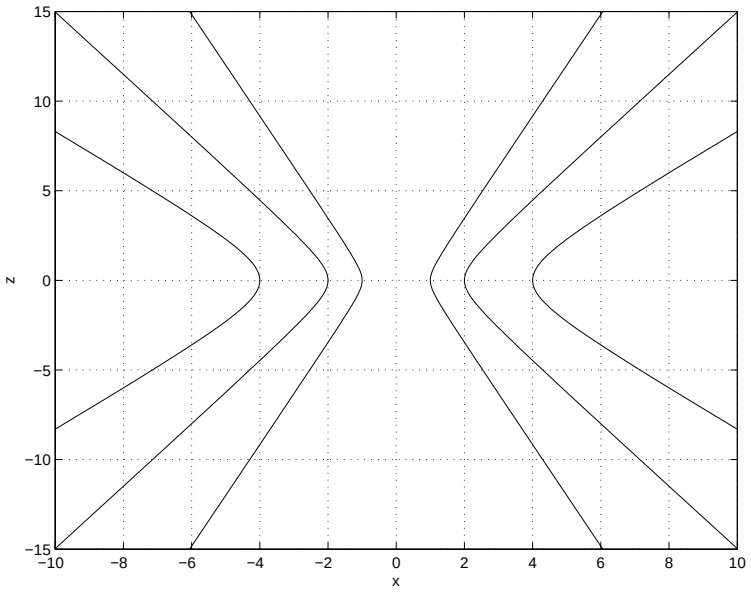


Figure 6.1: Some hyperbolae given by (6.22)

resembles that of the ground state trajectory in isolation, namely rotation about the z axis with rate of revolution

$$\frac{d\phi}{dt} = \frac{\hbar}{m_e a r},$$

and that later on, when the system is most likely to be found in the $2p_0$ state, the motion resembles that of the $2p_0$ state in isolation. But so far, the only comment that can be made about the relationship between the trajectories during the transition and the trajectories of the eigenstates in isolation is that the hyperboloids of revolution contain circles about the z axis. In other words, there is as yet no contradiction between the results of Chapter 3 and the notion that the transition should be 'visible' over the course of the trajectory under the hamiltonian we have chosen.

It is possible, though, that the presence of the perturbing hamiltonian will significantly alter the trajectories even when the wave function is 'close' to the $2p_0$ wave function. We certainly would not expect the transition trajectories to be circular about the z axis, though that is not yet ruled out. Since ψ_{2p_0} is not an eigenfunction of the new hamiltonian, it will

not be a stable state, and it is by no means clear at the outset how much the presence of even a small fraction of the ψ_{100} wave function will alter the trajectories. We know from our full knowledge of the time-dependent wave function how likely it would be for a transition to be observed if the perturbing hamiltonian were turned off at a given time, and the energy of the electron were measured; it is the numerical results which will answer the question of how clearly a transition is visible along trajectories.

In order to do any numerical integration, it is necessary to choose the field strength E_0 and the perturbing frequency ω_0, and in doing this, there are various factors that must be taken into account. First, recall that in order to use the hamiltonian $\hat{H}' = -\frac{1}{2}ezE_0e^{-i\omega t}$, we require that the perturbing frequency ω be close to the transition frequency ω_0 so that $\Omega = \omega_0 - \omega \ll \omega_0 + \omega$. Therefore, we cannot allow Ω to be too large, i.e., $\Omega \leqslant O(10^{13})$.

If we wish to be fairly confident that a transition will occur, it is also necessary that the coefficient c_b become large in magnitude at some time, i.e., roughly unity. Recall from (6.9) that $c_b \propto \nu/2\sigma$, and $\nu \propto E_0$. Also, the derivatives in (6.19) are proportional to $\nu/2\sigma$, and it is desirable for numerical integration that they evaluate to order 1. Therefore, $|\nu|$ should be significant compared to 2σ. Now, recall that $\sigma = \sqrt{\Omega^2 + \nu^2}$ so that

$$\frac{|\nu|}{2\sigma} = \frac{1}{2}\left[\frac{\Omega^2}{\nu^2} + 1\right]^{-1/2}.$$

Therefore we require that $|\nu|$ not be too large. Because $|\nu|$ is proportional to the field strength, we are free to choose a small value.

Another factor to consider is that there are two angular frequencies in the problem, namely σ and ω_0 from (6.13) and (6.17). For numerical stability it is best if these are within several orders of magnitude of each other. Therefore, σ should not be too small in comparison with ω_0. It is also desirable that c_b become significant in a reasonable time. From (6.9), we find that

$$|c_b(t)|^2 = \left(\frac{\nu}{\sigma}\right)^2 \sin^2\frac{\sigma}{2}t. \tag{6.23}$$

Therefore, having σ appropriately scaled will mean that there is a high probability of seeing a transition within a reasonable time.

The above considerations imply that:

1. $|\nu|$ cannot be too large because $[\Omega^2/\nu^2 + 1]^{-1/2}$ must be O(1),

2. $\sigma = \sqrt{\Omega^2 + \nu^2}$ cannot be more than several orders of magnitude smaller than ω_o and

3. we cannot increase σ by increasing Ω, because we require that $\Omega \leqslant O(10^{13})$.

With these points in mind, the parameters have been chosen as follows:

$$\begin{aligned} E_0 &= 8.8 \times 10^7 \text{ V/m}, \\ \Omega &= 1.55 \times 10^{12} \text{s}^{-1}, \end{aligned} \tag{6.24}$$

so that

$$\begin{aligned} \nu &= -5.1 \times 10^{12}, \\ \sigma &= 5.32 \times 10^{12}. \end{aligned} \tag{6.25}$$

The numerical integration was performed using MATLAB's built-in ordinary differential equation solvers. The results from the various solvers were compared, and the several solvers converged upon the final trajectories shown here. The solver *ode23s* was used to generate these results; it is a one-step solver based on a Rosenbrock formula of order 2. The results of numerical integration for two choices of initial conditions are shown in Figs. (6.2) and (6.3). Figs. (6.4) and (6.5) show the same trajectories split into five parts (the axes are the same). In these latter plots, the hyperboloid surfaces of revolution on which the trajectories lie, described at the end of the previous section, are discernible. Note also that though the axes of the plots are taken so as to best show the shape of the trajectories, the vertical axes vary in Figs. (6.4) and (6.5); the latter parts of the trajectories are more closely 'held in' and do not have as much vertical range. These latter figures have trajectories which more

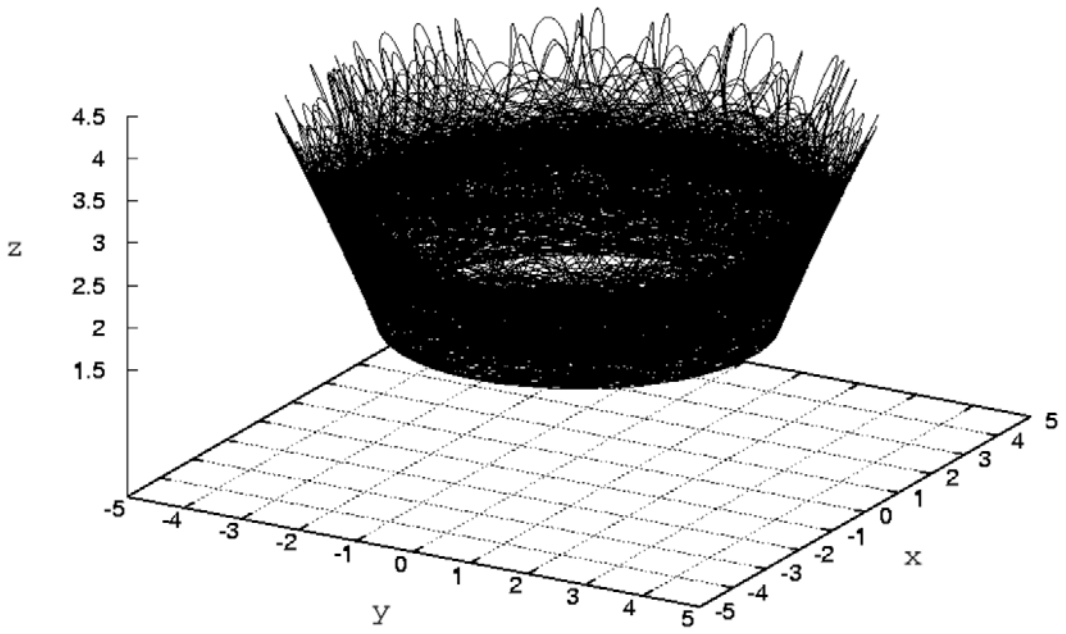


Figure 6.2: Transition trajectory, $\xi(0) = 4$, $\theta(0) = 1$

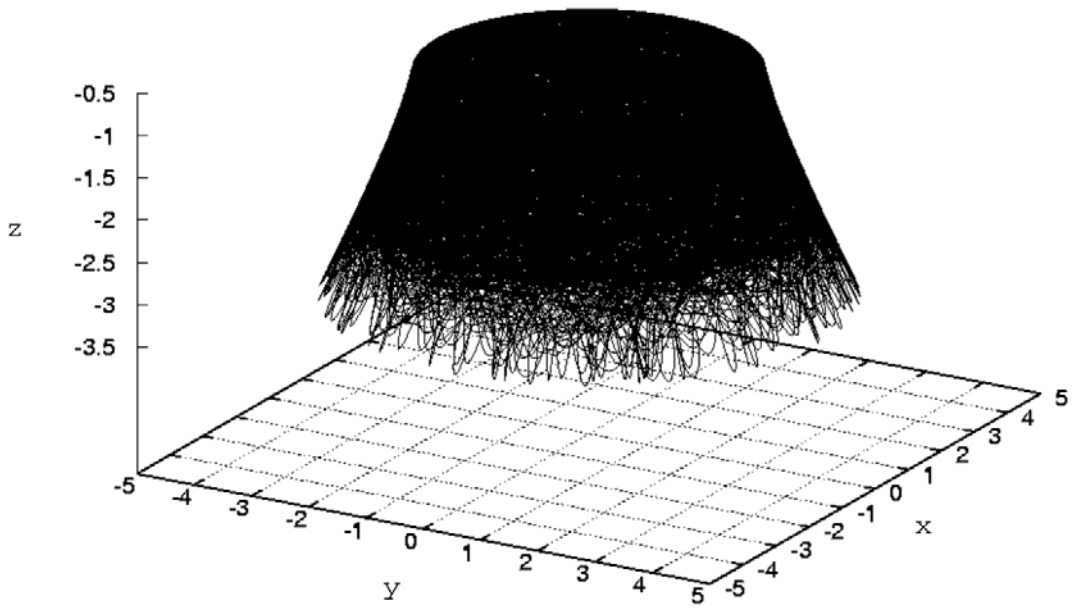
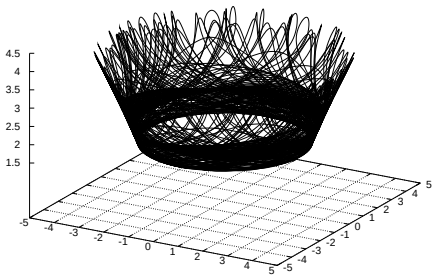
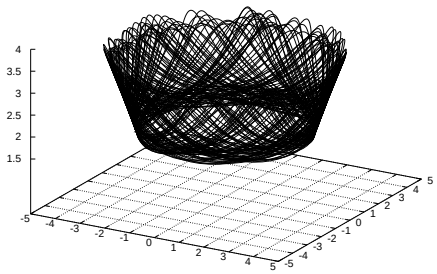


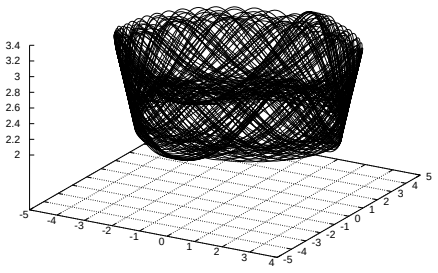
Figure 6.3: Transition trajectory, $\xi(0) = 3.2$, $\theta(0) = 2$



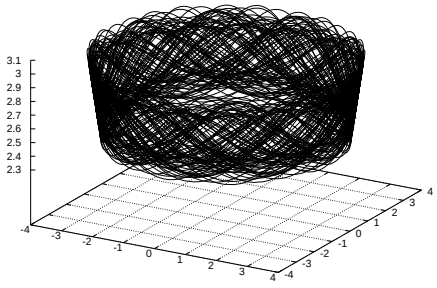
(a) $\tau = 0 - 1469$



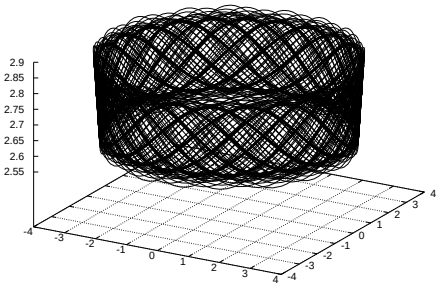
(b) $\tau = 1469 - 2992$



(c) $\tau = 2992 - 4844$

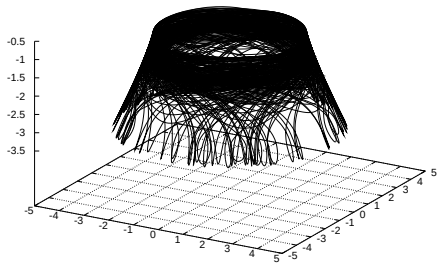


(d) $\tau = 4844 - 7196$

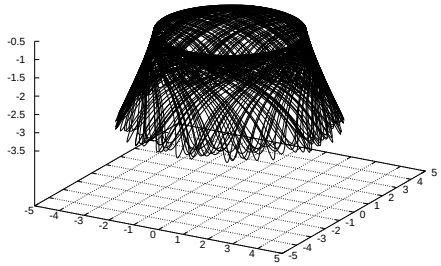


(e) $\tau = 7196 - 10000$

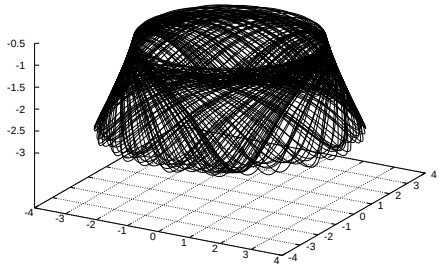
Figure 6.4: Transition trajectory, $\xi(0) = 4$, $\theta(0) = 1$ in five parts



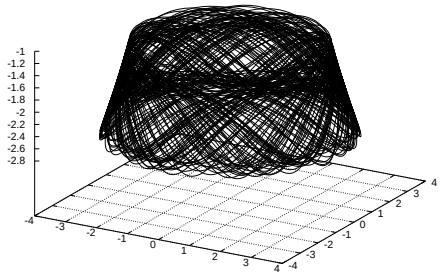
(a) $\tau = 0 - 1469$



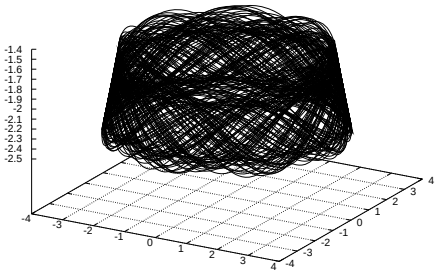
(b) $\tau = 1469 - 2992$



(c) $\tau = 2992 - 4844$



(d) $\tau = 4844 - 7196$



(e) $\tau = 7196 - 10000$

Figure 6.5: Transition trajectory, $\xi(0) = 3.2$, $\theta(0) = 2$ in five parts

closely resemble the familiar circles about the z axis, giving a preliminary indication that there is consistency with the eigenstate results.

The task now is to compare the numerical results with what one might expect in this transition problem. For example, in standard semiclassical treatments of this problem (see, for example, [82], pp. 282-285), the maximum probability of transition occurs when $\sin^2 \frac{1}{2}\Omega t = 1$, or $\Omega t = (2k+1)\pi$ for $k = 0, 1, 2, \ldots$. In our formulation, from (6.23) the maximum probability of transition occurs when $\sin^2 \frac{1}{2}\sigma t = 1$, or $\sigma t = (2k+1)\pi$ for $k = 0, 1, 2, \ldots$. In other words, the dependence on Ω is replaced with one on $\sigma = \sqrt{\Omega^2 + \nu^2}$. This is due to our choice of hamiltonian and the fact that the equations in (6.9) result from an exact integration of (6.8) rather than a perturbation approach. From the above, the first occurrence of the maximum probability of transition in our problem will occur at $t = \pi/\sigma$ or, in dimensionless time, $\tau = \pi\omega_0/\sigma$. From the numerical values chosen for the parameters above, this corresponds to $\tau \approx 9000$.

The causal interpretation allows us to examine the transition in greater detail by looking at the angular velocity $\dot{\phi}$ exhibited by the trajectories. At time $t = \tau = 0$, each trajectory begins at the $1s$ ground state wavefunction, with $c_a(0) = 1$ and $c_b(0) = 0$, and we expect the electron to revolve about the z-axis with angular frequency given by (3.2). When the wavefunction is approximately equal to the $2p_0$ eigenstate, viz., $c_a \approx 0$ and $c_b \approx 1$, then we expect $\dot{\phi}$ to be given roughly by (3.26).

Since the computations were performed in the scaled variables ξ and τ defined in (6.18), we must first rescale the $1s$ and $2p_0$ angular velocities in ϕ in order to assess the numerical results. For the $1s$ state, (3.2) becomes

$$\frac{d\phi}{d\tau} = \frac{\hbar}{m_e a^2 \omega_0 \xi} = \frac{8}{3\xi}. \tag{6.26}$$

The angular velocity for the $2p_0$ state is simply one-half the above result.

The values of the scaled angular velocity $d\phi/d\tau$ associated with the trajectory shown in

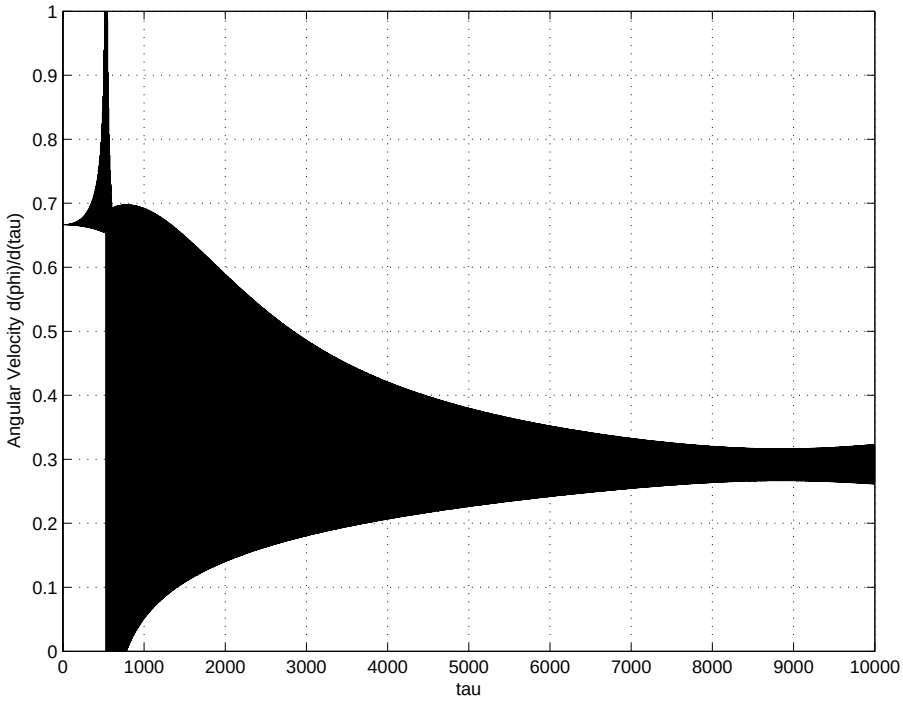


Figure 6.6: $\frac{d\phi}{d\tau}$ along the trajectory shown in Fig. 6.2

Fig. (6.2) are presented as a function of τ in Fig. (6.6). (In Fig. (6.7) the corresponding values of ϕ are shown.) Recall that this trajectory began with the value $\xi(0) = 4$. From Fig. (6.2), $d\phi/d\tau$ is observed to be roughly 2/3 near $\tau = 0$. This is in agreement with (6.26) – the electron is revolving about the z-axis at roughly the $1s$ rate.

Near $\tau = 9000$, roughly the time for $|c_b(\tau)|^2$ to achieve its maximum value, we observe that $d\phi/d\tau \approx 0.3$. At that time, $\xi \approx 4.5$. This is in agreement with the scaled $2p_0$ rate $4/(3\xi) \approx 0.3$. Thus, as was hoped, the trajectories for the transition problem do seem to reflect a change from one state to another, though neither the $1s$ nor the $2p_0$ states are eigenstates of the perturbed hamiltonian. It is intuitively satisfying that this should be the case, especially because in standard quantum mechanics, no continuous picture of the transition process is available, since the 'states' have no meaning unless the perturbation is turned off.

In the causal interpretation it is also possible to ascribe a value of energy along a trajec-

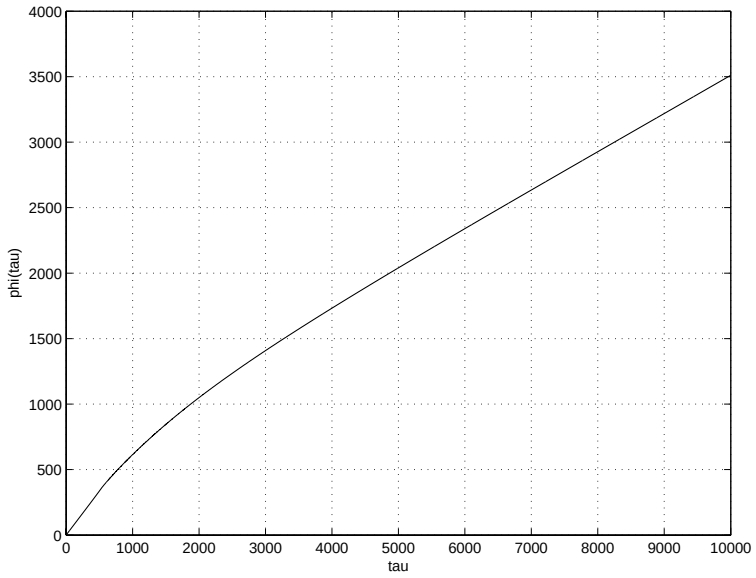


Figure 6.7: $\phi(\tau)$ along the trajectory shown in Fig. 1

tory and thereby examine the time-dependent behaviour of the energy during a transition. Note that this is in contrast to standard quantum mechanics, in which we can only compute probabilities of measuring energy eigenvalues E_1 or E_2 after the perturbation has been turned off. The energy could be seen as a more meaningful characterization of the state than the rate of ϕ revolution, perhaps because energy is more closely connected to the observation of transitions.

One method of computing the energy is to use the result $E = \partial S/\partial t$ implied by the quantum Hamilton-Jacobi equation (1.7). However, even when applied to the relatively simple wavefunction ψ in (6.11), this method is quite cumbersome. On the other hand, Holland's method of assigning values of an observable quantity A to points on a trajectory, which we outline below (see [61], pp. 91-93), is quite easily implemented in our problem.

Recall from Chapter 1, (1.18) and (1.19), that the local expectation value of a quantity A corresponding to the operator $\hat{A}$, along a trajectory, is defined

$$A(\mathbf{x}, t) = \frac{\mathrm{Re}\{\psi^* \hat{A} \psi\}}{\psi^* \psi}. \tag{6.27}$$

and the weighted average of $A(\mathbf{x},t)$ over trajectories agrees with the usual quantum mechanical expectation value for the observable $\hat{A}$.

To find the energy along the trajectory, we compute $E(\mathbf{x},t)$ using as our operator the hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'$ where, as before, $\hat{H}_0$ is the usual hydrogen hamiltonian, and

$$\hat{H}' = -\frac{1}{2} e E_0 e^{-i\omega t}(r\cos\theta).$$

Thus

$$E(\mathbf{x},t) = \frac{\mathrm{Re}\{\psi^*(\hat{H}_0+\hat{H}')\psi\}}{\psi^*\psi} = \frac{\mathrm{Re}\{\psi^*\hat{H}_0\psi\}}{\psi^*\psi} + \frac{\mathrm{Re}\{\psi^*\hat{H}'\psi\}}{\psi^*\psi}, \tag{6.28}$$

where $\psi(\mathbf{x},t)$ is given by (6.7). The first term in (6.28) is, after some manipulation, given by

$$\frac{\mathrm{Re}\{\psi^*(\hat{H}_0)\psi\}}{\psi^*\psi} = \frac{|c_a|^2 E_1\psi_{100}^2 + |c_b|^2 E_2\psi_{210}^2 + \psi_{100}\psi_{210}(E_2+E_1)\mathrm{Re}\{c_a c_b e^{-i\omega t}\}}{\psi^*\psi}$$

and the second term is simply

$$\frac{\mathrm{Re}\{\psi^*\hat{H}'\psi\}}{\psi^*\psi} = \frac{\mathrm{Re}\{\psi^*(-\frac{1}{2}eE_0e^{-i\omega t}(r\cos\theta)\psi)\}}{\psi^*\psi} = -\frac{1}{2}eE_0 r\cos\theta\cos\omega t$$

where, referring to (6.17),

$$\mathrm{Re}\{c_a c_b e^{-i\omega t}\} = \frac{\nu}{2\sigma}\left(\frac{\Omega}{\sigma}\cos\omega_0 t - \frac{\Omega}{\sigma}\cos\sigma t\cos\omega_0 t - \sin\sigma t\sin\omega_o t\right) = T'(t).$$

Therefore we have

$$E = \frac{|c_a|^2 E_1\psi_{100}^2 + |c_b|^2 E_2\psi_{210}^2 + \psi_{100}\psi_{210}(E_2+E_1)T'(t)}{\psi^*\psi} - \frac{1}{2}eE_0 r\cos\theta\cos\omega t. \tag{6.29}$$

This function can be evaluated along the trajectories shown in Figs. (6.2) and (6.3). The results for the first trajectory are shown in Fig. (6.8).

It should be noted that while this approach allows us to think about the energy defined along a trajectory, it is unlike the classical energy in that it is not an integral of motion.

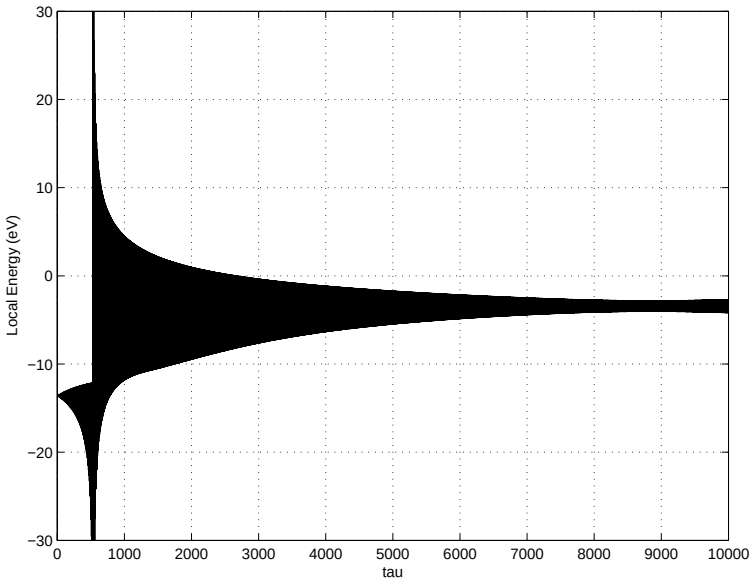
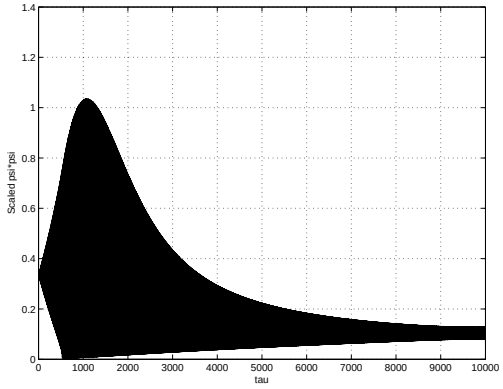


Figure 6.8: Energy along the trajectory in Fig. (6.2) (eV)

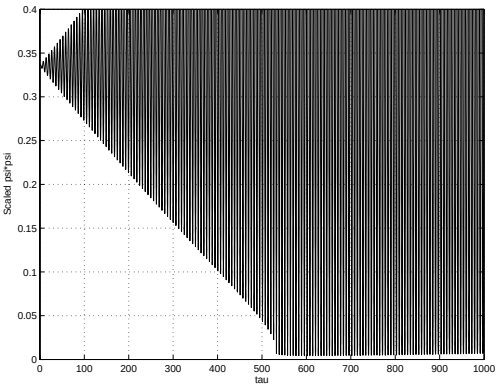
Indeed, the equation of motion (1.16) is only a first-order equation so that the structure of classical mechanics with energy as an integral of motion is not available here. The energy function given in (6.29) should therefore be referred to as a 'local energy' or 'local energy expectation value' rather than as 'the energy'. Having made this qualifying remark, note that at $\tau = 0$, the local energy is equal to the $1s$ ground state energy -13.6 eV, and that after the transition, the local energy oscillates near the value of $E_2 = -3.4$ eV, corresponding to the energy of hydrogenic $n = 2$ states.

This is quite encouraging. Like the rate of ϕ revolution, the trajectory shows a local energy expectation value which moves continuously from the $n = 1$ to (approximately) the $n = 2$ energy value. The fact that now both the quantities E and $d\phi/dt$ show qualitative features of a transition gives additional credibility to the notion that the causal trajectories make intuitive sense in describing quantum phenomena.

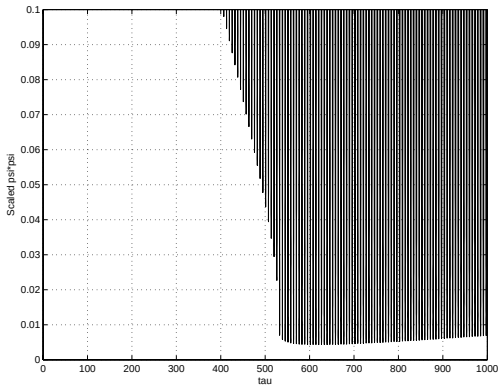
The local energy is not constant even in proximity of the $n = 1$ and $n = 2$ times, because of the extra oscillating perturbation $\hat{H}'$ that represents the semi-classical radiation field. A plot of the local energy along the trajectory shown in Fig. (6.3) is shown in Fig. (6.10).



(a) $|\psi|^2$ as a function of τ



(b) $|\psi|^2$: a closer view



(c) $|\psi|^2$: a very close view

Figure 6.9: The time-dependence of $|\psi|^2$

The spike in the local energy corresponds to a point along the trajectory that is near a zero of the wavefunction, and the quantum potential $Q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$ is steep. The dependence of $|\psi|^2$ is shown in Fig. 6.9. Note that while $|\psi|^2$ approaches zero, it does not quite reach zero. This is as it should be, because trajectories cannot pass through 'nodes' (at which $|\psi|^2 = 0$). Intuitively, one can understand the appearance of the spike in the local energy because the electron cannot spend very much time in regions where the wave function is very small, or where the quantum potential is steep– it receives a 'kick' from the quantum potential which corresponds to a sudden rise in its local energy.

Finally, note that we have computed trajectories to higher times in order to explore their

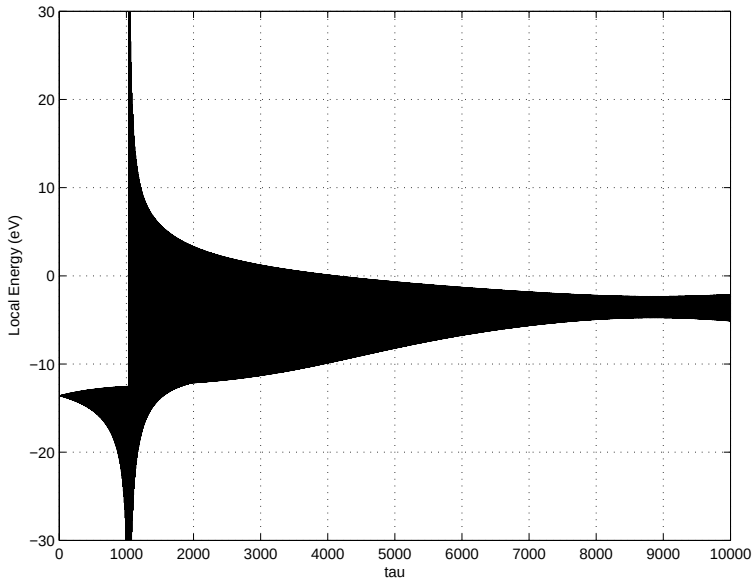


Figure 6.10: Energy along the trajectory in Fig. (6.3) (eV)

periodicity, or lack of same. At $\tau \approx 18000$, the scaled angular velocity $d\phi/d\tau$ is observed to oscillate about the $1s$ value. The local energy is also observed to oscillate about the $1s$ value of -13.6 eV. This is in accordance with $|c_b(\tau)|^2 \approx 0$ from (6.23) and the values of the parameters used in the calculation. We conclude that the transition has reversed and that the electron has returned to approximately the $1s$ ground state. Furthermore, two initial positions chosen very near each other, both on the same and on nearby hyperbolae of revolution, yield trajectories which remain near each other until at least $\tau \approx 20000$. This indicates that at least on the smaller time scale, the system is probably not chaotic.

6.4 Concluding Remarks

We have studied the problem of a $1s$ to $2p_0$ electronic transition in hydrogen – induced by an oscillating (semiclassical) radiation field – in terms of the causal interpretation of quantum mechanics, taking the spin of the electron into account via the momentum equation (1.16). The electron is assumed to be in a "spin up" eigenstate, with associated spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$,

during the transition. The electronic trajectories lie on invariant hyperboloid surfaces of revolution about the z-axis. The nature of the trajectories over these surfaces is quite complex due to the quasiperiodic nature of the equations of motion which, in turn, arise from the interplay of the $1s$-$2p_0$ transition frequency ω_0, the frequency ω of the oscillating radiation and E_0, the field strength.

As the electron moves over the invariant surface it also revolves about the z-axis due to the spin-dependent momentum term. The progress of the transition can be tracked by observing the local energy E and the angular velocity $\dot{\phi}$ of the electron. Beginning at values associated with the $1s$ ground state, both quantities are seen to evolve toward values associated with the $2p_0$ excited state as the wave function approaches the $2p_0$ wave function. These results are also available in [24].

The causal interpretation has offered a way to examine the phenomenon of transition which is not limited to computing the probabilities of measuring E_1 and E_2 at various times after the perturbation has been turned off. Indeed, this continuous picture of a quantum transition makes good intuitive sense and offers an idea of what 'actually' happens to the electron during the transition process– a process which was considered quite mysterious, as in the standard framework the question of what the energy 'really' is has no meaning without a measurement context.

6.5 Appendix

The usual approach to this transition problem is to use the hamiltonian

$$H = H_0 + H' = H_0 - ezE_0 \cos \omega t, \tag{6.30}$$

where the electric field is assumed to be in the z direction [49]. This hamiltonian will also stimulate only the $1s$ to $2p_0$ transition, as discussed in the text of this chapter. Thus, the wave function can be written

$$\psi(t) = c_a(t)\psi_{100}e^{-iE_1t/\hbar} + c_b(t)\psi_{210}e^{-iE_2t/\hbar}, \tag{6.31}$$

as before, but the system is not exactly solvable for $c_a(t)$ and $c_b(t)$. However, substituting into the Schrödinger equation gives

$$\begin{aligned} \dot{c_a} &= -\frac{i}{\hbar}H'_{12}e^{-i\omega_0 t}c_b, \\ \dot{c_b} &= -\frac{i}{\hbar}H'_{21}e^{i\omega_0 t}c_a \end{aligned} \tag{6.32}$$

in place of (6.8). This system of equations is not solvable exactly, and it is typical to use a perturbation approach beginning with $c_a(0) = 1$ and $c_b(0) = 0$. This gives

$$c_b(t) = \frac{-2iV_{12}}{\hbar}\int_0^t \cos(\omega t)e^{i\omega_0 t'}dt' \tag{6.33}$$

which can be written

$$c_b(t) = \frac{-2iV_{12}}{2\hbar}\int_0^t (e^{i(\omega_0+\omega)t'} + e^{i(\omega_0-\omega)t'})dt', \tag{6.34}$$

and integrating gives

$$c_b(t) = \frac{-V_{12}}{\hbar}\left(\frac{e^{i(\omega_0+\omega)t}-1}{\omega_0+\omega} + \frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}\right). \tag{6.35}$$

Now, recall that the perturbing hamiltonian $H' = -\frac{1}{2}ezE_0e^{-i\omega t}$ was claimed to be equivalent to $H' = -ezE_0\cos(\omega t)$ when $\omega_0 - \omega \ll \omega_0 + \omega$. In this approximation, the first term in (6.35) can be neglected, leaving

$$c_b(t) = \frac{-V_{12}}{\hbar}\frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}.$$

However, this is exactly the result which would have been obtained had we simply omitted the first term of (6.34), or written $e^{-i\omega t}$ rather than $\cos(\omega t)$ in (6.33). This in turn is equivalent to writing

$$H' = -\frac{1}{2}ezE_0e^{-i\omega t}$$

in the first place. For this hamiltonian, note that we use the matrix elements

$$\begin{aligned} H_{12} &= \frac{V_{12}}{2}e^{i\omega t} \\ H_{21} &= \frac{V_{12}}{2}e^{-i\omega t} \end{aligned} \tag{6.36}$$

for Hermiticity, in our derivation of (6.8). While the 'equivalence' of the two different perturbation hamiltonians is not complete in that (6.8) is solvable for our choice and not for the conventional one, the two are equivalent in the approximation that $\omega_0 - \omega \ll \omega_0 + \omega$ because if we were to choose $H' = -ezE_0\cos(\omega t)$, we could not get a better result for $c_b(t)$ (in this approximation) in any case, as we would have to use perturbation methods. Thus, one could view our choice of hamiltonian as an extension of the usual one, valid in the approximation that $\omega_0 - \omega \ll \omega_0 + \omega$.

Chapter 7

More General Transitions: the Question of Relaxation

7.1 Introduction

Thus far, we have seen how the de Broglie-Bohm causal theory can be applied to various states of the hydrogen atom. The eigenstates studied in Chapters 3 through 5 result in motion which is very simple to characterize geometrically, namely circular motion about the z axis. Even in the transition problem of Chapter 6, the motion can be characterized geometrically in terms of the invariant surfaces generated by rotating (6.21) about the z axis.

Thus, all of the hydrogen systems studied so far share the basic geometric property of rotation about the z axis; in the transition problem this is supplemented, as it were, by complicated oscillating motion in r and θ. The trajectories, as discussed at the end of Chapter 6, make intuitive sense, and the values of local energy and rate of ϕ rotation correspond in an intuitive way with the eigenstate values from the Schrödinger, Pauli and Dirac equations.

Though this is interesting and important in showing the details of how the causal theory

can be coherently applied, the properties of the trajectories have applications beyond simply showing that the causal theory yields intuitively satisfying descriptions of quantum systems. It is the purpose of this chapter to explore one such application.

In past chapters, we have not included discussion of the probability distribution of the initial conditions. We simply found general properties of the trajectories; in the first few cases these were simple enough that it was not necessary to compute specific trajectories, and in the case of the transition problem, we numerically found two different, but qualitatively similar, trajectories.

Recall that in the causal theory, (1.5) implies that if the system starts out with a spatial distribution $P = \rho = |\psi|^2$, then that distribution will be preserved. This is the basis of the statement that the causal theory duplicates all of the statistical predictions of standard quantum mechanics while still ascribing 'hidden' trajectories to quantum particles. However, Bohm and Hiley [18], and others [86, 87] have posed the question of what happens to a quantum system when it does *not* start out in the standard $|\psi|^2$ distribution. This topic was introduced briefly in Section 2.5.2.

Bohm and Hiley argued in [18] that if the wave function is sufficiently complicated, the non-standard distribution will eventually approximate the $|\psi|^2$ distribution due to the spreading out of the trajectories. Antony Valentini argues this as well, using an analogue of the classical H-theorem [86, 87]. Because the $|\psi|^2$ distribution is a 'stable' one, in the sense that once the distribution looks approximately like $|\psi|^2$ it will continue to do so due to the continuity equation [86, 87], the approach to $|\psi|^2$ can be seen as a form of 'relaxation' to a quantum equilibrium.

However, it seems to be unclear exactly how complex the wave function needs to be in order to ensure that this 'quantum relaxation' will occur. It is also unclear on what time scale relaxation occurs, when it does. Bohm and Hiley were convinced that in the context of quantum statistical mechanics this relaxation would ensure that one did not need to assume as a postulate of the theory that the distribution of initial conditions is always $P = \rho = |\psi|^2$

[18]. This reduction in the number of fundamental assumptions of the theory would be possible because even if the system started out in some other, 'non-quantum', distribution, the natural evolution would carry the system to a distribution which would approximate $|\psi|^2$ and, thereafter, the standard quantum mechanical predictions would be recovered.

Antony Valentini has shown that if there *were* quantum systems with a non-standard (i.e. non-$|\psi|^2$) distribution, then they would behave very strangely. In fact, they would violate the no-signalling rule [89, 86, 87] as well as other rules of quantum mechanics such as the uncertainty principle. Therefore, if somehow there were systems which were unlikely to relax to quantum equilibrium, perhaps because the time scales of their relaxation were very long, or for some other reason, and *if* the quantum $|\psi|^2$ distribution were not fundamental but was the result of this relaxation process, then these systems would be very strange, and would have properties that violate quantum mechanics.

The question of relaxation is thus an important one. Do *all* quantum systems relax to a $|\psi|^2$ distribution? If not, how complex does the wave function have to be in order to guarantee relaxation? What is the time scale of quantum relaxation? Is it possible that there exist non-equilibrium systems, i.e. systems in some distribution other than $|\psi|^2$? Many physicists would probably say that the $|\psi|^2$ distribution is fundamental and is an assumption that is necessary in quantum mechanics. Antony Valentini does not appear to believe this, and it appears that Bohm and Hiley were at least interested in exploring the question.

7.2 A Brief Discussion of the Bohm-Hiley Argument

In [18], Bohm and Hiley take several approaches relevant to the question of relaxation to the $|\psi|^2$ distribution, though they do not refer to the process as 'relaxation to equilibrium'. They first argue that for a complicated wave function composed of many different eigenstates, a distribution that is not equal to $|\psi|^2$ will evolve to the $|\psi|^2$ distribution in time. They also discuss mixed ensembles, rather than pure states, and finally discuss the inclusion of an

underlying stochastic process as an approach to answering the question of why we always observe the $|\psi|^2$ distribution

It is the first part of their argument that is directly relevant here. They consider N particles in a three-dimensional box, where the particles may interact with the walls of the box in such a way as to create a complex linear combination of stationary wave functions (eigenfunctions of the box hamiltonian). These stationary wave functions are periodic.

Bohm and Hiley write the wave function as

$$\Psi = \sum_{k_1,\ldots,k_N} c_{k_1,\ldots,k_N} e^{i\left(\sum_n \mathbf{k}_n \cdot \mathbf{x}_n - \sum_k \omega_k t\right)}. \tag{7.1}$$

Here, the term $e^{i\sum_n \mathbf{k}_n \cdot \mathbf{x}_n}$ is the eigenfunction of the hamiltonian, and the c_k's are the coefficients– these can, in general, be very complicated. For identical fermions, they would be restricted to antisymmetric functions, but Bohm and Hiley examine the general case. They argue that after the system has been left alone for 'a long time', the wave function would be a combination that includes a fairly wide range of k values. The $\mathbf{k}$'s are proportional to the particles' momenta.

Bohm and Hiley find that

$$\rho \mathbf{v}_j = \frac{1}{2m} \sum_{\{k\}} \sum_{\{k'\}} c^*_{\{k\}} c_{\{k'\}} (\mathbf{k}_s + \mathbf{k}'_s) e^{-i\left(\sum'_n (\mathbf{k}_n \cdot \mathbf{x}_n + \mathbf{k'}_n \cdot \mathbf{x'}_n) + \sum_{k,k'} (\omega_k - \omega'_k) t\right)}. \tag{7.2}$$

where $\mathbf{v}_j$ is the velocity of the j^{th} particle and $\rho = |\psi|^2$. Note that their use of (1.8) means that the particles cannot have spin; however, the necessity of the additional spin term in (1.16) was not known at the time that Bohm and Hiley wrote [18].

They then write:

> It is clear that the above is built out of a very large number of terms each of which oscillates with a phase that is in effect random relative to those of the others. The point in configuration space corresponding to $\mathbf{x}_1 ... \mathbf{x}_n$ moves in a chaotic way

through all the configuration space that is accessible to it. ([18] p. 183)

Now, for the expression given in (7.2), it is entirely possible that chaotic motion results, because it is clear that if the range of possible **k** values is sufficiently wide, the wave function and the velocities are very complicated functions. However, it seems that it is not *guaranteed* that chaos will result, nor is it clear how complicated the wave function and/or the coefficients must be, nor how wide the range of **k** values must be, in order to guarantee chaos. In addition, not all chaotic systems have the property that each trajectory ultimately explores the entire configuration space. Indeed, systems with this property are known as ergodic systems. In classical statistical mechanics, most systems are 'quasi-ergodic' and behave like ergodic systems. (See [84] for a good discussion of ergodicity in classical statistical mechanics). However, it is not clear that results from the classical case apply automatically to the quantum case, especially given that the underlying mathematical structure is quite different.

Bohm and Hiley continue, writing that if the distribution P is not equal to $|\psi|^2$, then we may write

$$P = \rho F, \tag{7.3}$$

where F is not identically equal to 1 and $\rho = |\psi|^2$. Now, by definition, the distribution P, because it is a distribution of particles flowing through the space with various velocities, satisfies a continuity equation

$$\frac{\partial P}{\partial t} + \sum_n \nabla_n \cdot \rho \mathbf{v}_n = 0, \tag{7.4}$$

as does ρ itself (see (1.5), which generalizes to an equation like (7.4) in the many-particle case). Furthermore, F also satisfies a continuity equation [18]:

$$\frac{\partial F}{\partial t} + \sum_n \mathbf{v}_n \cdot \nabla_n F = 0 = \frac{dF}{dt}. \tag{7.5}$$

Therefore, F is a constant of motion.

Bohm and Hiley argue that if one were to begin with a distribution that was highly localized in configuration space, then because the trajectories spread out to fill the space, this small volume of configuration space would eventually be spread out. This is because two nearby trajectories separated by δx in configuration space have "large phase differences between most of the contributions to the velocity" in (7.2) ([18] p. 183). The thread-like structure formed by the stretching and deforming of the small volume of configuration space will eventually evenly cover the whole space, and will be sufficiently mixed up that F can be taken to be effectively constant. And, if P was initially a normalized distribution, we know that

$$\int_\Omega P d\Omega = 1 = \int_\Omega \rho d\Omega$$

(where Ω and $d\Omega$ are the configuration space and its element, respectively). This means that when we say that F is effectively constant, F is effectively identically equal to 1, so that

$$P = \rho F \approx \rho.$$

In other words, we have recovered the $|\psi|^2$ distribution. Bohm and Hiley concluded that the assumption that $P = |\psi|^2$ is not necessary in their theory [18].

However, it should be noted that it is not clear that each trajectory will necessarily fill the space even when the wave function is given by (7.1). Also, there are some assumptions in (7.1) such as the form of the wave function, that will not hold in general. Of course, in general one would expect *more* complexity and hence more relaxation if the wave function were different than the one given in (7.1), but this is not a guarantee. The argument that F is effectively constant is a qualitative one, which might be made more precise by examining the classical ergodic theorem from statistical mechanics, though Bohm and Hiley have not done so in [18] Though their argument as it stands is credible, it seems by no means guaranteed that there will not be any physically meaningful exceptions. In addition, Bohm and Hiley

do not present detailed criteria for how complicated the wave function must be in order to ensure the type of behaviour on which they rely. (For the details of their argument, see [18] pp. 181-185.)

7.3 The Subquantum H-theorem

Bohm and Hiley also paved the way in [18] for drawing some connections between the process of quantum relaxation and relaxation processes in classical statistical mechanics. Indeed, they mention that a small volume element in configuration space gets drawn out and becomes a spread-out, thread-like structure ([18] p. 183). This is analogous to the mixing process described by Gibbs [46].

In classical statistical mechanics, one can define a quantity H by

$$H_{\text{class}} = \int p \ln p d\Omega \tag{7.6}$$

where the integral is over the phase space, and p is the probability distribution function on that space. Now, by Liouville's theorem,[1] dp/dt is zero along a trajectory, and it follows that

$$\frac{dH_{\text{class}}}{dt} = 0.$$

However, if one divides the phase space into small volumes or cells, Ω_i, each of volume δV, then one can define a 'coarse-grained' density function, $\bar{p}$, by setting $\bar{p}_i$ equal to the average value over the i^{th} cell:

$$\bar{p}_i = \frac{1}{\delta V} \int_{\Omega_i} p d\Omega. \tag{7.7}$$

[1]The proof of Liouville's theorem [84] relies on the fact that the coordinate and momentum variables satisfy Hamilton's equations. Thus, it is almost certainly the case that quantum trajectories defined by the causal theory do not satisfy Liouville's theorem

In analogy to (7.6) one then defines the coarse-grained H by

$$\bar{H}_{\text{class}} = \sum_i \bar{p}_i \ln \bar{p}_i. \tag{7.8}$$

The classical H-theorem states that the coarse-grained H satisfies

$$\bar{H}_{\text{class}}(t) \leq \bar{H}_{\text{class}}(0). \tag{7.9}$$

This version of the H-theorem is due to Gibbs and the Ehrenfests [46, 36]. It relies on the assumption that initially,

$$\bar{p} = p,$$

or, in other words, that there is no 'microstructure' in the initial conditions. This condition is sometimes taken to express that there is some finite level of measurement accuracy which represents the best possible state of knowledge of the distribution, and that there is no reason to suppose that the distribution would be different than this most closely measured approximation $\bar{p}$ [84].

The H-theorem does not imply that $\bar{H}_{\text{class}}$ is a monotonically decreasing function of time. However, it is known that $\bar{H}$ reaches a minimum at equilibrium [84], and the H-theorem is one way to understand the likelihood of an approach to equilibrium given the assumption that the initial conditions are not 'special'.

Antony Valentini [86, 87] has reconstructed a version of this theorem that he applies to quantum systems. However, the relevant space is the configuration space composed of all the coordinate variables of all the particles, and the notion of 'equilibrium' is replaced by the $|\psi|^2$ distribution. Valentini shows that if the distribution is given by $P \neq |\psi|^2$, and the function f is defined by

$$P = |\psi|^2 f,$$

then one can define a quantum H according to

$$H = \int_X dX |\psi|^2 f \ln f, \tag{7.10}$$

where X is the configuration space, with element dX. Note that there is a dissimilarity between the quantum and classical cases. In the classical case the relevant space is the phase space. In the quantum case there is no phase space (the governing differential equations (1.8) and (1.16) are first-order). Instead, we have a configuration space. Because of this, rather than applying Liouville's theorem, the fact that f is a constant of motion (as Bohm and Hiley showed in [18]) is exploited in the proof.

Now, the system may be coarse-grained in the same manner as in the classical case. Here the cells are in the configuration space rather than phase space. Otherwise, we can make coarse-grained functions $\bar{P}$ and $\bar{H}$ in the same manner as in (7.7). When we do this, it again follows, according to a very similar argument as in the classical case, that

$$\bar{H}_{\text{quantum}}(t) \leq \bar{H}_{\text{quantum}}(0). \tag{7.11}$$

Here, when the distribution is $|\psi|^2$, we have $\bar{H}_{\text{quantum}} = 0$, so the decrease in $\bar{H}_{\text{quantum}}$ is related to an approach to quantum equilibrium. This result is again based on the assumption that

$$\bar{P}(0) = P(0).$$

For the proof and further details and discussion, see [86, 87].

This is a general result which does not depend on any particular kind of wave function. However, the implicit context is one of quantum statistical mechanics: the wave function should be very complicated and there should typically be many particles. The implication is that these conditions would ensure that sufficient mixing occurs, and $\bar{H}_{\text{quantum}}$ decreases to equilibrium. Note that (7.11) leaves the possibility that in fact $\bar{H}_{\text{quantum}}$ is constant, due

to the fact that the inequality is not a strict one. There are, of course, various possibilities ranging from full relaxation to quantum equilibrium and a constant $\bar{H}_{\text{quantum}}$.

If we are to do as Bohm and Hiley suggested in [18] and use this kind of relaxation argument as the basis for eliminating the $|\psi|^2$ distribution postulate, then it becomes important to examine relaxation in greater detail. One of the advantages of the causal theory is that it applies to individual systems rather than only to ensembles; surely if we are to examine the possibility of reducing the number of postulates in the theory, we wish to be certain that this reduction also applies to individual systems.

7.4 Relaxation in Hydrogen

While we will not attempt to answer all of the questions posed in Section 7.1 in the remainder of this chapter, it is worth exploring the implications of the trajectories seen in earlier chapters for the question of relaxation. This examination will shed some light on the question of whether all quantum systems are guaranteed to undergo relaxation, and indicate something about the complexity a wave function must have in order to ensure that relaxation will occur.

7.4.1 Hydrogen Eigenstates

Consider the ground state hydrogen wave function from (3.1)

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}.$$

The wave function is symmetric in θ and ϕ and has an exponential decay in r, so that if a system had the initial distribution $P = |\psi|^2$, the radial distribution would be as shown in Figure 7.1. Note that there is a small, but nonzero, probability of finding the particle very far from the nucleus of the atom.

Recall that the trajectories for the ground state wave function are given by (3.2):

$$\frac{d\phi}{dt} = \frac{\hbar}{m_e a r}.$$

For these very simple trajectories, the question of relaxation is clear. Since r is a constant of motion, if the initial distribution is different from $|\psi|^2$ radially, i.e. if the initial distribution does not have an exponential decay in the density as a function of the radius, then there can be no full relaxation. The system will never approximate the $|\psi|^2$ distribution.

To see this clearly, consider the hypothetical initial distribution

$$P = \begin{cases} 0, & r < a \\ C, & a < r < 2a \\ 0, & 2a < r \end{cases} \tag{7.12}$$

where the constant C is chosen such that the distribution is normalized. In this case, all trajectories will remain in the region $a < r < 2a$. The probability of finding the particle, at *any* later time, in the other regions is identically zero, and thus the distribution will never evolve so as to approximate $|\psi|^2$. In a similar way, θ is a constant of motion, and if all trajectories were initially in some finite range of θ values, or indeed were distributed in any way not consistent with the θ symmetry in $|\psi|^2$, then at any later time this inconsistency would remain and full relaxation would not occur.

Note that there might be some partial relaxation in ϕ. Consider an initial distribution in which all the particles have $0 < \phi(0) < \pi/2$, with a variety of radii. The different rates $\frac{d\phi}{dt} = \frac{\hbar}{m_e a r}$ will result in a 'spreading' in ϕ, and eventually, it is quite conceivable that the ϕ distribution will be symmetric, as it is in a $|\psi|^2$ distribution. However, for this circular trajectory, this limited process of relaxation will not result in the system approximating a $|\psi|^2$ distribution overall; if it does not start with a flat distribution in θ and an exponentially decaying distribution in r, it will never attain these even approximately.

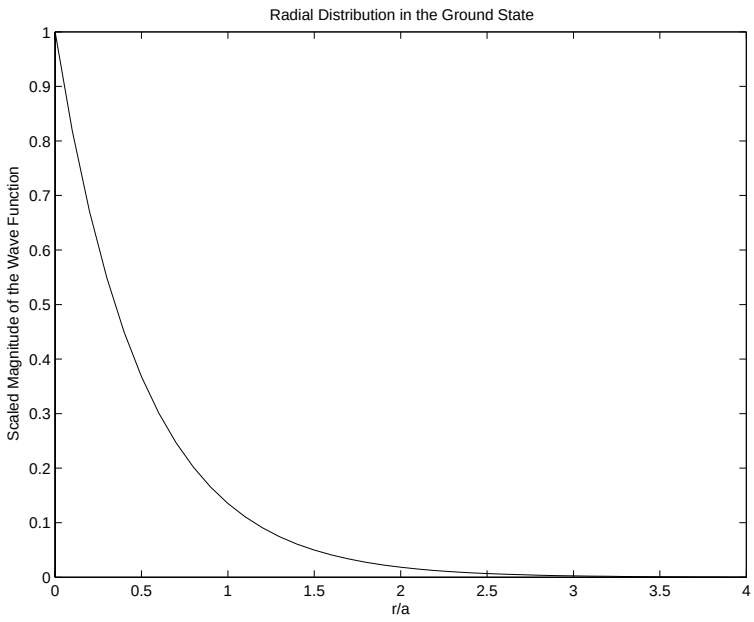


Figure 7.1: Radial Distribution: $|\psi|^2$ for the ground state

This will, of course, apply to all of the circular hydrogen eigenstate trajectories. As we have seen, this includes the eigenstate trajectories from the Schrödinger equation as well as from the Pauli and Dirac equations, so in this sense it is a very general result. Its implications are of some interest; clearly not *all* quantum systems will relax to quantum equilibrium even in a coarse-grained sense. It seems that more complexity is needed in order to relinquish the postulate that the distribution is always $|\psi|^2$ initially, and recover the standard distribution through time evolution, as Bohm and Hiley proposed in [18].

7.4.2 The $1s - 2p_0$ Transition in Hydrogen

We can also ask the question of whether relaxation occurs in the transition problem studied in Chapter 6. The trajectories during the $1s - 2p_0$ transition are more complex than the circular trajectories, and r and θ are not constants of motion. The ϕ motion is also more complicated. Might relaxation occur here, if not in the eigenstate systems?

The answer to this question is not difficult; though r and θ are not constants of motion, the transition trajectories of Chapter 6 do have another constant of motion, which characterizes

the invariant hyperbolae. Recall (6.21):

$$\xi = \frac{2}{A\sin\theta - 1}, \qquad A = \frac{2+\xi_0}{\xi_0 \sin\theta_0} > 1.$$

Here, A is the relevant constant of motion determined by the initial conditions. Each trajectory is constrained to lie on some hyperbola characterized by the number A.

Now, we cannot simply say that given an initial distribution in which all the trajectories were on the same hyperbola there would be no relaxation; while it is true that there would be no relaxation, the hyperbolae are of measure zero in $\mathbb{R}^3$, and so one hyperbola cannot contain all the trajectories.

Hence, suppose that the initial distribution placed all the trajectories in a 'rotated band' between two of the hyperbolae, for example in some range $a < A < b$. This would be analogous to the distribution given in (7.12). The entire rotated band is preserved as the system evolves in time. Now, the wave function, as given in (6.7), is

$$\psi(t) = c_a(t)\psi_{100}e^{-iE_1t/\hbar} + c_b(t)\psi_{210}e^{-iE_2t/\hbar}$$

where $c_a(t)$ and $c_b(t)$ are the oscillatory functions of time given in the previous chapter. With reference to (3.5), note that both ψ_{100} and ψ_{210} have an exponential decay in r, which will dominate the radial dependence for sufficiently large values of r. Clearly, the preservation of *all* arbitrary rotated hyperbolic bands of the form $a < A < b$ will not be consistent with a $|\psi|^2$ distribution;

Therefore, in the case of the transition studied in the previous chapter, the presence of nontrivial invariant sets prevents full relaxation. The distribution described above will never relax to a $|\psi|^2$ distribution precisely because the trajectories cannot leave the hyperbolae.

7.4.3 Other Transitions in Hydrogen

In this section, we examine the question of whether the same kinds of invariant sets exist in other transitions in hydrogen. To do this, we relinquish the requirement that the transition only be from the ground state to the first excited state. Also, we consider radiation other than z-polarized radiation (recall that in the previous chapter the electric field in the perturbing hamiltonian was assumed to be in the z-direction). If the perturbing hamiltonian can have light polarized in any direction $\mathbf{x}$, then more transitions are 'allowed'.

In this context, a transition between two states $|\psi_a\rangle$ and $|\psi_b\rangle$ is 'allowed' if the matrix element $\langle\psi_a| H' |\psi_b\rangle$ is non-zero, where H' is the perturbing hamiltonian. In the previous chapter, we had

$$H' = -\frac{1}{2}ezE_0e^{-i\omega t},$$

and the relevant matrix element was then proportional to $\langle\psi_{100}| z |\psi_{210}\rangle$. Generalizing the radiation from z polarized radiation only to any radiation will therefore mean considering matrix elements $\langle\psi_a| x |\psi_b\rangle$ and $\langle\psi_a| y |\psi_b\rangle$ as well.

It is well-known [49, 82] that there are selection rules governing which of these matrix elements are non-zero, and thus which transitions are allowed. It turns out that the only non-zero matrix elements are between wave functions such that the change in the quantum number m is either 0 or 1, and the change in ℓ is 1, i.e. $\Delta m = 0, \pm 1$ and $\Delta\ell = 1$. Note that in the case of our earlier transition, we were considering only z-polarized radiation, which permits only $\Delta m = 0$ transitions. Now we are free to consider $\Delta m = 1$ transitions as well. There is no constraint on the change in n, though the frequency of the incoming radiation will affect which transitions are stimulated.

The task is now to compute the causal trajectories to a sufficient degree of detail to see whether or not the allowed transitions give rise to the kind of invariant sets that occur in the $1s - 2p_0$ transition. If they do, then the relaxation argument of Section 7.4.2 can be applied to show that in general, full relaxation will not occur in *any* of these hydrogen transition

problems. If there are no such invariant sets, then it is possible that relaxation might occur, and some light might be shed on why it occurs in some transitions and not others.

To find the trajectories in general, we will examine the structure of the terms ∇S and $\nabla \log \rho \times \mathbf{s}$, which compose the total momentum (see (1.16)). In order to do this, note that these terms can be written

$$\nabla S = \frac{\hbar}{\psi^*\psi}\mathrm{Im}\{(\nabla\psi)\psi^*\}, \qquad \nabla \log \rho = \frac{2}{\psi^*\psi}\mathrm{Re}\{(\nabla\psi)\psi^*\}, \tag{7.13}$$

so that in order to examine whether the kind of simplification that occurred in (6.19) happens again, we need to understand the structure of $\mathrm{Im}\{(\nabla\psi)\psi^*\}$ and $\mathrm{Re}\{(\nabla\psi)\psi^*\}$.

Recall that in the $1s - 2p_0$ case, the r and θ differential equations were very similar in form, and in fact it was possible to 'divide out' the time dependence by taking the ratio of the first two equations of (6.19), and solve the resulting separable equation. Furthermore, the r and θ equations came only from the ∇S term in the momentum. This was because the wave function had no ϕ dependence, so that $\nabla \log \rho$ had no ϕ component. Consequently, $\nabla \log \rho \times \mathbf{s}$ had *only* a ϕ component, and contributed nothing to the r and θ momenta.

We will be considering transitions between two states, so that the wave function will always be written

$$\psi = c_a(t)\psi_a + c_b(t)\psi_b \tag{7.14}$$

where ψ_a and ψ_b are Schrödinger eigenstate wave functions and $c_a(t)$ and $c_b(t)$ are time-dependent coefficients analogous to the overall coefficients of (6.7), i.e. they include the $e^{-iE_it/\hbar}$ oscillations. In this chapter we will not solve the full differential equations for these coefficients, but will assume that they are unspecified complex functions of time.

To see if there is a geometric simplification such as the one of Chapter 6, recall that the structure of the Schrödinger hydrogen wave functions, from (3.5), is

$$\psi_{n\ell m} = N_{n\ell m}e^{-r/na}\big(\frac{2r}{na}\big)^{\ell}L^{2\ell+1}_{n-\ell-1}(2r/na)Y^m_{\ell}(\theta,\phi)$$

or

$$\psi_{n\ell m} = C_{n\ell m} e^{-r/na} \left(\frac{2r}{na}\right)^{\ell} L^{2\ell+1}_{n-\ell-1}(2r/na) P_{\ell m}(\cos\theta) e^{im\phi}$$

which can be written

$$\psi_{n\ell m} = R_{n\ell}(r) P_{\ell m}(\cos\theta) e^{im\phi}, \tag{7.15}$$

where the normalization constant (which is not critical here) is included in the radial function $R_{n\ell}(r)$. The important feature of these wave functions in this context is that their ϕ dependence is so simple. It will also be useful to recall the form of the gradient in spherical coordinates:

$$\nabla f = \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\phi}.$$

It will be necessary to examine the $\Delta m = 0$ and $\Delta m = 1$ transitions separately, as the relevant terms will have somewhat different structure in the two cases.

Transitions in which $\Delta m = 0$

From (7.15), it is clear that if $m = 0$ in both the wave functions, then there is no ϕ dependence. Thus both $\mathrm{Im}\{(\nabla\psi)\psi^*\}$ and $\mathrm{Re}\{(\nabla\psi)\psi^*\}$ have no ϕ component. This implies that in general as in the $1s - 2p_0$ transition, transitions in which $m = 0$ in both ψ_a and ψ_b have the property that the ∇S term contributes only to the r and θ momentum, and the $\nabla \log\rho \times \mathbf{s}$ is responsible only for the ϕ momentum.

Furthermore, if $m \neq 0$ but $\Delta m = 0$, then the ϕ component of $(\nabla\psi)\psi^*$ is simply $im\psi\psi^*/r\sin\theta$. This has no real part, so there is still no ϕ component of $\nabla\log\rho$, and the imaginary part is $m\psi\psi^*/r\sin\theta$. Thus the ∇S term now contributes $\frac{m\hbar}{r\sin\theta}$ to the ϕ component of the momentum. Because $\nabla\log\rho$ has no ϕ component, it is again the case that $\nabla\log\rho\times\mathbf{s}$ has *only* a ϕ component and does not contribute to either the r or θ momentum.

Now we must examine the r and θ components of ∇S. If they are of sufficiently similar form, we might be able to find a simplification like that of the $1s - 2p_0$ transition.

The radial part of $(\nabla\psi)\psi^*$ is given by

$$\frac{\partial\psi}{\partial r}\psi^* = (c_a\frac{\partial\psi_a}{\partial r} + c_b\frac{\partial\psi_b}{\partial r})(c_a^*\psi_a^* + c_b^*\psi_b^*).$$

Expanding gives

$$\frac{\partial\psi}{\partial r}\psi^* = |c_a|^2\frac{\partial\psi_a}{\partial r}\psi_a^* + |c_b|^2\frac{\partial\psi_b}{\partial r}\psi_b^* + c_ac_b^*\frac{\partial\psi_a}{\partial r}\psi_b^* + c_a^*c_b\frac{\partial\psi_b}{\partial r}\psi_a^*. \tag{7.16}$$

The first two terms of (7.16) have no imaginary parts and so do not contribute to ∇S. In the last two terms of (7.16), note that $\frac{\partial\psi_a}{\partial r}\psi_b^*$ and $\frac{\partial\psi_b}{\partial r}\psi_a^*$ are real, because the only imaginary parts of the wavefunctions (see (7.15)) arise in the $e^{im\phi}$ term and here, we have assumed that $\Delta m = 0$ so that these terms always cancel.

The only imaginary terms thus come from $c_ac_b^*$ and $c_a^*c_b$ which are complex conjugates of each other. Therefore,

$$\mathrm{Im}\{\frac{\partial\psi}{\partial r}\psi^*\} = \mathrm{Im}\{c_ac_b^*\}\left(\frac{\partial\psi_a}{\partial r}\psi_b^* - \frac{\partial\psi_b}{\partial r}\psi_a^*\right). \tag{7.17}$$

The above expression is a function of time, $\mathrm{Im}\{c_ac_b^*\}$, times a function of r and θ only.

Now we compare this to the $\hat{\theta}$ component of $(\nabla\psi)\psi^*$, which is similar to the radial part and is given by

$$\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^* = \frac{1}{r}(c_a\frac{\partial\psi_a}{\partial\theta} + c_b\frac{\partial\psi_b}{\partial\theta})(c_a^*\psi_a^* + c_b^*\psi_b^*). \tag{7.18}$$

Again, the first two terms in the expansion contain no imaginary parts and thus do not contribute to ∇S. Also, the resulting cross terms are real because again, the $e^{\pm im\phi}$ terms cancel. Therefore, we have

$$\mathrm{Im}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\} = \frac{1}{r}\mathrm{Im}\{c_ac_b^*\}\left(\frac{\partial\psi_a}{\partial\theta}\psi_b^* - \frac{\partial\psi_b}{\partial\theta}\psi_a^*\right) \tag{7.19}$$

This is a product of the same function of time as that which appears in (7.17), and

a different function of r and θ only. In summary, the momentum terms for the $\Delta m = 0$ transitions from the ∇S contribution are:

$$\begin{aligned} p_r &= \frac{\hbar}{\psi^*\psi}\mathrm{Im}\{c_a c_b^*\}\left(\frac{\partial\psi_a}{\partial r}\psi_b^* - \frac{\partial\psi_b}{\partial r}\psi_a^*\right) \\ p_\theta &= \frac{\hbar}{\psi^*\psi}\frac{1}{r}\mathrm{Im}\{c_a c_b^*\}\left(\frac{\partial\psi_a}{\partial\theta}\psi_b^* - \frac{\partial\psi_b}{\partial\theta}\psi_a^*\right) \end{aligned} \tag{7.20}$$

and the ϕ component comes from the $\nabla \log\rho \times \mathbf{s}$ term, and is

$$p_\phi = \frac{\hbar}{\psi^*\psi}\left(\mathrm{Re}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\}\cos\theta + \mathrm{Re}\{\frac{\partial\psi}{\partial r}\psi^*\}\sin\theta\right). \tag{7.21}$$

This yields the system of differential equations:

$$\begin{aligned} \frac{dr}{dt} &= \frac{\hbar}{\psi^*\psi}\mathrm{Im}\{c_a c_b^*\}\left(\frac{\partial\psi_a}{\partial r}\psi_b^* - \frac{\partial\psi_b}{\partial r}\psi_a^*\right) \\ \frac{d\theta}{dt} &= \frac{\hbar}{\psi^*\psi}\frac{1}{r^2}\mathrm{Im}\{c_a c_b^*\}\left(\frac{\partial\psi_a}{\partial\theta}\psi_b^* - \frac{\partial\psi_b}{\partial\theta}\psi_a^*\right) \\ \frac{d\phi}{dt} &= \frac{\hbar}{\psi^*\psi}\frac{1}{r\sin\theta}\left(\mathrm{Re}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\}\cos\theta + \mathrm{Re}\{\frac{\partial\psi}{\partial r}\psi^*\}\sin\theta\right). \end{aligned} \tag{7.22}$$

where we have used the relations $d\theta/dt = (1/r)p_\theta$ and $d\phi/dt = (1/r\sin\theta)p_\phi$.

Now, the first two differential equations are of very similar form, as they were in (6.19) in the case of the $1s - 2p_0$ transition. Indeed, we can write

$$\frac{dr}{d\theta} = r^2\frac{\frac{\partial\psi_a}{\partial r}\psi_b^* - \frac{\partial\psi_b}{\partial r}\psi_a^*}{\frac{\partial\psi_a}{\partial\theta}\psi_b^* - \frac{\partial\psi_b}{\partial\theta}\psi_a^*} \tag{7.23}$$

from the first two equations. This can be written

$$\frac{dr}{d\theta} = r^2\frac{P_a P_b}{R_a R_b}\left(\frac{\frac{dR_a}{dr}R_b - \frac{dR_b}{dr}R_a}{\frac{dP_a}{d\theta}P_b - \frac{dP_b}{dd\theta}P_a}\right) \tag{7.24}$$

This is valid when the denominator is nonzero. It will have a solution in some interval when the function on the right hand side is continuous and when its partial derivative with respect

to r is continuous.

The denominator of (7.24) vanishes when

$$\frac{\partial \psi_a}{\partial \theta}\psi_b^* - \frac{\partial \psi_b}{\partial \theta}\psi_a^* = 0.$$

From (7.15), it can be seen that this is equivalent to

$$R_a(r)R_b(r)\frac{dP_a(\cos\theta)}{d\theta}P_b(\cos\theta) - R_a(r)R_b(r)\frac{dP_b(\cos\theta)}{d\theta}P_a(\cos\theta) = 0.$$

This in turn reduces to

$$\frac{dP_a(\cos\theta)}{P_a} = \frac{dP_b(\cos\theta)}{P_b}$$

which implies, upon integration and exponentiation, that

$$P_a(\cos\theta) = KP_b(\cos\theta). \tag{7.25}$$

This will only be the case on an interval if $P_a = P_b$, or in other words, if the two states in the transition are in fact the same state: $\psi_a = \psi_b$. In this case, the system is in one of the eigenstates already considered in Chapter 3. Note that the term R_aR_b is not identically zero; it vanishes at most at isolated points.

The entire denominator can, therefore, only vanish at isolated points, and not on an interval. These points correspond to asymptotes of the $r-\theta$ curves resulting from integration of (7.24), and do not change the fact that (7.24) has solutions for almost all initial conditions. Such solutions define curves analogous to the hyperbolae of the previous chapter (see (6.21)). These curves can be explicitly computed in, for instance, the $x-z$ plane; the surfaces formed by rotating the curves about the z axis are invariant two-dimensional surfaces on which the trajectories must remain. The ϕ rotation is due to the third equation of (7.22).

Thus, the same kind of structure as was seen in the $1s-2p_0$ transition happens in all of the $\Delta m = 0$ transitions. The integration of (7.24) will involve a constant of integration

which will be a constant of motion, determined by the initial position. The distribution of this constant of motion is thus determined by the distribution of initial positions, so there is an implication for the question of relaxation. If the initial distribution does not distribute the constant of motion in a way that is consistent with the $|\psi|^2$ distribution, then full relaxation to the $|\psi|^2$ distribution cannot occur even in a coarse-grained sense, because trajectories can never leave the invariant surfaces.

Transitions in which $\Delta m = 1$

We now examine the ∇S and $\nabla \log \rho \times \mathbf{s}$ terms for transitions in which $\Delta m = 1$. We shall need to determine whether the r and θ differential equations are of sufficiently similar form as to have the same dependence on both time and ϕ, so that their ratio defines $dr/d\theta$ as a function of r and θ. To do this, we will have to find the r and θ components of both ∇S and $\nabla \log \rho \times \mathbf{s}$.

Beginning as usual with the r component of ∇S, we have the same expression as before, i.e. (7.16). But now, while the first two components are again real and thus do not contribute to ∇S (which involves only the imaginary part of $(\nabla\psi)\psi^*$), the second two terms are more complicated than before because the $e^{im\phi}$ terms no longer cancel.

We now have from (7.16)

$$\mathrm{Im}\{\frac{\partial\psi}{\partial r}\psi^*\} = \mathrm{Im}\{c_a c_b^* \frac{\partial\psi_a}{\partial r}\psi_b^* + c_a^* c_b \frac{\partial\psi_b}{\partial r}\psi_a^*\}, \tag{7.26}$$

and the only non-real term in the wave functions comes from the ϕ dependence. Assuming without loss of generality that $m_1 = m_2 + 1$, we have

$$\frac{\partial\psi_a}{\partial r}\psi_b^* = \frac{dR_a}{dr}R_b P_a P_b e^{i\phi}, \qquad \frac{\partial\psi_b}{\partial r}\psi_a^* = \frac{dR_b}{dr}R_a P_a P_b e^{-i\phi}. \tag{7.27}$$

We can therefore simplify (7.26):

$$\begin{aligned}\mathrm{Im}\{\frac{\partial\psi}{\partial r}\psi^*\} = \mathrm{Im}\{c_a c_b^*\}\frac{dR_a}{dr}R_b P_a P_b\cos\phi - \mathrm{Im}\{c_a c_b^*\}\frac{dR_b}{dr}R_a P_a P_b\cos\phi \\ + \mathrm{Re}\{c_a c_b^*\}\frac{dR_a}{dr}R_b P_a P_b\sin\phi - \mathrm{Re}\{c_a c_b^*\}\frac{dR_b}{dr}R_a P_a P_b\sin\phi \quad (7.28)\end{aligned}$$

which can be rewritten

$$\mathrm{Im}\{\frac{\partial\psi}{\partial r}\psi^*\} = \left(\frac{dR_a}{dr}R_b P_a P_b - \frac{dR_b}{dr}R_a P_a P_b\right)\left(\mathrm{Im}\{c_a c_b^*\}\cos\phi + \mathrm{Re}\{c_a c_b^*\}\sin\phi\right). \quad (7.29)$$

While this may not look terribly simple, it is again the case that the first term is a function of r and θ only, because of the fact that the ϕ dependence in the wave functions only occurs in the exponentials. The second term is a function of time and ϕ. To simplify the notation, let

$$H(\phi,t) = \mathrm{Im}\{c_a c_b^*\}\cos\phi + \mathrm{Re}\{c_a c_b^*\}\sin\phi.$$

This means that (7.29) can be written

$$\mathrm{Im}\{\frac{\partial\psi}{\partial r}\psi^*\} = \left(\frac{dR_a}{dr}R_b P_a P_b - \frac{dR_b}{dr}R_a P_a P_b\right)H(\phi,t). \quad (7.30)$$

It is necessary to see if a similar structure occurs in the θ component of ∇S, and also in the components of $\nabla\log\rho\times\mathbf{s}$.

The θ component of ∇S can be found in a similar manner as the r component. Again we have (7.18), but now that $\Delta m = 1$ the wave functions contribute imaginary parts. We have, analogously to (7.26),

$$\mathrm{Im}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\} = \frac{1}{r}\mathrm{Im}\{c_a c_b^*\frac{\partial\psi_a}{\partial\theta}\psi_b^* + c_a^* c_b\frac{\partial\psi_b}{\partial\theta}\psi_a^*\} \quad (7.31)$$

which becomes

$$\begin{aligned}\mathrm{Im}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\} = \mathrm{Im}\{c_a c_b^*\}\frac{1}{r}\frac{dP_a}{d\theta}P_b R_a R_b\cos\phi - \mathrm{Im}\{c_a c_b^*\}\frac{1}{r}\frac{dP_b}{d\theta}P_a R_a R_b\cos\phi \\ + \mathrm{Re}\{c_a c_b^*\}\frac{1}{r}\frac{dP_a}{d\theta}P_b R_a R_b\sin\phi - \mathrm{Re}\{c_a c_b^*\}\frac{1}{r}\frac{dP_b}{d\theta}P_a R_a R_b\sin\phi \quad (7.32)\end{aligned}$$

and again this can be simplified:

$$\begin{aligned}\mathrm{Im}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\} &= \left(\frac{1}{r}\frac{dP_a}{d\theta}P_b R_a R_b - \frac{1}{r}\frac{dP_b}{d\theta}P_a R_a R_b\right)(\mathrm{Im}\{c_a c_b^*\}\cos\phi + \mathrm{Re}\{c_a c_b^*\}\sin\phi) \\ &= \left(\frac{1}{r}\frac{dP_a}{d\theta}P_b R_a R_b - \frac{1}{r}\frac{dP_b}{d\theta}P_a R_a R_b\right)H(\phi,t).\end{aligned} \quad (7.33)$$

This has the same time and ϕ dependence as the radial component in (7.30), and again the other factor is only a function of r and θ. Thus, the r and θ components of ∇S are given by

$$\begin{aligned}(\nabla S)_r &= \frac{\hbar}{\psi^\dagger\psi}\mathrm{Im}\{\frac{\partial\psi}{\partial r}\psi^*\} = \frac{\hbar}{\psi^\dagger\psi}P_a P_b\left(\frac{dR_a}{dr}R_b - \frac{dR_b}{dr}R_a\right)H(\phi,t) \\ (\nabla S)_\theta &= \frac{\hbar}{\psi^\dagger\psi}\mathrm{Im}\{\frac{1}{r}\frac{\partial\psi}{\partial\theta}\psi^*\} = \frac{\hbar}{\psi^\dagger\psi}\frac{R_a R_b}{r}\left(\frac{dP_a}{d\theta}P_b - \frac{dP_b}{d\theta}P_a\right)H(\phi,t).\end{aligned} \quad (7.34)$$

So far, this seems quite promising. The r and θ components of ∇S have sufficiently similar structure as to define $dr/d\theta$ as a function of r and θ only, which is ultimately what we require. However, unlike in the $\Delta m = 0$ transitions, here, the term $\nabla\log\rho\times\mathbf{s}$ does not necessarily only have a ϕ component. In fact, it now has all three components, so the r and θ components found in (7.29) and (7.33) only contain part of the total r and θ momentum.

In the $\Delta m = 0$ transitions, recall that $\nabla\log\rho\times\mathbf{s}$ had only a ϕ component because the ϕ component of $\nabla\log\rho$ was zero. This was because the ϕ component of $(\nabla\psi)\psi^*$ had no real parts. For simplicity of notation, let

$$A \equiv \nabla\log\rho.$$

Recall from (3.19) that the cross product of two vectors can be written in spherical coordi-

nates as

$$\mathbf{A} \times \mathbf{s} = \begin{vmatrix} \hat{e}_\theta & \hat{e}_\phi & \hat{e}_r \\ A_\theta & A_\phi & A_r \\ s_\theta & s_\phi & s_r \end{vmatrix} \tag{7.35}$$

which in this case, because we are assuming that the spin vector is in the $\hat{e}_z$ direction, becomes

$$\mathbf{A} \times \mathbf{s} = \begin{vmatrix} \hat{e}_\theta & \hat{e}_\phi & \hat{e}_r \\ A_\theta & A_\phi & A_r \\ s_\theta & 0 & s_r \end{vmatrix} \tag{7.36}$$

and in this case this means that

$$\nabla \log \rho \times \mathbf{s} = \frac{\hbar}{2} \begin{vmatrix} \hat{e}_\theta & \hat{e}_\phi & \hat{e}_r \\ A_\theta & A_\phi & A_r \\ \cos\theta & 0 & -\sin\theta \end{vmatrix}. \tag{7.37}$$

Thus, to find the r and θ components of $\nabla \log \rho \times \mathbf{s}$ it is necessary only to find A_ϕ.

Now, recall from (7.13) that $\nabla \log \rho$ can be written in terms of the real part of $(\nabla\psi)\psi^*$, so to find the ϕ component of $\nabla \log \rho$ we must find the ϕ component of $\mathrm{Re}\{(\nabla\psi)\psi^*\}$. This is given by

$$\mathrm{Re}\{\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}\psi^*\} = \frac{1}{r\sin\theta}\mathrm{Re}\{(im_1c_a\psi_a + im_2c_b\psi_b)(c_a^*\psi_a^* + c_b^*\psi_b^*)\}. \tag{7.38}$$

Now, the first two terms in the expansion (i.e. those involving $|\psi_a|^2$ and $|\psi_b|^2$) will have no real parts because of the i in the coefficients. Therefore the only real parts will be contributed by the cross terms and we have

$$\begin{aligned} \mathrm{Re}\{\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}\psi^*\} &= \frac{1}{r\sin\theta}\mathrm{Re}\{c_ac_b^*im_1\psi_a\psi_b^* + c_a^*c_bim_2\psi_a^*\psi_b\} \\ &= -\frac{1}{r\sin\theta}\mathrm{Im}\{c_ac_b^*m_1\psi_a\psi_b^* + c_a^*c_bm_2\psi_a^*\psi_b\} \end{aligned} \tag{7.39}$$

Because we assumed that $m_1 = m_2 + 1$, this can be simplified using the fact that

$$\psi_a \psi_b^* = R_a R_b P_a P_b e^{i\phi}, \quad \psi_b \psi_a^* = R_a R_b P_a P_b e^{-i\phi}. \tag{7.40}$$

This means that the terms in

$$\begin{aligned}\mathrm{Re}\{\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}\psi^*\} = -\frac{1}{r\sin\theta}\,(&\mathrm{Re}\{c_a c_b^*\}\mathrm{Im}\{\psi_a\psi_b^*\}m_1 + \mathrm{Im}\{c_a c_b^*\}\mathrm{Re}\{\psi_a\psi_b^*\}m_1 \\ &+\mathrm{Re}\{c_a^* c_b\}\mathrm{Im}\{\psi_b\psi_a^*\}m_2 + \mathrm{Im}\{c_a^* c_b\}\mathrm{Re}\{\psi_b\psi_a^*\}m_2)\end{aligned} \tag{7.41}$$

can be written

$$\begin{aligned}\mathrm{Re}\{\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}\psi^*\} &= -\frac{R_a R_b P_a P_b}{r\sin\theta}(\mathrm{Re}\{c_a c_b^*\}(-\sin\phi)(m_2 - m_1) + \mathrm{Im}\{c_a c_b^*\}\cos\phi(m_2 - m_1)) \\ &= -\frac{R_a R_b P_a P_b}{r\sin\theta}(\mathrm{Re}\{c_a c_b^*\}\sin\phi + \mathrm{Im}\{c_a c_b^*\}\cos\phi).\end{aligned} \tag{7.42}$$

This means that the term we are seeking, A_ϕ, is given by

$$\begin{aligned}A_\phi &= \frac{2}{\psi^*\psi}(-\frac{R_a R_b P_a P_b}{r\sin\theta})(\mathrm{Re}\{c_a c_b^*\}\sin\phi + \mathrm{Im}\{c_a c_b^*\}\cos\phi) \\ &= -\frac{2}{\psi^*\psi}(\frac{R_a R_b P_a P_b}{r\sin\theta})H(\phi,t).\end{aligned} \tag{7.43}$$

Note that this is the *same* time and ϕ dependence $H(\phi,t)$ that occurs in the r and θ terms of ∇S, which is very promising.

Now we are in a position to find the r and θ components of $\nabla\log\rho\times\mathbf{s}$ without difficulty. They are given by

$$(\nabla\log\rho\times\mathbf{s})_r = -A_\phi s_\theta = -\frac{1}{r}\frac{\hbar}{\psi^*\psi}R_a R_b P_a P_b H(\phi,t) \tag{7.44}$$

and

$$(\nabla \log \rho \times \mathbf{s})_\theta = -A_\phi s_r = -\frac{1}{r}\cot\theta \frac{\hbar}{\psi^*\psi} R_a R_b P_a P_b H(\phi, t). \tag{7.45}$$

Now we can find the r and θ components of the total momentum by adding ∇S from (7.34) and $\nabla \log \rho \times \mathbf{s}$ together:

$$\begin{aligned} p_r &= (\nabla S)_r + (\nabla \log \rho \times \mathbf{s})_r = \frac{\hbar}{\psi^*\psi} P_a P_b \left(\frac{dR_a}{dr} R_b - \frac{dR_b}{dr} R_a - \frac{R_a R_b}{r} \right) H(\phi, t) \\ p_\theta &= (\nabla S)_\theta + (\nabla \log \rho \times \mathbf{s})_\theta = \frac{\hbar}{\psi^*\psi} \frac{R_a R_b}{r} \left(\frac{dP_a}{d\theta} P_b - \frac{dP_b}{d\theta} P_a - P_a P_b \cot\theta \right) H(\phi, t) \end{aligned} \tag{7.46}$$

This gives rise to the system of differential equations

$$\begin{aligned} \frac{dr}{dt} &= \frac{\hbar}{\psi^*\psi} P_a P_b \left(\frac{dR_a}{dr} R_b - \frac{dR_b}{dr} R_a - \frac{R_a R_b}{r} \right) H(\phi, t) \\ \frac{d\theta}{dt} &= \frac{\hbar}{r^2 \psi^*\psi} R_a R_b \left(\frac{dP_a}{d\theta} P_b - \frac{dP_b}{d\theta} P_a - P_a P_b \cot\theta \right) H(\phi, t) \end{aligned} \tag{7.47}$$

where it should be understood that we have left the ϕ differential equation out because it is not relevant to the question of whether the r and θ components have sufficiently similar structure to give rise to invariant sets of the kind seen previously.

And it appears that they do have sufficient structure. Dividing the two equations of (7.47) gives

$$\frac{dr}{d\theta} = r^2 \frac{P_a P_b}{R_a R_b} \frac{\left(\frac{dR_a}{dr} R_b - \frac{dR_b}{dr} R_a - \frac{R_a R_b}{r} \right)}{\left(\frac{dP_a}{d\theta} P_b - \frac{dP_b}{d\theta} P_a - P_a P_b \cot\theta \right)} \tag{7.48}$$

This is a separable equation whose solution $r(\theta)$ contains a constant of integration determined by the initial condition. It will have solutions when the denominator is nonzero. As in the case of (7.24), this condition is satisfied by almost all points in the space, for the equation

$$\frac{dP_a}{d\theta} P_b - \frac{dP_b}{d\theta} P_a - P_a P_b \cot\theta = 0$$

can be integrated and exponentiated, yielding the condition

$$\frac{P_a}{P_b} = A \sin\theta. \tag{7.49}$$

When this relation holds on an interval, rather than at specific points, it holds identically for $\theta \in [0, \pi]$. In this case, θ *itself* is the constant of motion we seek. If

$$\frac{d\theta}{dt} = 0$$

on the trajectories, then the motion is constrained to cone-shaped surfaces. In general, the $r(\theta)$ curves given by (7.48) are rotated about the z axis as ϕ changes in a manner determined by the ϕ differential equation (which we have not written explicitly). The resulting surfaces are invariant.

Both (7.24) and (7.48) give rise to nontrivial invariant sets characterized by constants of motion that are determined by initial conditions. Thus, in both cases, if the relevant constants are not initially distributed in a manner consistent with the $|\psi|^2$ distribution, then at later times the overall distribution will not necessarily approach $|\psi|^2$, for the reasons given in the last section.

7.5 Concluding Remarks

These results mean that for all transitions in hydrogen considered here, there is sufficient structure in the equations of motion that quantum relaxation will not occur. Recall that the transitions we have considered are those stimulated by semi-classical radiation, for which the transition occurs between two Schrödinger eigenstates and in which the spin is constant and in the z direction, In these transitions, if the initial distribution is such that the constant of motion is not distributed as it would be in a $|\psi|^2$ distribution, then because the trajectories are constrained to remain on the invariant surfaces, the distribution will not evolve so as to

approximate a $|\psi|^2$ distribution.

However, one could argue that these transitions are very simple systems. We have assumed that the spin orientation is constant in the z direction, which is a simplification. The Schrödinger equation is non-relativistic, and furthermore, the semiclassical approximation for light is an approximation of a more complicated interaction that would involve the magnetic field, a full description of the photons as quanta, etc.

Even so, it remains the case that for eigenstates in the Schrödinger as well as the Pauli and Dirac equations, relaxation will not occur because the trajectories are so simple– circles about the z axis. And in all allowed transitions in the Schrödinger hydrogen atom, assuming non-polarized semi-classical radiation, relaxation also does not occur because of the invariant sets, or constants of motion, which arise.

This is in some sense a powerful conclusion, for it addresses the question of whether the $|\psi|^2$ distribution is a necessary postulate of the de Broglie-Bohm theory. These results seem to say that it *is* a necessary postulate, for there are physically meaningful situations in which an arbitrary initial distribution will not 'naturally' evolve in time to a $|\psi|^2$ distribution. Therefore, at least at the level of individual systems in the Schrödinger context, the causal theory does require the assumption that a system always has a $|\psi|^2$ distribution, in order to make the same predictions as quantum mechanics. While it may be possible to remove the $|\psi|^2$ distribution postulate in the statistical theory, where the wave functions are always *greatly* more complex than they are here, at the axiomatic level it is a desirable feature of the causal theory that it describes individual systems, where the standard theory does not. And at the individual level it appears that quantum relaxation does not occur reliably enough to allow the $|\psi|^2$ distribution postulate to be removed.

Chapter 8

Conclusions

8.1 The Hydrogen Application

The application of the causal theory to the hydrogen atom has yielded some interesting results, both simple and intuitive, and has also had some broader implications. From the computation of the electron trajectories in the simplest of the cases considered here to the most general systems considered (probably the general transitions of Chapter 7), the causal theory has successfully described the individual hydrogen atom in a meaningful, intuitive, and consistent way.

First, we have shown that in the Schrödinger, Pauli and Dirac contexts, the hydrogen atom in the causal theory has the property that in the usual eigenstates, the electron orbits about the z axis in a circular manner. The 'usual eigenstates' are states which are eigenstates of the total angular momentum M, the z component of the total angular momentum, M_z, and the hamiltonian. In the Pauli case these are also taken to be eigenstates of the total orbital angular momentum operator L^2. In the Schrödinger case, the eigenstates are eigenstates of the energy, the orbital angular momentum and the z-component of the orbital angular momentum.

Though this all sounds quite specific, if one were to consider a hydrogen atom in 'some

eigenstate' of the relevant angular momentum operators, then one could without loss of generality choose the z axis in such a way that the above conditions were recovered. Therefore the choice of eigenstates is not as specialized as it might seem.

Not only are the possible orbits of the electron about the proton very simple, they are consistent between the Schrödinger, Pauli and Dirac contexts. We saw this consistency in Tables 3.1 and 4.1. When the nonrelativistic limits of the results from the Dirac equation are computed they are consistent with the Pauli equation trajectories.

This means that we have an example of the consistency and intuitive appeal of the causal theory, where previously, we had to rely on such simple results as the one given in (1.10) for an appreciation of the intuitive appeal and coherence of the theory. Furthermore, to the extent that we subscribe to the causal theory's realist underpinnings, we have a description of what the electron of the hydrogen atom does when the atom is isolated and in one of the given eigenstates.

We have also computed the rates of revolution about the z axis. These rates of revolution are given in Table 8.1. Where the Pauli and Dirac states also happen to be spin eigenstates, the rates of revolution agree with the corresponding Schrödinger rates. However, in the last case presented in the table, the Schrödinger hamiltonian yields no eigenstate analogous to the Pauli and Dirac states; here the rates of revolution are different.

We also know from the eigenstate calculations that in the Schrödinger, Pauli and Dirac hydrogen atoms the trajectories are sufficiently orderly that quantum relaxation to equilibrium cannot occur. This is essentially because both r and θ are constants of motion; if they are not initially distributed according to $|\psi|^2$ then under time evolution they will not approach the $|\psi|^2$ distribution, as discussed in Chapter 7. So, even if we did not wish to subscribe to the notion that the trajectory of the electron in isolation in an eigenstate is meaningful, the hydrogen trajectories found here give something more. They allow us to examine the question of what would happen to a non-$|\psi|^2$ distribution under time evolution in *any* of the hydrogen eigenstates considered, under either the Schrödinger, Pauli or Dirac

Schrödinger Trajectories		**Pauli/Dirac Trajectories**	
n, ℓ, m	$\mathbf{d\phi/dt}$	n, ℓ, j, m	$\mathbf{d\phi/dt}$
1, 0, 0	$\pm\frac{\hbar}{m_e a r}$	$1, 0, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{m_e a r}$
2, 0, 0	$\pm\frac{\hbar}{2m_e a r}(\frac{1}{1-\frac{r}{2a}}+1)$	$2, 0, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{2m_e a r}(\frac{1}{1-\frac{r}{2a}}+1)$
2, 1, 0	$\pm\frac{\hbar}{2m_e a r}$	$2, 1, \frac{3}{2}, \pm\frac{3}{2}$	$\pm\frac{\hbar}{2m_e a r}$
2, 1, ±1	$\pm\frac{\hbar}{2m_e a r}$	$2, 1, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{m_e r^2}(3-\frac{r}{2a})$
		$2, 1, \frac{3}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{2m_e r a}\frac{8\cos^2\theta-\sin^2\theta}{4\cos^2\theta+\sin^2\theta}$

Table 8.1: Angular rates of revolution for hydrogen eigenstates

equations, and to conclude that the distributions would not in general approach $|\psi|^2$.

We have also seen that the causal theory may be applied to transition problems, and that various interesting features may result. The $1s-2p_0$ transition problem described in Chapter 6, for example, gave rise to mathematically interesting structures such as the two very different time scales on which the system oscillates, and the invariant sets which define a constant of motion for the system. Furthermore, there was a clear connection between the computed trajectory and the transition, because the local energy expectation value along the trajectory and the rate of revolution $d\phi/dt$ indicated a continuous transition between the $1s$ and $2p_0$ values.

As in the eigenstate cases, the first transition problem showed sufficiently orderly trajectories that there was not sufficient mixing for quantum relaxation to occur. This is due to the existence of nontrivial invariant sets; if under the given initial distribution the particles were distributed among these invariant sets in a way inconsistent with $|\psi|^2$, then because the sets are invariant and the trajectories are constrained to remain on them, the distribution could never approach $|\psi|^2$.

Lastly, we found that this result could be generalized to include a larger class of transition problems. This class consists of all those hydrogen transition problems which assume a

constant spin in the z direction, and stimulation by semi-classical radiation polarized in any direction (rather than just in the z direction as was the assumption of Chapter 6). All such transition problems have the kind of structure that was seen in the $1s - 2p_0$ transition, namely nontrivial invariant sets. Therefore, by the same argument that was given for the $1s - 2p_0$ transition, systems undergoing any of these transitions would not undergo full quantum relaxation if they were to begin in a non-$|\psi|^2$ distribution.

The implications of the hydrogen study for the question of relaxation are interesting in that Bohm and Hiley proposed in [18] that it might be possible to explain the $|\psi|^2$ distribution via time evolution rather than requiring it as a postulate in the theory. The fact that this is not possible for hydrogen in the situations studied here indicates that it is certainly not possible for *all* individual systems in isolation (or as in the case of the transition problems, in relative isolation). If the postulate is to be removed by some such time evolution explanation, it must be for more complex systems probably composed of more particles. It would be very interesting to see exactly how complex such a system would have to be, and indeed, characterizing the complexity of the dynamical systems generated by the causal theory via (1.8) and (1.16) is an interesting problem in general.

8.2 Response to Criticisms of the Causal Theory

In Sections 2.3 and 2.4 we presented several critiques of the causal theory. It is worth examining how the results presented for the hydrogen atom and quantum relaxation fit into the framework of how the theory has been evaluated. Has the application of the causal theory to hydrogen enabled us to better respond to criticisms of the theory?

The most fundamental criticism of the causal theory, as was seen in Chapter 2, was that its predictions are fundamentally unobservable. First, one can point out that the trajectories are not the only predictions of the theory; it is a full-fledged interpretation of quantum mechanics from which the usual expectation values may be derived. Also, as was pointed

out in the earlier discussion, questions may be asked and answered in the causal theory that are not considered allowable questions in the standard theory. Our examination of the transition process in much more detail than is permissible in the standard theory illustrates this point.

Though the trajectories computed are not directly observable, the relevance to the question of relaxation helps form a response to the criticism that the predictions of the causal theory are non-physical. Clearly, the direct examination of whether or not a given postulate is a necessary feature of a theory has implications for physics. While the standard theory has not, so far, presented a way to investigate the question of *why* the probabilities are given by $|\psi|^2$, the causal theory offers some approaches to investigating this question. The calculations done in Chapter 7 are a concrete first step in this kind of investigation. Thus, the causal theory can offer results with physical relevance despite the fact that the detailed nature of the trajectories is 'hidden'. The implication of the results given here is that it is not possible to use relaxation to explain the $|\psi|^2$ distribution for individual systems such as the hydrogen atom in an eigenstate, nor for 'simple' systems such as the transition problems studied in hydrogen. However, it may still be the case that for a sufficiently complicated wave function, the $|\psi|^2$ distribution arises, at least approximately, from the natural time evolution of the system.

Another criticism that was discussed in Chapter 2 was the statement that because the observations predicted by the causal theory are the same as those predicted by standard quantum mechanics, no 'new physics' can emerge from the theory. Now, it has been argued here and elsewhere [18, 86, 87, 88] that the question of relaxation and the statistical approach to quantum equilibrium is something 'new' with physical content which is relevant to an understanding of quantum theory. But even at a more basic level, the examination of the hydrogen eigenstate trajectories has also contributed something: the detailed discussion of the consistency of the Schrödinger, Pauli and Dirac eigenstates. In standard quantum theory, no analogous comparison of the electron behaviour can be obtained, and while the

stationary state energies arising from the three different hamiltonians can be compared, our trajectory computations form a more intensive comparison of the three frameworks that was not available from standard theory.

One of the advantages of the causal theory, as discussed in the first two chapters of this work, is that it carries not only an algorithmic way to treat quantum phenomena, but a realistic and explanatory picture associated with those phenomena. It is now more clear what is meant by that assertion. Take for example the $1s - 2p_0$ transition problem of Chapter 6. The wave function is composed of two oscillating contributions from the $1s$ and $2p_0$ wave functions. The time scale of these oscillations, and the time scale of the transition frequency ω_0, combine to yield complicated oscillatory motion. The mathematical structure of the wave functions yields the shape of the invariant surfaces on which the trajectories are constrained. Then, the trajectory may be seen to oscillate at disparate time scales over the invariant surface.

The transition itself can be seen along the trajectories, as discussed earlier, by plotting values of both local energy and $d\phi/dt$. The transition is thus described by a continuous process, though the motion is complicated. It is not necessary to picture a mysterious 'quantum jump' as is sometimes done in discussions of transition phenomena in the standard theory. Nor is it necessary to claim that the question of what the system is 'really' doing between measurements is an unreasonable or meaningless question. This explanatory framework does not answer all of the questions of physics, nor even of quantum mechanics, but in terms of previously mysterious phenomena such as transitions, and the double slit experiment (see Chapter 2), it offers some insight.

The physical situations addressed here are not the same as the ones that, for example, Englert *et al.* [39] discussed, and so their criticisms are not addressed by these results. However, the fact that for the hydrogen systems considered here, the causal theory gives rise to intelligible and consistent applications does at least imply that there are physically meaningful contexts in which the causal theory is not 'surrealistic'. Furthermore, it seems

that we can begin to answer the objection that there is no 'new physics' to be found through an examination of the causal theory. In the following section, several avenues of research which seem promising and which are based on the work presented here are discussed.

8.3 Avenues for Further Research

There are several further research topics that would follow naturally from the work presented here. There are others that are less closely related to the study of the causal theory and its application to hydrogen but which would be interesting and fruitful research topics. It is the purpose of this section to describe several of these.

8.3.1 Extensions of Problems Studied Earlier

We have studied transition problems in hydrogen only using the Schrödinger equation, and assuming that the spin is constant and in the z direction. While this is important in that the Schrödinger equation is typically used to describe transitions in textbooks [82, 49] it would be interesting to model transitions in hydrogen using the Pauli or Dirac equations. This could, at first, be done in the same way that transitions were examined in Chapter 7, namely by assuming that

$$\psi = c_a\psi_a + c_b\psi_b \tag{8.1}$$

where ψ_a is one of the wave functions defined by (4.7) or (4.8), or (5.4) or (5.5), and ψ_b is another. By making the assumption that c_a and c_b are (unspecified) complex-valued functions of time, the transitions can be studied without a fully time-dependent analysis, which might well yield invariant sets or some other kind of structure, as was the case for the Schrödinger analysis of the same problem. Even if one assumes that c_a and c_b are constants, quite complicated motion can result, even in the Schrödinger case.

It would also be possible to include a better model of radiation in hydrogen transition problems. Even in the Schrödinger case, a better radiation model could be quite interesting,

because with a different hamiltonian, there is no guarantee that the invariant sets of Chapters 6 and 7, or the qualitative behaviour of the local energy or the rate of ϕ revolution, would appear. Thus, broadening the hamiltonian to account for the magnetic as well as the electric field, and/or treating the incoming radiation not as continuous but as quantized photons might have interesting results.

With the Pauli or Dirac eigenstates, these refinements over the semi-classical approximation might be better left until the semi-classical version was completed. This in itself would be a natural extension of the transitions problems discussed in Chapters 6 and 7. Including a specific hamiltonian, be it due to the semiclassical approximation or better model, would add the detailed time dependence to the model given in (8.1), and thereby allow the computation of explicit trajectories. These trajectories might show qualitative features of the transition as the trajectories of Chapter 6 did.

It is possible that the fact that the spin is no longer constant in the Pauli and Dirac hydrogen eigenstates would introduce sufficient complexity in the wave function so as to allow quantum relaxation to occur. Recall that in Chapter 6, the differential equations given in (6.12) came from the ∇S term, while (6.16) was a result of the 'extra' spin-dependent term $\nabla \log \rho \times \mathbf{s}$. This structure occurred again in Section 7.4.3 for transitions in which $\Delta m = 0$. When $\Delta m = 1$, the structure began to be more complicated, though there was still a sufficiently simple structure that invariant sets again occur, and full quantum relaxation is prevented.

Thus, while the trajectories for transitions involving the Pauli or Dirac hydrogen wave functions would be interesting in their own right, they could have further implications for quantum relaxation. If they did introduce sufficient complexity so as to allow for relaxation, this change would have implications for the amount of complexity required for relaxation. This in turn would have implications for the possibility of removing the $|\psi|^2$ postulate from the causal theory in the relativistic (Dirac) or fully spin-dependent (Pauli) case. Yet another possibility is that adding a better model of the radiation would yield enough complexity for

relaxation to occur, even in the Schrödinger case. Therefore, a study of transitions under the Pauli and Dirac equations, and/or under a more detailed model of the incoming radiation, might be quite fruitful.

8.3.2 Relaxation

The results that we have obtained with regards to relaxation are naturally a small part of the overall relaxation question, as they relate only to the hydrogen atom. If the claims of Bohm and Hiley [18] and Valentini [86, 87, 88, 89] are to be further explored, it will be necessary to examine more complicated wave functions and characterize not only whether relaxation occurs but also the time scale of relaxation. Valentini has already taken some steps towards finding characteristic time scales of relaxation based on the quantum H-theorem in [86, 87]. However, because the H-theorem, as we have seen here, allows for the possibility that no relaxation occurs at all, it would be nice to have a better understanding of when in general it can occur and use a more stringent criterion than the H-theorem to find the time scale.

When Bohm and Hiley stated that the trajectories of their model 'box' systems would fill the configuration space, they referred to the notion of ergodicity [18] (see the discussion of their relaxation argument in Section 7.2). An ergodic system may be defined as one in which each invariant set has either zero measure, or the measure of the whole space. Furthermore, an ergodic system has a unique stable distribution (see [65] or [21] for a discussion of ergodic dynamical systems). This has an interesting implication for quantum systems as defined by the causal theory: could it be the case that ergodicity is what characterizes whether or not full relaxation to the $|\psi|^2$ distribution occurs? If so, then one must compare the notion of 'quantum equilibrium,' where the distribution is $|\psi|^2$ at least in a coarse-grained sense, to a classical equilibrium density which would not change with time. In general, $|\psi|^2$ is time-dependent.

Another property of ergodic systems is that the average of an integrable quantity over an entire trajectory is the same as the average of that quantity of the entire space [65]. This is

also known as the 'ergodic hypothesis' in classical statistical mechanics [84], the hypothesis being that sufficiently complicated (statistical) systems are ergodic. Recall that in the debate between Ghose and Marchildon (see 2.4.2 and [44, 73]), Ghose suggests that the causal theory is not consistent with the standard theory unless the causal system in question is ergodic. While it was argued in Chapter 2 that this conclusion relies on choosing a sub-ensemble of the causal trajectories, the question of time-series behaviour posed by Ghose might also be answerable through an examination of ergodicity and relaxation. Indeed, it seems that the two are connected.

In an ergodic system whose spatial distribution is the standard $|\psi|^2$ distribution, the average of a quantity over any trajectory (or the time average) would be the usual $|\psi|^2$ expectation value. Because this applies to any individual trajectory, one might be tempted to examine averages along each trajectory and compare them to $|\psi|^2$ expectation values, interpreting the $|\psi|^2$ values as the 'standard quantum result' and the trajectory average as the 'causal theory result'. In the ergodic case where the system begins in a $|\psi|^2$ distribution, the two results would agree.

This is the approach Ghose has taken. However, the distribution Ghose assumes is not the $|\psi|^2$ distribution because of the fact that he considers a sub-ensemble (see the discussion of Ghose's argument in Section 2.4.2). In general in the causal theory, a sub-ensemble considered on its own will not have the same statistical properties as the full quantum system with the $|\psi|^2$ distribution, as Valentini has shown in [86, 87, 89].

At this point, relaxation becomes relevant. Bohm and Hiley's argument might suggest that it is ergodic systems, in general, that relax to the $|\psi|^2$ quantum equilibrium [18]. This means that the spatial averages of quantities, and hence the trajectory (time) averages in the ergodic case, approach $|\psi|^2$. This will be the case for any trajectory. Thus, a sub-ensemble may be chosen, and the time averages along trajectories in the sub-ensemble will be the same as the standard quantum expectation values. This is made possible by the combination of the ergodicity of the system and the relaxation process. The ergodicity ensures that the

trajectory average over time is the same as the spatial average, and the relaxation ensures that eventually, the spatial average approximates the $|\psi|^2$ distribution.

In summary, the causal theory gives expectation values consistent with the standard quantum results *if* the initial distribution is the $|\psi|^2$ distribution. It may also give expectation values consistent with standard quantum mechanics in a coarse-grained sense if the system relaxes and approaches the $|\psi|^2$ distribution. Furthermore, if the system is ergodic *and* relaxes to approximately the $|\psi|^2$ distribution, then it will have the additional property that the time averages of quantities along the trajectories (even if a sub-ensemble is chosen) will agree with the standard quantum mechanical averages.

This kind of reasoning probably explains why, according to Ghose, only ergodic systems defined by the causal theory have time series that are consistent with $|\psi|^2$ expectation values. It would be an interesting research problem to substantiate this idea. Such substantiation would require both general research on the properties of ergodic causal quantum systems and specific study of the kinds of systems for which Ghose posed his criticism of the causal theory in [45, 44]. An important first step in this research program would be to show that, indeed, ergodicity characterizes relaxation.

8.3.3 Nonlocality and Entanglement

The causal theory could also be fruitfully applied to the question of nonlocality and entangled quantum systems. Some preliminary calculations in this direction were done by Dewdney, Kyprianidis and Holland, [31, 29] and presented in Peter Holland's book [61]. One of the relevant results is a calculation of the electron trajectories in the Stern-Gerlach experiment. In this calculation, the system is a pair of spin 1/2 particles entering two Stern-Gerlach devices, which are oriented in z' and z directions. The authors begin with two entangled particles described by a combined wave function:

$$\psi_0(z_1', x_2) = f_1(z_1')f_2(z_2)\frac{1}{\sqrt{2}}(u_+v_- - u_-v_+). \tag{8.2}$$

In this expression, z_1' and z_2 are the coordinates of particles 1 and 2 in the z' and z directions, $f_1(z_1')$ and $f_2(z_2)$ are normalized Gaussian packets, and u and v denote the spin eigenfunctions, i.e. $\sigma_{z_1} u_\pm = \pm u_\pm$ and $\sigma_{z_2} v_\pm = \pm v_\pm$. The authors assume that the magnetic field interaction is brief, and they neglect the magnetic field in other directions than z' and z (for particles 1 and 2 respectively). They only discuss the z components of particle motion, suppressing the other components (this is valid classically).

The authors then proceed to solve the Pauli equation in the case that a spin measurement is made on each particle, using a Stern-Gerlach device. Their results are quite compelling: they show each wave packet, $f_1(z_1')$ and $f_2(z_2)$, splitting into two non-overlapping packets, corresponding to spin up and spin down in the z' and z directions. Each particle will always appear in one and only one packet, and which packet a particle arrives in depends only on the initial positions. Furthermore, the authors compute the spin vector and show the continuous evolution of the spin from various starting points to one of the two outcomes, 'up' and 'down', associated with the two packets. If the initial distribution is $|\psi|^2$ then, as usual, the final probabilities for the outcomes are the same as they are in standard quantum mechanics. This continuous version of the Stern-Gerlach experiment is no small achievement for the causal theory, and has considerable appeal.

While these results are intuitively appealing and show that it is possible to consider the spin as a continuous variable while recovering the discreteness predicted by standard quantum mechanics, these calculations by no means represent the full potential of the causal theory's application to entangled systems. For example, while it is becoming clear that there is nonlocality in quantum mechanics, the physical *cause* of this nonlocality is not clear. In other words, it is somewhat of a mystery what forces or aspects of quantum systems 'enforce' quantum correlations across distances. The causal theory offers the quantum potential and the guiding wave concept as available conceptual tools with which one might begin to explore this general question. Such exploration could perhaps begin with more calculations of the detailed or hidden behaviour of various different entangled systems. In the case of hydrogen

transitions, the fact that the transition was apparent along the trajectory, and that the local energy and rate of ϕ revolution characterize the transition, was not apparent from the statement of the causal theory. Rather, these features emerged from the numerical computations. In addition, structures that led to insight into the problem of relaxation emerged from the differential equations. This kind of insight could emerge from a study of the details of entangled systems as well.

It is quite widely accepted that no signalling is possible using nonlocal quantum correlations (see for example [49, 18, 61, 12] and many others). This result is sometimes referred to as the 'no-signalling theorem' or the 'no-signalling result'. However, it is not clear physically why it should be the case that signalling via quantum entanglement is not possible, though it is clear that the result emerges quite naturally from the standard quantum formalism. Perhaps the more explanatory framework of the causal theory could offer some insight; for example, perhaps there are symmetries in the wave function which produce exactly counteracting forces from the quantum potential so as to 'mask' possible signals.

Furthermore, there have recently been some authors who question whether the no-signalling rule, well-accepted though it is, is really fundamental to quantum theory [79, 64]. These authors argue that the no-signalling theorem, which is usually thought to be a very basic result of quantum theory, is a result of the theory only because of the tensor product formalism which statements of multi-particle quantum theory typically assume. They argue that the actual dynamic laws of quantum mechanics do not imply the no-signalling rule, but that it is only the tensor product formulation that does so. They also give argue that the tensor product formulation actually *assumes* something equivalent to the no-signalling theorem, and therefore that the no-signalling result begs the question.

The causal program offers an opportunity to study this question in more detail. Under the causal theory, one could simply find out, through direct computation, what happens to some entangled systems, and thereby use the dynamic laws of the theory directly rather than appealing to the tensor product formulation. Peter Holland states in [61] that the

no-signalling result emerges directly from the computation given, which was for the Stern-Gerlach experiment described above. However, no more general work based on the dynamical laws of quantum theory, either the standard theory or the causal program, seems to be available which duplicates this claim. The currently accepted proofs of the no-signalling rule rely on the tensor product formalism rather than on the Schrödinger equation (or other central dynamical equations of quantum mechanics). If one were convinced, as Kennedy and Peacock seem to be [64, 79], that the standard no-signalling proofs are question-begging, then it would be of great importance to either prove this result by more rigorous means, or find a system which refutes it.

Yet another reason to study entangled systems under the causal theory is that there is as yet no 'good' quantification of the amount of entanglement in a system of more than two particles [6, 38, 63]. While there is such a quantification in the two-particle case, it would be useful for quantum computing and for better understanding of entanglement in general to have such a function. Because in the causal theory the nonlocality emerges essentially from the fact that the wave ψ is assumed to be a physical wave propagating not in real space but in configuration space, it might be possible to study the degrees of entanglement in various systems though the relationship between these spaces induced by the system dynamics. Alternatively, the form of the quantum potential could be a useful tool for characterizing or quantifying entanglement. In general, it is not difficult to argue that the study of entangled systems under the causal theory would be of considerable interest in various contexts.

8.3.4 The Classical Limit

There is also the question of the classical limit: when do quantum systems behave like classical systems? It is to be hoped that a good quantum theory will give rise to classical physics in the appropriate limits, and indeed standard quantum mechanics does so to some extent. The causal theory may have something to offer towards understanding the classical limit of quantum theory and the correspondence between classical and quantum systems.

For example, comparing (1.7) with the classical Hamilton-Jacobi equation (1.6), which reads

$$\frac{\partial S_c}{\partial t} + \frac{(\nabla S_c)^2}{2m} + V = 0, \tag{8.3}$$

we see that the quantum version of the Hamilton-Jacobi equation (1.7) contains an 'extra' term

$$Q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$$

which is the quantum potential. Thus, when the quantum potential vanishes (or is negligible), the quantum Hamilton-Jacobi equation becomes (or approximates) the classical one.

There is, of course, also the distinction that in the quantum case, the generating function S is determined by the wave function, which is in turn determined by the quantum mechanics of the system. However, because the causal program operates in a Hamilton-Jacobi framework, the relationship between the two scales can be studied in a novel way. This study might include examining systems for which the quantum potential vanishes and comparing the quantum and classical generating functions. It might then be possible to make some generalizations based on these comparisons. Then, it would be interesting to find the quantum potentials and generating functions for entangled systems and understand them in the context of the classical limit and the relationships between other quantum and classical generating functions.

8.4 Final Remarks

In this chapter, we have discussed several topics in quantum mechanics and given suggestions of research problems. In all of these areas, there is potential for the causal theory to be a valuable tool and give insight into unsolved problems of importance. These problems range from quite applied problems such as the trajectory computations presented in earlier chapters and their implications for the question of quantum relaxation, to quite general questions such

as the relationships between quantum and classical systems. It seems that the causal theory has a great deal to offer, and it is the author's hope that the theory will continue to gain support in the physics community.

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