State-Dependent Classical Potentials

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Abstract

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Since the inception of quantum mechanics, the classical limit has been an area of unease. Explanations proposed on this matter include the usage of Plank's constant, the decoherence parameter of the master's equation, or the quantum potential of Bohm's theory. An equally obscure related topic is the mixing of classical and quantum quantities in the dynamical equations.

In this thesis, the subject of classical-quantum mixing will be studied. A method will be explored which will demonstrate one of several candidate methods whereby mixing may be removed and replaced by fully quantum non-relativistic equations. Through use of the quantum potential concept and the Feynman path integral, state-dependent forms of the classical scalar and vector potentials will be derived by assuming the existence of separate component wave functions for the particle and potential. The specific wave component ψ_e attributed to the potential, will hold the effects of an environment. The resulting equations are devoid of classical potentials and can therefore be considered as purely quantum - no mixing takes place. The standard classical potentials emerge from the state-dependent equations by a condition which will be referred to as state-dependence reduction (SDR). Through SDR, the semi-quantum and purely quantum equations are qualitatively and quantitatively equivalent.

The new purely quantum equations will be used both to interpret gauge symmetry and to clarify the reasoning behind the Aharonov-Bohm effect. It will be argued that the freedom of gauge is related to the freedom to choose from many different and distinct environments which reproduce the same experimental outcome. Likewise, the

AB-effect is understood through the environment from which the topological structure of the electromagnetic field is represented. Several aspects of the environment responsible for the effective potentials will be calculated numerically for well-known physical situations including one-dimensional scattering, two-dimensional double-slit setup, two-dimensional Aharonov-Bohm effect, and the two-dimensional Dirac equation.

The proposal of using state-dependent potentials to replace the semi-quantum equation represents a consistent generalization and unification of the quantum and classical potentials, and may offer some experimental results yet untapped.

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Dedication

To my wife Cinzia, the most beautiful soul I know; my children Jessica and Daniel who have brought enormous joy to my life; and God of this universe whose creativity and artistic beauty are evidenced through physics.

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List of Abbreviations

Acronym	Description
AB	Aharonov-Bohm
BQM	Bohm's Quantum Mechanics
CSE	Closed Schrödinger's Equation
IFM	Influence Functional Method
MHJE	Modified Hamilton-Jacobi Equation
NRQM	Non-relativistic Quantum Mechanics
PDE	Partial Differential Equation
QFT	Quantum Field Theory
SDCP	State-Dependent Classical Potential
SDP	State-Dependent Potential
SDR	State-Dependence Reduction
SDVP	State-Dependent Vector Potential
SQM	Standard Quantum Mechanics
TDSE	Time-Dependent Schrödinger's Equation

Introduction

For over a decade, scientists and philosophers have laboured to understand quantum theory. Like every new theory of physics, quantum theory has provided a new and previously unknown domain of scientific discovery. But unlike other theories, it has struggled to reveal the previous known domain (the classical world) as a limiting case. The theory of special relativity, for example, requires the general laws of nature to be co-variant with respect to Lorentz transformations[1]. The Galilean transformation of classical mechanics is easily obtained from special relativity in the limit of small relative velocities $v \ll c$, where c is the speed of light. With quantum theory, the situation is not so simple.

The difficulty with quantum mechanics is that unlike special relativity, the notion of measurement is not precisely defined. For example, the exact role of the observer is not unanimously agreed upon. Is the observer simply a very complex quantum system, or a unique as yet undiscovered world of consciousness? Is the universe primarily quantum, with the classical world emerging from it, or does it require both a quantum and a classical description, as proposed by Bohr[2]?

A modern explanation to this question is provided by decoherence theory[3]. The claim is that the world is primarily quantum and that the classical world is a complex quantum system. The main feature of this theory is derived from the understanding

that the difference between classical and quantum behaviours is related to the notion of interference. Unlike the quantum world, the classical world does not display interference. From this basic concept, a decoherence parameter is defined. When the decoherence vanishes, interference disappears and classical behaviour emerges.

Although decoherence theory provides a refined and very elaborate framework for explaining the classical world from the quantum world, it relies on the introduction of large scale environment systems to provide the decoherence or classicality mechanism. But how is decoherence related to the correspondence principle? Particularly, how can decoherence describe the use of classical potentials in Schrödinger's equation? Are these potentials, such as the Coulomb force between two electrons, to represent a large decohering environment? How can the decoherence mechanism which relies on the "spontaneous dynamical diagonalization of the density operator for a macroscopic object" [3] provide a solution to phenomenological uses of potential wells and potential barriers?

The current thesis deals with these issues by providing a candidate solution to the problem of classical and quantum mixing in non-relativistic quantum mechanics. It will be proposed that classical potentials which are generally believed to summarize the effects of a secondary interacting system, can be better understood by substituting it for an environment wave function. The new wave function represents the overall influence of the secondary system on the quantized particle. Viewed this way, classical potentials become state-dependent - a concept which closely resembles the quantum potential of Bohm's ontological view of quantum mechanics[4]. This thesis will provide a simulation of *a world without potentials* - a world composed only of wave functions and therefore a world of amplitudes.

Attempting such a problem appears challenging enough. However, the problem is compounded by the many different points of view taken with respect to the interpretation of quantum mechanics. Providing a simulation of a world without potentials, will therefore necessitate adopting one interpretation consistently. In addition, the specific interpretation chosen must provide insight which is not gained by other interpretations. For this reason, Bohm ontological interpretation[5] will be used throughout the thesis.

The main advantage of Bohm's interpretation is that it provides a deterministic picture of the inner workings of the quantum world. Take the standard double-slit gedanken experiment for example. In the conventional approach, the interference pattern produced at the scintillator screen by a stream of electrons aimed towards the slit region is explained by giving the probability amplitude $\psi^*\psi$. The wave function is a superposition ($\psi = \phi_1 + \phi_2$) of separate wave functions for each slit. The probability for a particle at the screen is given by $P = |\phi_1 + \phi_2|^2$[6]. Since the total wave function is a complex number, the probability will contain cross terms from both the real and imaginary parts of ϕ_1 and ϕ_2. The characteristic interference pattern emerges in this way.

In Bohm's deterministic interpretation, the wave function is treated as a force field. The quantum force is given by $-\nabla Q_\psi$ where $Q_\psi = -(\hbar^2/2m)\nabla^2 R/R$ and $R = \psi^*\psi$. The pattern at the scintillator screen is created by varying the initial location of the electron as it leaves the electron gun. The problem is solved using $m\ddot{x} = -\nabla V - \nabla Q|_{x=x(t)}$, where $x(t)$ is the trajectory of the particle from the source to the screen. Solving this equation for a range of initial conditions results in a pattern at the screen equal to the pattern formed by the conventional method.

Although Bohm's approach resembles the method of classical mechanics, it does so at the expense of introducing a very strange force field encapsulated by the quantum potential. In attempting to describe this new force, David Bohm has appealed to the notion of 'active' information. The specific mathematical quality of Q_ψ which gives rise to active information is called 'state-dependence' and refers to the functional dependence of Q_ψ on the wave function ψ.

The idea of active information is only one of several views of the quantum potential. An example of another view is that Q_ψ represents a substratum fluid force[2]. However, not all advocates of Bohm's theory agree with the need for Q_ψ. Dürr, Goldstein, and Zanghì[7] for example, propose that 'Bohmian mechanics', is better formulated without reference to a quantum potential.

Despite the lack of consensus towards the precise meaning behind the quantum potential, what is generally accepted is the usefulness of Q_ψ as an aid in visualizing the inner workings of quantum phenomenon. The quantum potential when viewed graphically provides the landscape traveled by a particle throughout its journey. Several striking visualizations of Q_ψ have been provided by Dewdney and Hiley[8]. The current thesis provides an additional, rather lengthy catalog of quantum potentials for several well-known physical systems.

The quantum potential provides two additional important and related functions which form the subject of the current thesis - namely, the classical limit and the process of quantization. In the present work, the implications of mixing classical and quantal quantities in non-relativistic quantum mechanics will be studied. Bohm's theory is a strong candidate for addressing this problem since the quantum potential provides both the vehicle for determining the classical limit, and the means for

quantizing classical equations. Bohm's theory holds that in the classical limit, Q_ψ tends to zero ($Q_\psi \rightarrow 0$). Furthermore, the published work on this subject[4][9][5][10] seems to indicate a pattern in the way classical equations are modified through the process of quantization. It appears that a classical equation such as the classical wave equation $\nabla\phi = 0$ or the Hamilton-Jacobi equation, is modified by the inclusion of a quantum correction term - the quantum potential Q_ψ. This suggests that a resolution to the question of the validity of mixing classical and quantal quantities in dynamical equations is whether a quantum potential term has or has not been included in the determination of the precise form of the scalar and vector potentials. By combining this observation with the fact that quantum field theory does not contain the problem of mixing - it may be concluded that the answer rests mainly with the notion of state-dependence.

The notion of state-dependence is at the heart of the quantum formalism. Every physical quantity in quantum mechanics is identified through a hermitian operator - the derived expectation values are thus state-dependent. How then, can the classical scalar and vector potentials, which are not state-dependent quantities, be candidates for physical status, whereas the physical reality of the quantum potential - a state-dependent quantity - is all but dismissed? To be consistent with the quantum formalism, it would appear that the quantum potential has more right to physical status than the classical potentials present in the Schrödinger Hamiltonian.

The lack of state-dependence in the use of the classical potentials is a strong contributor to several unresolved issues of current quantum theory. One problem is that unlike the quantum potential, the classical potentials do not have a mechanism for varying the degree of classicity - it is an all or nothing situation. But several of

today's loosely resolved or completely unresolved issues have their origins in semi-classical or non-relativistic quantum mechanics. The Aharonov-Bohm(AB) effect[11] for example, is based on observations derived from the non-relativistic Schrödinger's equation where a mixing of classical and quantal concepts are present. Additionally, the more general problem of the reality of gauge potentials[12] has at its core, the problem of surplus structure[13]. Presently, there is no way to faithfully map a specific vector potential to a physical situation[12]. By shedding light on the implications of mixing, the AB-effect and other issues of gauge symmetry may be made clearer.

A relationship between the quantum potential Q_ψ and the classical potentials $(V, \boldsymbol{A})$ has already been pointed out on several occasions[4][5]. It has been noted that Q_ψ enters the modified classical equations the same way as the classical potential. This is the very reason why Q_ψ has been called a quantum potential despite possessing some unusual nonlocal properties and a stability towards amplitude amplification (form-dependence). Beyond this, no further extrapolation of the relationship between Q_ψ and $(V, \boldsymbol{A})$ has been explored. A simple example of the connection between Q_ψ and $(V, \boldsymbol{A})$ may be given directly from Schrödinger's equation. In situations where the phase is constant, the time-dependent Schrödinger's equation has a real component given by $-V(x) = Q_\psi = -(\hbar/2m)\nabla^2 R/R$ where $R = |\psi|$. Under these circumstances, the scalar and quantum potentials are equal in magnitude.

The idea that Q_ψ and V are more closely related than admitted by Bohm's theory offers the immediate advantage of uniting Q_ψ and V in a consistent manner in the Schrödinger's equation and in the resulting modified Hamilton Jacobi equations (MHJE). This is important because in the current Bohm theory, the potential V enters in a dual fashion. It determines the form of the quantum field via the Schrödinger's

equation, and it contributes to the particle trajectory through the MHJE. It is mysterious how an agent (V) which determines ψ and the particle trajectory $x(t)$ is not affected by any of these, but at the same time has a twofold influence on the particle mechanics. By replacing the classical potential with a state-dependent form, the dual use of V in Bohm's ontological interpretation can be alleviated.

Finally, it must be noted that the method used to arrive at the results of this thesis involves the Feynman path integral. The path integral method has the advantage that any one system of a two system physical situation can be integrated or summarized away. This allows for two interacting systems, to be treated as a single system in the presence of an environment functional or kernel. The environment functional encapsulates the effective interaction potential of the two systems. But since it is essentially an amplitude, it must be viewed as a state-dependent quantity. In this way, it resembles closely the quantum potential and shares a common feature - state-dependence. The specific property of the Feynman path integral - its ability to encapsulate features of a second interacting system without the need to deal directly with its coordinates - was stated by Feynman[14] as being the main advantage of his path integral method.

Chapter 1

Justification for State-Dependent Classical Potentials

In this chapter, for the purpose of exploring a relationship between the quantum and classical potentials, the essential features of Bohm's quantum mechanics (BQM) will be compared against standard quantum mechanics (SQM). Although the more economical approach of Dürr, Goldstein, and Zanghì[7] is possible, here instead, the quantum potential will be presented as a vital component of BQM - one which highlights the core of Bohm's ontological theory of quantum mechanics. However, it will be shown from inductive arguments, that the quantum potential reveals an unnecessary complication when compared to SQM. The complication supports the arguments of Dürr, Goldstein, and Zanghì[7] but is here resolved differently. A resolution to the apparent complication will be offered by both comparison to quantum field theory (QFT) and by conjecture to the appropriate implications for BQM. The results of the analysis is a hypothesis which proposes that classical potentials be replaced by intermediate state-dependent potentials (SDP). But unlike the quantum potential, state-dependence from these new potentials will come not from the particle wave function, but from some unspecified environment wave function ψ_e. The function

ψ_e is responsible for providing the effective interaction between the particle and the environment, both acting in the same configuration space. State-dependence not only restores consistency in BQM, it also allows for a closer correspondence between NRQM and QFT.

1.1 Comparative review of SQM and BQM

Standard quantum mechanics and Bohm's quantum mechanics differ not only in their formalism but also in the interpretation of their respective formalisms. A complete comparative review would require a lengthy chapter covering topics such as conceptual developments, the theory of measurement, the concept of probability and the role of statistics[2]. However, for purposes of the present work, only three areas need be mentioned including, the objects of the formalisms, the explanations given to the classical limit, and the explanation of the methods of achieving quantized form for the dynamical equations. The study is somewhat simplified by the fact that SQM and BQM both depend on the same wave function ψ. Furthermore, the predicted experimental outcomes of the theories are the same.

Regarding the objects of the formalism, in SQM, a system of particles is completely described by its wave function, evolving according to Schrodinger's equation - which may be symbolized as a single element set (ψ). In BQM, a system of particles is described by a set of two elements ψ and $\boldsymbol{r}_i(t)$ - the set $(\psi, \boldsymbol{r}_i)$ - where $\boldsymbol{r}_i(t)$ is the precise path of the i^{th} particle. To remain consistent with the results of SQM, BQM requires that along with the Schrödinger wave function, an additional equation exist for the evolution of the particle paths. Dürr, Goldstein, and Zanghì[7] show that the

simplest choice, 'compatible with Galilean and time-reversal invariance', is the form,

$$\dot{r}_i(t) = \frac{\hbar}{m_i} Im \frac{\nabla_i \psi}{\psi}(r_1, ..., r_N) = \frac{\nabla_i S(r_1, ..., r_N)}{2m_i}.$$

This is simply the equation for the current density ($J = \rho v$), where ρ is the probability density. Unlike SQM however, the velocity in BQM is taken literally rather than statistically. It appears, therefore, that the only addition to SQM to arrive at BQM is the statement that particles have well-defined paths. The paths are guided by a state-dependent velocity field ($v = \nabla S/2m$) where $S = (\hbar/2i)\log(\psi/\psi^*)$. Hence, the first difference between SQM and BQM is the complement of the set (ψ) in the set $(\psi, \boldsymbol{r}_i)$.

From a mathematical or axiomatic perspective, the set $(\psi, \boldsymbol{r}_i)$ is sufficient for describing BQM. As explained by Dürr, Goldstein, and Zanghì[7], no additional reference to quantum potentials are necessary. This method has the advantage of simplicity and economy of form. However, the more striking features of BQM are illustrated by way of the quantum potential Q_ψ. This object of the BQM formalism not only encapsulates the special features of the quantum world but also reveals the classical limit and helps to clarify the effects of quantization on classical dynamical equations. In SQM, the classical limit is the point at which $\hbar \to 0$. The process by which the quantum world is entered, is through quantization where classical dynamical variables become operators on a Hilbert space. In BQM, the classical limit is approached as $Q_\psi \to 0$. This suggests that the difference between classical and quantized equations is the presence of Q_ψ. This result is precisely what was arrived at by Bohm. There are several examples of this. The modified Hamilton-Jacobi equation (MHJE) originally derived by de-Broglie[2] for a single particle is one such equation.

The MHJE equation reads,

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V(x) + Q_\psi(R) = 0 \tag{1.1.1}$$

where

$$Q_\psi(R) = -\frac{\hbar^2}{2m}\frac{\nabla^2 R(x,t)}{R}$$

and $R(x,t) = |\psi|$. This equation emerges by a polar substitution of ψ for $R(x,t)e^{iS(x,t)/\hbar}$ in Schrödinger's equation. The classical and modified Hamilton-Jacobi versions differ by the presence of Q_ψ. Quantum field theoretic (QFT) versions of this equation also exist. The equation of a quantized neutral, spin 0, massless field ($\phi(\boldsymbol{x},t)$) is[10],

$$\Box\phi = \frac{\delta Q_\psi[\phi(\boldsymbol{x}),t]}{\delta\phi(\boldsymbol{x})}|_{\phi(x)=\phi(x,t)} \tag{1.1.2}$$

where

$$Q_\psi[\phi,t] = -(1/2R)\int d^3\delta^2 R/\delta\phi^2.$$

Again, the classical wave equation $\Box\phi = 0$ is altered by the presence of Q_ψ. Yet another example is provided by Bohm[9] for the quantized equation of an electromagnetic field using normal mode coordinates,

$$\ddot{q}_{k,u} + k^2c^2q_{k,u} = \frac{\partial}{\partial q^*_{k,u}}Q_\psi[q_{k,u},t] \tag{1.1.3}$$

where

$$Q_\psi[q_{k,u},t] = \left(\frac{\hbar^2}{2R}\sum_{k\prime,u\prime}\frac{\partial^2 R}{\partial q_{k\prime,u\prime}\partial q_{k\prime,u\prime}}\right)$$

and where $q_{k,u}$ are the coordinates of the electromagnetic field associated with oscillations of wave number, k, and polarization direction, u. Here again, the classical limit is attained as Q_ψ becomes 0. In summary, the two major differences between SQM and BQM are the addition of well-defined particle trajectories in BQM and their

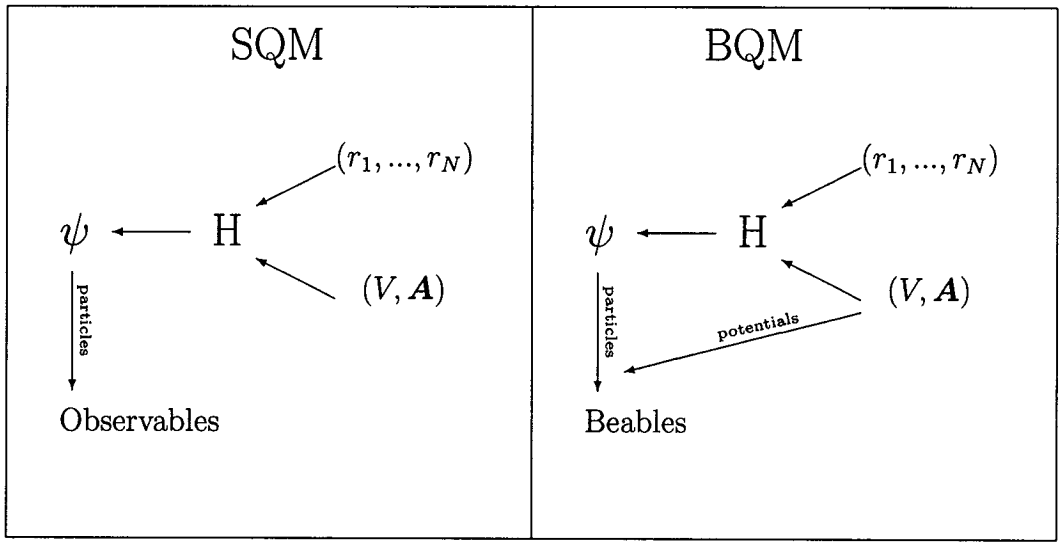

Figure 1.1: The relationship among objects of the formalism in non-relativistic SQM and BQM

respective views on quantization and the related classical limit. All other differences may be taken as originating from these basic two.

The results of SQM and BQM can be illustrated graphically by an arrow diagram. For NRQM, the diagram (fig. 1.1) depicts the relationship among objects of the respective formalisms. The direction of the arrows show dependence of one object on another. In the SQM diagram (left side of fig. 1.1), the functional form of ψ is determined once the potential $(V, \boldsymbol{A})$ is known. No further relationship exists among objects. All other physical quantities are derived by mathematical operation against the wave function. Obviously, to uniquely determine ψ, the appropriate boundary conditions, Dirichlet or Neumann must be applied.

In the NRQM version of the BQM diagram (right side of fig. 1.1), the relationships among objects is somewhat more involved. Like BQM, the quantum wave is

determined by the potentials $V, \boldsymbol{A}$, but due to the introduction of the particle path, an additional relationship is forged. The particle trajectory is determined by both the quantum wave ψ via the quantum potential Q_ψ, and the classical potentials $V, \boldsymbol{A}$. Furthermore, as indicated by the direction of the arrows, neither ψ nor $V, \boldsymbol{A}$ are affected by the particle path.

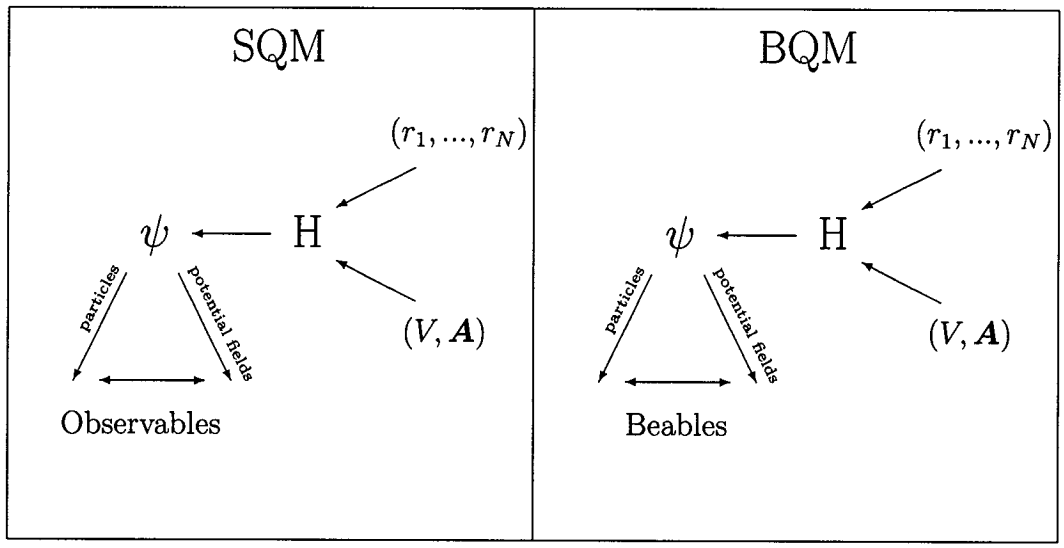

Figure 1.2: The relationship among objects of the formalism in SQM and BQM for quantum field theory

In the passage to QFT (fig. 1.2), very little difference is noticed other than the fact that the potentials are now field operators, like the configuration space variables of NRQM, and the co-dependency between particle and field coordinates. The diagrams of figs. 1.1 and 1.2 bring to light the exact essential disparity between SQM and BQM. The products of SQM are probabilities. The products of BQM are deterministic equations for the input variables. Bell has coined the term beables[15] to describe the products of BQM. This is in contrast to the observables of SQM.

1.2 Dual Role of Classical Potentials in BQM

In the analysis of the previous section, it was explained that the chief differences between SQM and BQM were in the assumptions regarding the physical outcomes derived from the quantum wave. For SQM, it is the statistical expectation values, for BQM it is the deterministic well-defined beables of Bell. The situation is somewhat muddled in the non-relativistic case where the exact placement of the classical potentials are vague - neither as system variables, nor as interaction components of the Hamiltonian. This should seem quite surprising in light of the successes of NRQM.

As previously mentioned, in the QFT diagrams of fig. 1.2, there exists an almost perfect symmetry between SQM and BQM. The NRQM diagrams of fig. 1.1 do not demonstrate this symmetry. Notice that the classical potentials have a dual influence on the particle trajectories. They both determine the form of ψ (the quantum potential Q_ψ) and participate in the particle dynamics through the modified force law $m\ddot{r}(t) = -\nabla Q_\psi - \nabla V$. The question this raises is - can the dependencies be modified so as to alleviate this problem, but without affecting the results of SQM, which are well established?

The first indicator towards resolving the unnecessary complication in BQM is that the classical potentials $V, \boldsymbol{A}$ are neither system variables, nor Hamiltonian elements. The fact that they appear in the Hamiltonian does not affirm their status. But rather, it is for this reason that the complication occurs to begin with. To better understand the specific role of $V, \boldsymbol{A}$ in NRQM, a theory is needed which allows for a mechanism by which classical and quantized forms of the fields can be arrived at by some mathematical method based on physical grounds, not by merely postulating the requirement of a quantized field. For this reason, the Feynman path integral

and environment functional (related to the Feynman-Vernon influence functional[16]) will be used (see chapter 2). The idea is that although the Feynman path integral can be solved for an action involving classical potentials (for a single system), an equivalent system can be arrived at by starting from a quantum field theoretic action (for two interacting systems) and obtaining the classical potential through specific mathematical techniques, such as those applied by Dente[17], which integrate away the second system. In this case, the potentials may be seen not as objects of the non-relativistic Hamiltonian, but as functions representing the effective influence of an environment. It is in this respect that $V, \boldsymbol{A}$ are neither system variables nor Hamiltonian elements. The proposal of this thesis is that V and $\boldsymbol{A}$ are a part of the system wave function - a structure of the internal space.

1.3 Quantum Field Theory

In this section QFT will be looked at more closely. Two aspects of QFT relevant to this thesis will be expanded - the beables of BQM, and the influence function method of Feynman.

In Bohm's theory, the quantized field has an ontological representation just like the trajectories of non-relativistic BQM. The field strength is a beable and may be calculated directly from the modified classical equations with appropriate initial conditions, and having a precise form for the Quantum potential. Equations 1.1.2 and 1.1.3 are examples of deterministic quantized field equations of BQM. As beables, the potential field and therefore the classical potential are the same physical field with the exception of a quantum correction. The degree of classicity of the potential field depends on how active the quantum potential is. When the state of the quantized

system is such that $Q_\psi \to 0$, such as in the case of coherent states[5] the potential field is classical by all respects. But this does not imply that the wave function necessarily vanishes - there may be several ways for the condition $Q_\psi = 0$ to be met. For example, if Q_ψ is the sum of two parts of a total quantum potential ($Q_\psi = Q_1 + Q_2$), the system will behave classically if $Q_1 = -Q_2$ - the wave function will generally not vanish.

The quantum potential provides a compelling picture of the classical limit and process of quantization, but its reliance on the wave function means that it is victim to the same mysteries as SQM. What would be more interesting is a method by which different systems may be made to obey equivalent behaviors - behaviors which may be described by some effective function or functional of an interacting system. Such a method could be construed as indicating that the role of classical potentials is to summarize a set of equivalent systems, each producing the same non-relativistic experimental outcome. The gauge potentials, in this light, would represent not one physical situation but a class of equivalent physical situations.

To demonstrate how different systems may produce equivalent behaviours, a statistical version of the Feynman environment functional[18], namely the Feynman-Vernon theory influence functional method (IFM)[16] will be presented. The IFM will be explored closer in the next chapter. Here, a brief review will be given. The basic idea behind the IFM proceeds as follows: let us assume that we are interested in the behaviour of a system whose coordinate is q, interacting with another system whose coordinate is Q. If we are concerned only with the system q and make no measurements on the system Q, then the IFM shows that it is possible to integrate away all references to the variable Q and produce a functional whose path integral depends on contributions from the q coordinates. Let $S_q[q(t)]$ be the action of the

system q, $S_Q[Q(t)]$ the action of the system Q, and $S_i[q(t), Q(t)]$ be that of the interaction between both systems. Now, the probability of transition from a state ϕ to χ will involve the Kernel $J = K(q_f, t_f; q_i, t_i)K^*(q_f^{'}, t_f; q_i^{'}, t_i)$. For the system of q and Q this forms a double-path integral given by,

$$J = \int\int exp(i[S_q[q(t)] - S_q[q^{'}(t)] + S_i[q(t), Q(t)] - S_i[q^{'}(t), Q^{'}(t)] + S_Q[Q(t)] - S_Q[Q^{'}(t)]])Dq(t)DQ(t)Dq^{'}(t)DQ^{'}(t).$$

If we are only concerned with measurements made to q, this equation can be written in the form,

$$J = \int\int e^{i[S_q[q(t)]-S_q[q^{'}(t)]]}T[q(t), q^{'}(t)]Dq(t)Dq^{'}(t)$$

where T is a functional which defines the amplitude for the Q system to travel between its end points Q_i and Q_f for any given path q. The total amplitude for any specific path q is then the product of a free-particle kernel and the functional T. The functional T is called the influence functional because it holds the influence of the system Q (the environment) which is relevant to the system $q(t)$.

An interesting point about the influence functional is that if T can be approximated by the form $\exp i\int [q(t) - q^{'}(t)]V(t)dt$, then the system q behaves as if acted upon by a classical potential V. This form of the influence functional may result from an infinite number of different systems Q. It explains without ambiguity, how the classical potentials of NRQM could come about. Moreover, since the influence functional is essentially an amplitude, the influence of system Q on system q is state-dependent in nature although effectively described by a classical potential.

1.4 Gauge Symmetry and Aharonov-Bohm Effect

Physics has a long tradition of being the subject of interpretive inspection. Often, it is the role of mathematicians or philosophers to provide an unbiased and fresh look at issues pertaining to the interpretation of physical theories. Without a doubt, from its discovery in 1959, the Aharonov-Bohm effect[11] has been the source of such activities in areas including the meaning and reality of gauge potentials, localities, observabilities, and the closed curve or holonomy interpretation[19]. The AB effect presents a dilemma - how can a finite vector potential influence the wave function in areas of vanishing magnetic flux[11]? This problem can be tackled by studying purely mechanical aspects of the electromagnetic force or alternatively, by interpreting the AB-effect as a manifestation of a geometrical aspect of local gauge symmetry.

However, in light of the previous discussion on the IFM, it is difficult to see how any conclusions can be made regarding the interpretation of AB-effect without a clear picture of the validity and limits of the appearance of classical elements in Schrödinger's equation. If the IFM is taken literally, the roles played by $V, \boldsymbol{A}$ in the quantum equation become irrelevant, since they are merely averaged functions containing the summarized effect of an interacting environment. The environment has been factored out and very little interpretive value can be acquired. For example, the observation that the phase picked up by the electron is independent of the path taken towards the screen, but is dependent on the number of windings n of the magnet field-producing coil, is of a secondary nature. The phase for n windings ($e^{ni\pi BR^2}$) is meaningful only in relation to the way in which the phase factor is mapped back to the original influence functional. Additionally, the holonomy interpretation is devoid of meaning unless this can be related back to some physically meaningful aspect of the

sum of amplitudes of the environment system. Furthermore, the surplus structure of gauge potentials[12][13] may just represent the infinite environments of the Feynman environment functional. Further will be said on this matter in the final chapter, once a form for a state-dependent version of the vector potential has been postulated.

1.5 State-Dependent Classical Potentials

Before suggesting candidate methods for deriving state-dependent forms of the classical potentials, some preliminary observations are in order.

To begin with, it is well known that the scalar potential can be used interchangeably as a boundary condition. The problem of a particle in a box may be treated in two ways. We can solve the free Schrödinger's equation and apply Dirichlet (or Neumann) boundary conditions at the box walls as $\psi(L,t) = 0$ for all t and where L is the width of the box. We could alternatively solve the equation for a particle and a scalar potential where the potential is $V(x) = \infty$ for all $|x| > L$. The equations are equivalent and yield similar results. This suggests, as expected, that $V(x)$ holds the environment boundary. A state-dependent version of the classical potentials must somehow reflect this boundary property.

A second observation is that the equations of BQM - namely, the modified classical equations are not specific to BQM. The essential statement of BQM is the existence of well-defined particle trajectories ($r_i(t)$) or beables. It is always possible to formulate SQM as two coupled real equations rather than one complex-valued partial differential equation. If written as two coupled equations, a quantum potential would emerge from SQM. This prescription is employed for example in the WKB approximation where the quantum potential is dropped in the limit $\hbar \to 0$. Furthermore, the form

of Q_ψ is apparent under certain physical situations where the phase of the wave function is constant $S(x,t) = C$. In this situation, the potential becomes $-V(x) = -(\hbar/2m)\nabla^2 R/R$. The classical and quantum potentials are equal in magnitude - the condition which brings about this relationship is $S \rightarrow C$.

1.5.1 Method of SDCP

In this section, three methods will be proposed for deriving state-dependent forms of classical potentials (SDCP). Several assumptions shall be made. The special property of the Feynman path integral - the influence or environment functional - will be taken literally as indicating an equivalence-type principle between potentials and environments. As previously indicated, this will imply an infinite number of environments for a specific potential. The environment functional concept will then be combined with the inferred method of quantization according to BQM.

Method I:

Although not a part of the formalism of BQM, a review of the results of published work on the subject reveals a pattern in the process of quantization. Equations (1.1.2) and (1.1.3) are two such examples. The book by Holland[10] lists several additional equations of the same type including the quantized classical Schrödinger's equation. These equations have embedded in them a direct method for obtaining SDPs. In eq. (1.1.2) for example, the quantum potential is a functional of the amplitude of the wave function $R[\phi(x), t]$. If it was somehow possible to solve, or rather reverse the equation in terms of $\phi(x)$, then a relationship between the potential field ϕ and the wave function (amplitude) R would follow. Under such conditions, the potential field

could be expressed as a SDCP $\phi_\psi(R,t)$. The classical potential would be regained as $Q_\psi \to 0$, or more precisely as $\phi_\psi \to \phi(x)$. As previously indicated, the condition of classicity does not mean that the wave function vanishes. It may also imply a form for Q_ψ in which $Q_1 = -Q_2$ for a total quantum potential $Q_\psi = Q_1 + Q_2$.

Method II:

Consider a system q interacting with a system Q. Suppose the system can be described by an action

$$S(q,Q) = S_q(q) + S_i(q,Q) + S_Q(Q).$$

The system Q may describe an electromagnetic field and q may stand for matter coordinates[18]. The Feynman path integral for the amplitude for an event $\xi_{q,Q}$ is obtained from the Kernel

$$K = \int \exp\left\{\frac{i}{\hbar}[S_q(q) + S_i(q,Q) + S_Q(Q)]\right\} DqDQ.$$

Defining an environment functional according to

$$T_e[q] = \int \exp\left\{\frac{i}{\hbar}[S_i(q,Q) + S_Q(Q)]\right\} DQ$$

the Kernel will become

$$K = \int \exp\left\{\frac{i}{\hbar}[S_q(q)]\right\} T_e[q] Dq.$$

The environment functional $T_e[q]$ expresses "the modifying effect of the field on the action of the particles"[18]. Therefore, a second method for obtaining a SDCP is to derive an environment functional for a potential system. Then, using approximate methods, cast the kernel into differential form. This equation would contain the

particle wave function ψ_s and the environment wave function ψ_e. The differential form could then be compared with Schrödinger's equation and an effective SDP derived.

Once again, notice that the environment functional $T_e[q]$ is essentially an amplitude. It is the amplitude that the system Q follows along its path endpoints for a fixed path q. Since it is possible in general to choose a different environment to reproduce the same $T_e[q]$, the SDP will represent an infinite number of environments.

Method III:

The wave function ψ at (q_1, t_1) is related to ψ at (q_2, t_2) by Huygens' principle,

$$\psi(q_1, t_1) = \int_{-\infty}^{\infty} \left\{ \int_{q_i}^{q_f} \exp\left(\frac{im}{\hbar} S_q(q)\right) T_e[q] Dq \right\} \psi(q_2, t_2) dq_2.$$

If this equation can be approximated by an equation having the new form,

$$\psi(q_1, t_1) = \int_{-\infty}^{\infty} \left\{ \int_{q_i}^{q_f} \exp\left(\frac{im}{\hbar} S_q(q)\right) Dq \right\} T_e'(q_2, t_2) \psi(q_2, t_2) dq_2,$$

then Schrödinger's equation would immediately follow. This would require assumptions about the dynamics of the path of integration DQ and would result in a less general physical domain for the system. The total wave function would be composed of two distinct components $\psi_e = T_e'(q, t)$ and $\psi_s = \psi(q, t)$. Comparing the new equation with Schrödinger's equation would yield state-dependent forms of the classical potentials.

Chapter 2

Method of State-Dependent Classical Potentials

For over two decades, an increasing amount of attention has been paid to issues pertaining to the investigation of transitions from quantum to classical behaviour. Due to the successful realization of interference phenomenon in larger systems, it is today understood that quantum behaviour is not limited to microscopic scales. H. Zurek [20] points out a number of recent developments in mesoscopic quantum effects including; a gravity-wave detector[21]; nonclassical squeezed states [22]; and quantum states from superconducting currents of Josephson junctions [23][24][25]. The mathematical framework for dealing with mesoscopic quantum systems is in the form of a diffusion coefficient $D(t)$. This coefficient describes the rate at which off-diagonal elements responsible for interference vanish - the rate of decoherence. Decoherence is a spontaneous property of a quantum system in interaction with an environment. The term *environment* usually refers to a system containing a large number of quantum objects such as a spin or oscillator bath[20]. Hence, the environment can be given properties such as temperature, and entropy. The higher the temperature, the greater the rate of decoherence and hence the time for which a microscopic system

loses its quantum behaviour through leakage into the environment.

This chapter will begin by describing the role played by the Feynman Kernel in the description of a system q coupled to an environment Q. Understandably, q is an environment to Q just as Q is to q. However, the term *environment* will be ascribed to the system whose dynamics are being summarized either by some form of approximation or by integrating away all specific reference to its coordinates. Feynman's path integral will be used to derive a wave function ψ_e whose existence will provide information to Schrödinger's equation about the environment, without reference to an external potential function (Method III of sect. 1.5.1). The modified Schrödinger's equation is potential-free, but is effectively equal to that containing a scalar or vector potential. The similarity between this method and methods which use space-time substitutions to evaluate the path integral will be highlighted. Finally, it will be shown that the resulting state-dependent potentials are in the form of a quantum potential, thereby resolving the aforementioned BQM complication.

2.1 Influence Functional and the Environment Functional

Richard Feynman's famous paper[14] in which he unveiled what he called "a third formulation of non-relativistic quantum theory" ends with a demonstration of what he considered to be the main advantage of the path integral approach.

> ...The formulation is mathematically equivalent to the more usual formulations. There are therefore, no fundamentally new results. However, there is the pleasure in recognizing old things from a new point of view.

> Also, there are problems for which the new point of view offers a distinct advantage. For example, if two systems A and B interact, the coordinates of the systems, say B, may be eliminated from the equations describing the motion of A.

The path integral approach therefore, provides a way for studying a quantum system consisting of two subsystems (say q and Q) as though it were a single system q - the histories of any of the systems (say Q) can be integrated out. The result is a path integral for a single path Dq. The question therefore, is whether the single path integral can be converted back into a differential form, namely a Schrödinger-like equation. Methods to obtain differential forms for the path integral are well known and have been solved for several mathematical structures[26][27].

In light of the previous information, it seems natural that the starting point for developing a state-dependent potential would be to use the Feynman path integral method. The integration resulting from the elimination of the Q variable results in a state-dependent functional from which the dynamics of q are derived.

The following convention will be used in the calculations. The quantum system of interest will be labeled with the subscript s - its coordinate will be q and its action will be $S_s[q]$. The systems will interact with the environment-baring system Q, which will be labeled with the subscript e. Its action will be given by $S_e[Q]$. The interaction between system q and Q will be labeled with the subscript i, the interaction action will be $S_i[q, Q]$. The combined system (q, Q) forms a closed system - no further interactions take place. Furthermore, it will be assumed that the system action $S_s[q]$ is a free action - the emerging state-dependent potentials should not depend on any other classical potential. The amplitude that the system will be found at point q_i at

time t_i, given that it was at the point q_f at time t_f, is given by the path integral [18],

$$K(b,a) = \int_{q_i}^{q_f} \left[\exp\left(\frac{i}{\hbar}S_s[q]\right)\right] T_e[q(t)]Dq(t). \tag{2.1.1}$$

The functional $T_e[q(t)]$ will here be referred to as the environment functional. It is the amplitude that the Q system will be found at Q_f at time t_f, given that it was at the point Q_i at time t_i for a specific path $q(t)$. The functional dependence of T_e on $q(t)$ is derived from,

$$T_e[q(t)] = \int_{Q_i}^{Q_f} \left[\exp\left(\frac{i}{\hbar}S_e[Q] + S_i[q,Q]\right)\right] DQ(t). \tag{2.1.2}$$

The total system path integral of eqs. (2.1.1) and (2.2.2) is derived from the usual path integral for the combined system,

$$K(b,a) = \int_{q_i}^{q_f}\int_{Q_i}^{Q_f} \left[\exp\left(\frac{i}{\hbar}(S_s[q] + S_e[Q] + S_i[q,Q])\right)\right] DQ(t)Dq(t). \tag{2.1.3}$$

As pointed out by Feynman, if q is the coordinate of a non-relativistic particle and T_e evaluates to

$$T_e[q(t)] = \exp\left(\frac{i}{\hbar}\int q(t)V(t)\right),$$

then the problem simplifies to that of a quantized particle under the influence of a scalar potential $V(q,t)$. This is a trivial situation where the Hamiltonian $H = \nabla^2/2m + V(q)$ is regained.

In practical applications (statistical outcomes), the probability $J = K(q_f,q_i)K^*(q_f,q_i)$ is required. The probability is calculated from the rule of combining amplitudes which results in the double path integral,

$$J = \int\int \exp\left(i[S_s[q(t)] - S_s[q'(t)] + S_i[q(t),Q(t)] - S_i[q'(t),Q'(t)] + S_e[Q(t)] - S_e[Q'(t)]]\right) Dq(t)DQ(t)Dq'(t)DQ'(t).$$

The environment action is here termed the *reservoir* instead, for analogy with thermodynamical systems. The reservoir allows for a direct calculation of transition probabilities, and density matrices written in terms of the propagators. The transition probability is

$$P_{n\to m} = \int \phi_m^*(q_f)\phi_m(q'_f)J(q_f,q'_f;q_i,q'_i)\phi_n(q_i)\phi_n^*(q'_i)dq_i dq'_i dq_f dq'_f$$

and the density matrix written in terms of the propagation is

$$\rho(q_f,q'_f,t) = \int dq_i dq'_i J(q_f,q'_f;q_i,q'_i)\rho(q_f,q'_f,0).$$

The form of J used to find information about q assumes an initial state for the reservoir and sums (or traces) over all final states of the reservoir - a similar method is applied to the environment system. The propagation J is similar to eq. (2.1.1) but its statistical character necessitates a double path integral

$$J(q_f,q'_f;q_i,q'_i) = \int\int \exp\left(i[S_s[q(t)] - S_s[q'(t)]]\right)F[q(t),q'(t)]Dq(t)Dq'(t)$$

where the functional F - called the influence functional - is given by,

$$F[q(t),q'(t)] = \sum_f \int\int \exp\left(i[S_i[q(t),Q(t)] - S_i[q'(t),Q'(t)] + S_e[Q(t)] - S_e[Q'(t)]]\right)DQ(t)DQ'(t).$$

Written this way, the general form of the influence functional stems from the matrix,

$$F = < K'[Q,t]\phi_e(0)\phi_e(0)K'^*[Q',t] > . \qquad (2.1.4)$$

The statistical method outlined above is due to Feynman and Vernon[16] and serves as the basis for a host of calculations where a simple quantum system is coupled to a large bath of quantum objects[20]. The method is employed when techniques for solving the path integral exist. Its strength lies in its ability to describe behaviour of an environment without the need to know its exact details at every moment.

2.2 Environment Wave Function ψ_e

In this section, method III of sect. 1.5.1 will be applied to arrive at a state-dependent version of the classical scalar and vector potential. The basic idea is to assume that the potentials used in Schrödinger's equations depend upon an environment wave function or kernel which somehow encapsulates the complexities of a second system. It has been argued throughout this text that this is a natural part of Feynman's path integral method and even he claimed this to be a central strength of his method. The problem with a two coordinate system (q, Q) in interaction is that it does not admit a solution to the integral for the sum of paths for a wave function,

$$\int_{\infty}^{\infty} K(q, Q, t; q', Q', t')\psi_s(q', t')dq' \tag{2.2.1}$$

where ψ_s is the wave function for the system s. In this equation, the resulting wave function must depend on the specific path taken along Q. Since this produces in general, different contributions to the integral, only if somehow the paths q are equal to or at least effectively equal for each path Q, do we get a meaningful result in the integral. One way to make this unambiguous is to specify an amplitude for the different values of $q(t)$. This may be for example, a distribution weighting for each value of q. In any way, it is an amplitude and will be labeled as $\psi_e(q, t)$ to express that it is an amplitude resulting from some statistical functional of the environment Q integrated for a fixed q. Under these assumptions, eq. (2.2.1) would become,

$$\int_{\infty}^{\infty}\int_{q_i}^{q_f}\left[\exp\left(\frac{im}{\hbar}(S_s[q])\right)\psi_e(\dot{q}, q, t)\right]Dq(t)\psi_s(q', t')dq'. \tag{2.2.2}$$

The exact details of how ψ_e is derived is unknown. Instead, taking advice from method III of sect. 1.5.1, the usual prescription of evaluating the integral for a small time increment $\triangle t$ where difference $\triangle q$ is $q_{t-\triangle t} - q_t$, will be followed. The specific

final form for the partial differential equation will not contain explicit reference to potentials, only amplitude. The aim therefore, is to extract from the path integral both the wave function of the particle ψ_s and the wave function of the environment ψ_e. This can be accomplished by searching for ways by which the environment functional may be cast in the same form as the wave function. That this is possible can be seen by writing eq. (2.2.2) for an incremental time $\triangle t$

$$\int_{\infty}^{\infty} \exp\left(\frac{im}{2\hbar\triangle t}(\triangle q)^2\right) \exp\left\{L_{V,A}\left(\frac{\triangle q}{\triangle t}, q+\frac{1}{2}\triangle q\right)\right\}\psi_s(q+\triangle q,t)d(\triangle q) \quad (2.2.3)$$

where $L_{V,A} = \frac{e}{c}\dot{q}\cdot\boldsymbol{A} - V(q)$ is the electromagnetic Lagrangian. Inserting the expression for $L_{V,A}$ and expanding around $\triangle q = 0$ yields,

$$\begin{aligned}
&\int_{\infty}^{\infty} \exp\left[\frac{im\triangle t}{2\hbar}\left(\frac{\triangle q}{\triangle t}\right)^2\right] \\
&\times \exp\left[-\frac{i\triangle t}{\hbar}V(q) - \frac{i\triangle t}{\hbar}\triangle q_l \triangle q_m \nabla_m V(q) + \ldots\right] \\
&\times \exp\left[-\frac{ie}{\hbar c}\triangle q_l A_l + \frac{ie}{2\hbar c}\triangle q_l \triangle q_m \nabla_l A_m + \ldots\right] \\
&\times \left[\psi_s(q,t) + \triangle q_m \nabla_m \psi_s + \frac{1}{2}\triangle q_m \triangle q_n \partial_m \partial_n \psi_s + \ldots\right]
\end{aligned} \quad (2.2.4)$$

where $l, m = 1, 2, 3$. This equation can be simplified with the following two observations. First, note that for the scalar potential, the only surviving member is the first term. Hence, the terms within the exponent can be written as a function of q and t. For reasons which will appear obvious in the next steps, the function will be chosen as a log function ($\triangle t V(q) = A_0 = (i\hbar)\ln\psi_e$). Here A_0 is the fourth component of the

vector potential. The equation becomes

$$\begin{aligned}
&\int_{\infty}^{\infty} \exp\left(\frac{im}{2\hbar\triangle t}(\triangle q)^2\right) \\
&\times \exp\Big[\ln\psi_e(q,t)\Big] \\
&\times \exp\left[-\frac{ie}{\hbar c}\triangle q_l A_l + \frac{ie}{2\hbar c}\triangle q_l \triangle q_m \nabla_l A_m + ...\right] \\
&\times \left[\psi_s(q,t) + \triangle q_m \nabla_m \psi_s + \frac{1}{2}\triangle q_m \triangle q_n \partial_m \partial_n \psi_s + ...\right].
\end{aligned} \tag{2.2.5}$$

Next, note that all terms for ψ_s starting from the second onward will correspond with the terms for vector potentials if the following substitution is made, $\boldsymbol{A} \rightarrow (ie\hbar/c)\nabla \ln\psi_e$. Note however, that if the electric field is unrelated to the vector potential - if it originates from an external source - then $\triangle t V(q) = (i\hbar)\ln\psi_e' \neq A_0$. In this case, since V is a function of $q + \triangle q$ in eq. (2.2.4) it can immediately be combined with ψ_e. Otherwise the scalar potential would be constrained by the vector $\nabla\psi_e$. The substitution for the vector potential amounts to eliminating the magnetic field. Situations where the magnetic field does not vanish will be looked at in sect. 2.3.3. The equation now reads,

$$\begin{aligned}
&\int_{\infty}^{\infty} \exp\left(\frac{im}{2\hbar\triangle t}(\triangle q)^2\right) \\
&\times \exp\left[\ln\psi_e(q,t) + \triangle q_m \nabla_m \ln\psi_e + \frac{1}{2}\triangle q_m \triangle q_n \partial_m \nabla_n \ln\psi_e + ...\right] \\
&\times \left[\psi_s(q,t) + \triangle q_m \nabla_m \psi_s + \frac{1}{2}\triangle q_m \triangle q_n \partial_m \partial_n \psi_s + ...\right].
\end{aligned} \tag{2.2.6}$$

The term in the exponential is simply the expansion of $\ln\psi_e$. Finally, the results of method III are obtained

$$\int_{\infty}^{\infty}\int_{q_i}^{q_f} \left[\exp\left(\frac{im}{\hbar}(S_s[q])Dq(t)\right)\right] \psi_e(q',t)\psi_s(q',t)dq'. \tag{2.2.7}$$

The total transformation applied, amounts to making the following replacement

$$(\boldsymbol{A}, \frac{e}{c}A_0) \Rightarrow \left(\frac{ihe}{c}\nabla \ln \psi_e, \frac{ihe}{c}\partial_t \ln \psi_e\right). \tag{2.2.8}$$

With this, we get back Schrödinger's equation for a free particle, provided that the integral of eq. (2.2.1) evaluates to $\psi'(q,t) = \psi_s\psi_e$. That this is true, can be shown by a simple substitution into the free particle kernel of eq. (2.2.1),

$$\psi_e(q,t)\psi_s(q,t) = \int_{\infty}^{\infty} K_{free}(q,t;q',t')\psi_e(q',t')\psi_s(q',t')dq'. \tag{2.2.9}$$

To better understand the implications of the above results, eq. (2.2.7) will be re-expressed in its expanded form in terms of ψ_e and ψ_s. The result is

$$\begin{aligned}\psi'(q,t)+\triangle t\Bigg[-\partial_t\psi_s(q,t) + \frac{i\hbar}{2m}\nabla^2\psi_s(q,t)+ \\ \left(\frac{\partial_t\psi_e}{\psi_e} + \frac{\nabla^2\psi_e}{\psi_e} + \frac{\nabla\psi_e}{\psi_e}\cdot\frac{\nabla\psi_s}{\psi_s}\right)\psi_s\Bigg] + O((\triangle t)^2).\end{aligned} \tag{2.2.10}$$

This equation resembles that obtained by time scaling methods of Duru and Kleinert[28], Kapoor[26], and others[29][30]. Using a point canonical transformation, which is a form of a classical canonical transformation useful in a quantum framework, the potential term is put into a solvable form. This results in a shifting of the classical potential term to include some correction terms. For the case of a transformation known as the 'scaling of time'[26] method, Schrödinger's equation becomes,

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V - \frac{\hbar^2}{8m}\left[\frac{f''}{f} - \left(\frac{f'}{f}\right)^2\right]\right)\psi \tag{2.2.11}$$

where f is a function related to the coordinate transformation. This equation is obtained by substituting for the Hamiltonian $H(q,p) = \frac{p^2}{2m} + V(q)$, an auxiliary Hamiltonian $H'(q,p) = \alpha(q)\left(\frac{p^2}{2m} + V(q) - E\right)$ where $\alpha(q)$ is a local scaling function. The auxiliary Langrangian obtained from H' is placed in a path integral with appropriate

transformation made to the path variables. Schrödinger's equation is then derived in the usual way.

The difference between eq.(2.2.10) and eq.(2.2.11) is that in the former, the transformation is applied to the wave function (internal space), whereas in the latter, the transformation is applied to the coordinates.

2.3 Potential-Free Schrödinger's Equation

The previous section has shown that it is possible to eliminate the classical potential terms from Schrödinger's equation and replace them with an environment wave function ψ_e. The combined wave travels as a closed system and is consequently a free system. For this reason, eq. (2.2.10) will be referred to as the closed Schrödinger's equation (CSE). Although the particular method outlined has effectively eliminated the magnetic field, the vector potential still plays an active role in the dynamics. Subsection 2.3.3 will suggest one way to reinstate magnetic effects.

The next step is to compare the CSE against Schrödinger's equation in the presence of classical potential terms. Since the combined wave of the CSE ($\psi_s\psi_e$) forms a closed system, the total combined particle-environment system (q, Q) travels as though free. The simple form of the equation is,

$$i\hbar\frac{\partial(\psi_s\psi_e)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2(\psi_s\psi_e). \tag{2.3.1}$$

To reproduce the behavior of standard quantum mechanical systems involving a particle and a potential, the CSE will be rewritten in a more familiar form. First, notice that terms may be rearranged to obtain the new equation

$$i\hbar\frac{\partial\psi_s}{\partial t} = -\frac{\hbar^2}{2m}\left[\nabla + \frac{\nabla\psi_e}{\psi_e}\right]^2\psi_s + \left(-i\hbar\frac{\partial_t\psi_e}{\psi_e}\right)\psi_s. \tag{2.3.2}$$

Next, by making the following substitutions, which will be referred to as state-dependent vector potentials (SDVP),

$$\begin{aligned} \boldsymbol{A}_{\psi_e} &= \Re(\frac{i\hbar c}{e}\nabla \ln \psi_e) \\ \boldsymbol{G}_{\psi_e} &= \Im(\frac{i\hbar c}{e}\nabla \ln \psi_e) \\ -cA^0_{\psi_e} &= \Re(\frac{i\hbar c}{e}\partial_t \ln \psi_e) \\ -cG^0_{\psi_e} &= \Im(\frac{i\hbar c}{e}\partial_t \ln \psi_e), \end{aligned} \tag{2.3.3}$$

an equation involving state-dependent potentials is arrived at according to

$$i\hbar\frac{\partial \psi_s}{\partial t} = -\frac{\hbar^2}{2m}\left[\nabla - \left(\frac{ie}{\hbar c}\right)\boldsymbol{A}_{\psi_e}\right]^2 \psi_s + eA^0_{\psi_e}\psi_s + \{V_{\psi_e} + iW_{\psi_e}\}\psi_s, \tag{2.3.4}$$

where

$$\{V_{\psi_e} + iW_{\psi_e}\} \rightarrow \left\{Q_e + Q_{es} + i\frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_s}}{m} + i\frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_e}}{m} + ieG^0_{\psi_e}\right\}. \tag{2.3.5}$$

The environment quantum potential and the coupling quantum potential are respectively,

$$Q_e = -\frac{\hbar^2}{2m}\left(\frac{\nabla^2 R_e}{R_e}\right) \qquad \text{and} \qquad Q_{es} = \frac{1}{m}\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{G}_{\psi_s}. \tag{2.3.6}$$

Although V_{ψ_e} can be set to zero, this does not rule out the existence of terms $\boldsymbol{G}_{\psi_e}$ and $G^0_{\psi_e}$.

2.3.1 State-Dependent Scalar Potential V_ψ

Having arrived at Schrödinger's equation with SDCPs, the equivalence between standard non-relativistic Schrödinger's equation in the presence of an external scalar potential and the CSE can be developed. There are two situations of interest - the equation with a vector potential and the equation without. When a vector potential

is present, the state-dependent scalar potential is given by eq. (2.3.5). The real and complex components on the left hand side are equated to the real and complex components of the right-hand side. The reduction of the state-dependent equations to standard form is,

$$V_{\psi_e} \rightarrow V(\boldsymbol{x}) = \Re\left\{Q_e + Q_{es} + i\frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_s}}{m} + i\frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_e}}{m} + ieG^0_{\psi_e}\right\} \tag{2.3.7}$$

and

$$W_{\psi_e} \rightarrow W(\boldsymbol{x}) = \Im\left\{Q_e + Q_{es} + i\frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_s}}{m} + i\frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_e}}{m} + ieG^0_{\psi_e}\right\} \tag{2.3.8}$$

or simply $V(\boldsymbol{x}) = Q_e + Q_{es}$ and $W(\boldsymbol{x}) = (1/m)\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_s} + (1/m)\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_e} + eG^0_{\psi_e}$. The conditions by which the non-relativistic and CSE are equal will be referred to as state-dependence reduction (SDR). If the imaginary component of the scalar potential is not present, the resulting equation describes the time rate of change of the environment amplitude according to

$$\hbar\frac{\partial_t R_e}{R_e} + \frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_e}}{m} + \frac{\boldsymbol{G}_{\psi_e}\cdot\boldsymbol{A}_{\psi_s}}{m} = 0. \tag{2.3.9}$$

The asymmetry between ψ_s and ψ_e appears odd at first in light of the symmetrical appearance of either component in the CSE. However, the symmetry is destroyed by the SDR condition which requires the scalar potential reduce to a predefined function of the particle coordinate.

When the vector potential is not present, the scalar potential will have to shoulder the load taken by the SDVP A_{ψ_e} in eq. (2.3.4). For this purpose it is best to rewrite eq. (2.3.1) without A_{ψ_e} namely,

$$i\hbar\frac{\partial\psi_s}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi_s + \{V_{\psi_e} + iW_{\psi_e}\}\psi_s \tag{2.3.10}$$

where

$$V_{\psi_e} + iW_{\psi_e} = \left\{ -i\hbar \frac{\partial \psi_e}{\psi_e} - \frac{\hbar^2}{2m} \frac{\nabla^2 \psi_e}{\psi_e} - \frac{\hbar^2}{m} \frac{\nabla \psi_e}{\psi_e} \cdot \frac{\nabla \psi_s}{\psi_s} \right\}. \tag{2.3.11}$$

Separating real and complex components gives the equations

$$V_{\psi_e} = \left\{ \frac{\partial S_e}{\partial t} + \frac{(\nabla S_e)^2}{2m} + \frac{\nabla S_e \cdot \nabla S_s}{m} - \frac{\hbar^2}{2m} \frac{\nabla^2 R_e}{R_e} - \frac{\hbar^2}{m} \frac{\nabla R_e}{R_e} \cdot \frac{\nabla R_s}{R_s} \right\}, \tag{2.3.12}$$

or

$$V_{\psi_e} = \left\{ A^0_{\psi_e} + \boldsymbol{A}_{\psi_e}{}^2 + \boldsymbol{A}_{\psi_e} \cdot \boldsymbol{A}_{\psi_s} + Q_e + Q_{es} \right\} \tag{2.3.13}$$

and

$$W_{\psi_e} = \left\{ -\hbar \frac{\partial R_e}{R_e} - \frac{\hbar}{m} \frac{\nabla R_e}{R_e} \cdot \nabla S_e - \frac{\hbar}{m} \frac{\nabla R_e}{R_e} \cdot \nabla S_s - \frac{\hbar}{m} \frac{\nabla R_s}{R_s} \cdot \nabla S_e - \frac{\hbar}{2m} \nabla^2 S_e \right\}, \tag{2.3.14}$$

or

$$W_{\psi_e} = \left\{ G^0_{\psi_e} + \frac{\boldsymbol{G}_{\psi_s} \cdot \boldsymbol{A}_{\psi_e}}{m} + \frac{\boldsymbol{G}_{\psi_e} \cdot \boldsymbol{A}_{\psi_s}}{m} + \frac{\boldsymbol{G}_{\psi_e} \cdot \boldsymbol{A}_{\psi_e}}{m} + \nabla \cdot \boldsymbol{A}_{\psi_e} \right\}. \tag{2.3.15}$$

The terms which were managed by the SDVP A_{ψ_e} are now handled by the scalar potentials. This implies that the vector potential is present even when the components of $\boldsymbol{A}$ do not appear in the non-relativistic equation. This should not seem surprising since the role of the vector potential has been assigned to the environment phase S_e - a term which is always present. If however, the phase S_e is a constant of time and space, then eqs. (2.3.13) and (2.3.15) will reduce to eqs. (2.3.7) and (2.3.8).

2.3.2 State-Dependent Vector Potential A_ψ

It is tempting to describe the condition for the reduction of eq. (2.3.4) to an equivalent non-relativistic Schrödinger's equation in the presence of a vector potential, as simply setting the SDVP $(\boldsymbol{G}_{\psi_e}, G^0_{\psi_e})$ to zero. However, as previously remarked, eq. (2.3.7)

simply requires that V_{ψ_e} vanish. This does not mean that the SDVP $\boldsymbol{G}$ is zero. The condition is instead that $V(\boldsymbol{x}) = Q_e + Q_{es} \rightarrow 0$. Hence, for the case of a non-vanishing vector potential, the environment potential will have the same magnitude as the coupling potential but with opposite signs ($Q_e = -Q_{es}$). Although the potential equations have been simplified somewhat, the rate of change of the environment is complicated by an additional term

$$\hbar \frac{\partial_t R_e}{R_e} + \frac{\boldsymbol{G}_{\psi_e} \cdot \boldsymbol{A}_{\psi_s}}{m} + \frac{\boldsymbol{G}_{\psi_e} \cdot \boldsymbol{A}_{\psi_e}}{m} = 0. \tag{2.3.16}$$

Furthermore, the vector potential requires that the condition $(\boldsymbol{A}_{\psi_e}, A^0_{\psi}) \rightarrow (\boldsymbol{A}(\boldsymbol{x}), A^0)$ be met. But this is a trivial matter since this deals primarily with a vanishing magnetic field. The usual substitution $\boldsymbol{A}_{\psi_e} = \boldsymbol{A}(\boldsymbol{x}) = \nabla S$ is exactly what has been defined up front.

2.3.3 Non-vanishing environment magnetic field

This section will attempt to show that although the CSE amounts to an elimination of the magnetic field, it is nonetheless possible to re-introduce finite magnetic effect. The suggestion outlined here provides only one of many ways this may be accomplished. It is expected however, that the CSE, which deals with a one-component complex scalar wave function, is not in a framework to naturally deal with magnetic fields. Method I of sect. 1.5.1 would be a more appropriate method for dealing with this problem.

As previously mentioned, the curl of $\boldsymbol{G}$, which is $\nabla \times (ie\hbar/c) \nabla \ln \psi_e = 0$. This is expected since the state-dependent vector potential involves the gradient of one function. An obvious first attempt at restoring the magnetic field in $\boldsymbol{G}$ would be

to use a three-component wave function $(\psi_e^1, \psi_e^2, \psi_e^3)$. The idea would be to replace ψ_e with $\psi_e^1\psi_e^2\psi_e^3$, but this would not re-introduce finite magnetic effects, since $\nabla\times(ie\hbar/c)\nabla \ln \psi_e^1\psi_e^2\psi_e^3$ is still zero. This does however offer a clue, for regardless of the functional form of the new SDP, the gauge invariant Dirac phase integral must result for the wave function.

To better display how a three-component wave function might restore magnetic effects, it is instructive to rewrite the line segment $\boldsymbol{G}_u dq^u$ in matrix form

$$\begin{bmatrix} \boldsymbol{G_1} & 0 & 0 \\ 0 & \boldsymbol{G_2} & 0 \\ 0 & 0 & \boldsymbol{G_1} \end{bmatrix} \begin{bmatrix} dq_1 \\ dq_2 \\ dq_3 \end{bmatrix} = \begin{bmatrix} \partial_1 \ln \psi_e^1 & \partial_2 \ln \psi_e^1 & \partial_3 \ln \psi_e^1 \\ \partial_1 \ln \psi_e^2 & \partial_2 \ln \psi_e^2 & \partial_3 \ln \psi_e^2 \\ \partial_1 \ln \psi_e^3 & \partial_2 \ln \psi_e^3 & \partial_3 \ln \psi_e^3 \end{bmatrix} \begin{bmatrix} dq_1 \\ dq_2 \\ dq_3 \end{bmatrix}. \quad (2.3.17)$$

The gauge invariant Dirac phase integral is reproduced since the matrix equation is nothing but a long way of writing $\boldsymbol{G}\cdot d\boldsymbol{q} = \nabla \ln(\psi_e^1, \psi_e^2, \psi_e^3)\cdot d\boldsymbol{q}$. But this form has the advantage that it allows us to see how the various components of $\boldsymbol{G}$ and ψ_e are related. What is observed is that the off-diagonal elements, which result in an exact differential for ψ_e, are responsible for the vanishing magnetic field. Therefore, a suggested method for restoring magnetic effects is to eliminate the off-diagonal terms. The new wave function is still a gauge invariant quantity. To see this, take the integral of the matrix equation,

$$\begin{bmatrix} \boldsymbol{G_1} & 0 & 0 \\ 0 & \boldsymbol{G_2} & 0 \\ 0 & 0 & \boldsymbol{G_1} \end{bmatrix} \begin{bmatrix} dq_1 \\ dq_2 \\ dq_3 \end{bmatrix} = \begin{bmatrix} \partial_1 \ln \psi_e^1 & 0 & 0 \\ 0 & \partial_2 \ln \psi_e^2 & 0 \\ 0 & 0 & \partial_3 \ln \psi_e^3 \end{bmatrix} \begin{bmatrix} dq_1 \\ dq_2 \\ dq_3 \end{bmatrix} \quad (2.3.18)$$

The result is,

$$\frac{i}{\hbar}\int \boldsymbol{G}\cdot d\boldsymbol{q} = \ln(\psi_e^1\psi_e^2\psi_e^3) - F(q_1, q_2, q_3) \quad (2.3.19)$$

or in exponential form,

$$\exp\left\{\frac{i}{\hbar}\int \boldsymbol{G}\cdot d\boldsymbol{q} + F\right\} = (\psi_e^1\psi_e^2\psi_e^3). \quad (2.3.20)$$

The function F could then be eliminated by setting appropriate conditions on ψ_e.

2.4 The Dirac equation and ψ_e

The state-dependent vector potential has so far been developed in the context of non-relativistic quantum theory. The minimal substitution guarantees that the SDVP for both vanishing and non-vanishing magnetic fields lead to consistent results for other equations, including the Klein-Gordon equation and the Dirac equation. This is easily demonstrated starting with the Dirac equation in the Dirac representation,

$$\Big(i\gamma^u\partial_u - m\Big)\psi = 0. \tag{2.4.1}$$

The 'gamma' matrices are related to 'alpha' and 'beta' matrices as $(\gamma^0, \boldsymbol{\gamma}) \equiv (\beta, \beta\boldsymbol{\alpha})$ which are derived from the Pauli matrices according to

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{2.4.2}$$

In expanded form, the four components of the Dirac spinor generate four partial differential Dirac equations given by,

$$\begin{aligned} i\Big[\partial_0\psi_1 + \partial_1\psi_4 - i\partial_2\psi_4 + \partial_3\psi_3\Big] &= m\psi_1 \\ i\Big[\partial_0\psi_2 + \partial_1\psi_3 + i\partial_2\psi_3 - \partial_3\psi_4\Big] &= m\psi_2 \\ i\Big[-\partial_0\psi_3 - \partial_1\psi_2 - i\partial_2\psi_2 - \partial_3\psi_1\Big] &= m\psi_3 \\ i\Big[-\partial_0\psi_4 - \partial_1\psi_1 + i\partial_2\psi_1 + \partial_3\psi_2\Big] &= m\psi_4. \end{aligned} \tag{2.4.3}$$

For vanishing magnetic fields, the components of momentum are shifted from the SDVP by the minimal substitution

$$\partial_u = (\partial_0, \boldsymbol{\partial}) \rightarrow D_u \rightarrow (\partial_0 + \partial_0 \ln\psi_e, \boldsymbol{\partial} - \boldsymbol{\partial}\,\mathbf{ln}\,\boldsymbol{\psi_e}). \tag{2.4.4}$$

To see what effect this has on the spinor, take the first of the four equations above and apply the substitution of D_u for ∂_u

$$\begin{aligned} & i\Big[\partial_0\psi_1 + \partial_1\psi_4 - i\partial_2\psi_4 + \partial_3\psi_3\Big] + \\ i\Big[\psi_e^{-1}\psi_1\partial_0\psi_e + \psi_e^{-1}\psi_4\partial_1\psi_e - i\psi_e^{-1}\psi_4\partial_2\psi_e + \psi_e^{-1}\psi_3\partial_3\psi_e\Big] &= m\psi_1. \end{aligned} \tag{2.4.5}$$

Then, if both sides of eq. (2.4.5) are multiplied by ψ_e and repeated for the other three equations, a new Dirac spinor is gained which is the old spinor multiplied by ψ_e. The new equation contains only state-dependent vector potentials, not quantum potentials.

2.5 The total quantum potential along the particle path $x(t)$

It is time to pause to review two major differences between the new emerging quantum potentials Q_e and Q_{es} and the quantum potential of Bohm's theory Q_ψ (Q_s). First, unlike Bohm's quantum potential, which appears only in the modified Hamilton Jacobi equations, the environment potentials are part of Schrödinger's equation. They are therefore, essentially independent of the particle path, although their presence in the modified Hamilton-Jacobi equations does not prevent them from being calculated for $x(t)$ along a specific path of the particle. Also, although the total force (F_T) along a specific path has not changed since $F_T = -\nabla Q_T = -\nabla Q_s - \nabla V = -\nabla Q_s - \nabla Q_e - \nabla Q_{es}$, the precise definition of the classical limit has changed. The original condition $Q_s \to 0$ has become $Q_T \to V$, where Q_T is the total quantum potential. The more general condition requires that Schrödinger's equation and the CSE

are equal. The complete reduction according to SDR, is $(V_\psi, \boldsymbol{A}_\psi) \xrightarrow{\text{SDR}} (V, \boldsymbol{A})$, where the set $(V_\psi, \boldsymbol{A}_\psi)$ contains the state-dependent potentials. Furthermore, the current method has defined a new quantity not present in BQM - the state-dependent vector potential $\boldsymbol{G}$. This quantity may be taken as more fundamental than Q_ψ. For instance, Q_ψ may be derived from $\boldsymbol{G}_s$ by $Q_s = \nabla \cdot \boldsymbol{G}_s - \boldsymbol{G}_s \cdot \boldsymbol{G}_s$. Since $\boldsymbol{G}_s$ involves first-order differentiation, it naturally emerges from the Dirac equation (2.4.5) - the quantum potential Q_ψ does not have a Dirac counterpart.

Chapter 3

Numerical Methods

The increase in computational power has stimulated numerous methods for solving quantum mechanical systems. Not only have the methods increased in accuracy, but the visualizations techniques have provided an intuitive and insightful window into the world of the nano scale. As well, the methods go far beyond simple one-dimensional non-relativistic mechanics to include three-dimensional Dirac equation and the inclusion of magnetic effects. If the richness in algorithms were not enough, today there are available packages such as the QuantumKernel of Bernd Thaller and Manfried Liebmann which allow direct calculations and visualization within math software such as Mathematica[31].

The aim of this chapter is to provide visualizations of various state-dependent potentials including the vector and quantum potentials. Several general properties of SDPs will be deduced. The first step is to derive the environment wave function. Although the partial differential equation appears to pose no difficulty, it nonetheless presents a situation for which a lack of information exists for applying boundary and initial conditions. There is an infinite spectrum of possible environments to choose from and very little information on how to select a preferred environment. Appeal

will therefore be made to trial and refinement. The environment yielding the most reasonable compromise between computational efficiency and visual appeal will be selected.

3.1 Method of Suzuki and Raedt

Computations of this chapter are based on the framework of De Raedt[32] and Suzuki[33], and the specific Mathematica implementation provided by Thaller[34] and Liebmann[35]. The Mathematica implementation will be discussed in the next section. The central objective in the numerical method is to search for solutions to the time-dependent Schrödinger's equation (TDSE) for which the norm of the wave function is conserved perfectly at all times. This requirement is referred to in the texts[32] as unconditional stability. To obtain unconditional stability in the TDSE, a unitary approximation is made to the time-step operator $U(\tau) = e^{-i\tau H}$. The specific unitary approximation is obtained using the Trotter-Suzuki method of expressing the exponential of a sum of two matrices as an infinite ordered product of the exponentials of two individual matrices.

For a Hamiltonian consisting of two parts (free particle and potential energy), the Trotter-Suzuki method expresses the exponential of the sum of the two matrices as an infinite ordered product of the exponentials of the matrices:

$$e^{x(A+B)} = \lim_{m\to\infty} \left(e^{xA/m} e^{xB/m}\right)^m . \tag{3.1.1}$$

The index m is the order of the two Hamiltonian matrices ($M \times M$). By expanding both sides through a Taylor series, the error magnitude is found to be[33],

$$\|e^{x(A+B)} - e^{xA/m} e^{xB/m}\| \leq \frac{x^2}{2m^2} \|[A,B]\| e^{|x|(\|A\|+\|B\|)/m}. \tag{3.1.2}$$

If A and B commute, then the right-hand side is zero.

The Trotter formula has been generalized to include more than two matrices in the Hamiltonian. By setting $x = -im\tau$, where τ is the time step, the generalized Trotter-Suzuki formula is,

$$\|e^{-i\tau(A_i+...+A_n)} - e^{-i\tau A_1}...e^{-i\tau A_n}\| \leq \frac{\tau^2}{2} \sum_{1\leq i\leq j\leq n} \|[A_i, A_j]\| e^{|x|(\|A\|+\|B\|)/m}. \quad (3.1.3)$$

This formula is very useful not only in cases where more than three contributions exist in the Hamiltonian, but also in situations where the Hamiltonian has been decomposed into several contributions. The first-order approximation to eq. (3.1.3) is,

$$U_1(\tau) = e^{-i\tau A_1}...e^{-i\tau A_n}. \quad (3.1.4)$$

To see that U_1 is actually a unitary approximation to the time-step operator $e^{-i\tau H}$, notice first that the hermitian conjugate of U is,

$$U_1^\dagger(\tau) = e^{i\tau A_n}...e^{i\tau A_1}. \quad (3.1.5)$$

The product of terms is $U_1(\tau)U_1^\dagger(\tau) = I$ or $U_1(\tau)^{-1} = U_1^\dagger(\tau)$ from which it is seen that U_1 is actually a unitary approximation.

To obtain higher-order approximations, several symmetrization techniques have been developed[32] including a fractal symmetrization decomposition which is used in the Mathematica implementation of the next section. As a brief demonstration of the techniques, the example of Raedt[32] will be concisely outlined. Start with the dimensionless form of the Hamiltonian for a non-relativistic particle experiencing an external two-dimensional vector potential which reads,

$$H = -\frac{1}{4\pi^2}\left\{\left[\frac{\partial}{\partial x} - iA_x(x,y)\right]^2 + \frac{\partial^2}{\partial y^2}\right\} + V(x,y). \quad (3.1.6)$$

The first step is to discretize the derivatives (first and second order) with respect to the space coordinates x and y. The resulting difference equations to the fourth order in the space mesh $\delta = \triangle x, \triangle y$ are,

$$\begin{aligned} H\psi_{l,k}(t) = \frac{1}{48\pi^2\delta^2}\Big\{ & [1 - i\delta(A_{l,k} + A_{l+2,k})]\psi_{l+2,k}(t) \\ & + [1 + i\delta(A_{l-2,k} + A_{l,k})]\psi_{l-2,k}(t) \\ & - 16[1 - i\delta/2(A_{l,k} + A_{l+1,k})]\psi_{l+1,k}(t) \\ & + \psi_{l,k+2} + \psi_{l,k-2} - 16\psi_{l,k+1} - 16\psi_{l,k-1}(t) \\ & + [60 + 12\delta^2 A_{l,k}^2 + 48\pi^2\delta^2 V_{l,k}]\psi_{l,k}(t) + O(\delta^5)\Big\}. \end{aligned} \tag{3.1.7}$$

The indices k and l are the grid points for the space mesh ranging from $k, l = 1, ..., L_{x,y}\delta$ where L is the number of grid points in the specific direction.

The next step is to apply the product formula to difference equation 3.1.7. But at this point, it is helpful to pause and reflect on whether a more optimized form exists - a form more suited for computational purposes. One such method is to expand ψ in terms of a creation operator $c^\dagger$. By rewriting the wave function as,

$$|\psi(t)\rangle = \sum_{l=1}^{L_x}\sum_{k=1}^{L_y} \psi_{l,k} c_{l,k}^\dagger |0\rangle \tag{3.1.8}$$

or

$$|\psi(m\tau)\rangle = e^{-im\tau H}|\psi(t=0)\rangle \tag{3.1.9}$$

the resulting first order unitary approximation is

$$U_1(\tau) = \prod_{n=1}^{9} e^{-i\tau A_n} \tag{3.1.10}$$

where the A_ns are expressed in terms of the creation and annihilation operators $c^\dagger, c$. The remaining task is to translate these equations into a specific computer implementation.

3.1.1 Mathematica Mathlink Implementation

Specific implementations of the Raedt-Suzuki framework for solving the TDSE, the Pauli equation, and the Dirac equation, have been supplied by Thaller[34] and Manfried Liebmann[35]. The paper by Manfried Liebmann includes specific algorithms for one, two, and three-dimensional Schrödinger's equation; two and three-dimensional Pauli equation; and the two and three-dimensional Dirac equation. Liebmann has also developed a Mathlink interface[31] using compiled C++ object for solving single-particle systems within the Wolfram Mathematica software environment. In addition, several helper functions are provided for the visualization of the output from the time evolution of the wave function.

The remaining work of obtaining the various state-dependent potentials can proceed using standard Mathematica methods. Once the specific TDSE system has been solved, the environment wave function can be derived in one of two ways. One method is to solve the partial differential equation (2.3.7) numerically. Since the PDE involves the wave function ψ_s, the amplitude will be interpolated first to produce an 'interpolation function' (Appendix A). A second method involves using the CSE with appropriate boundary conditions.

3.2 Computation of the One-Dimensional Scattering Environment

Illustrations of the SDVP and quantum potential for the single particle and environment will be produced for the common one-dimensional potential barrier and potential well. To obtain the environment, eq. (2.3.7) must be solved. In one-dimension, the

equation reads,

$$\frac{d^2R_e}{dx^2} + 2\frac{dR_e}{dx}G_s(x,t) - 2V(x)R_e(x) = 0 \tag{3.2.1}$$

where

$$G_s(x,t) = \frac{1}{R_s}\frac{dR_s}{dx}. \tag{3.2.2}$$

Before solving the equation for R_e, the space matrix is calculated for each time increment by solving Schrödinger's equation. The resulting space matrix for R_s is then converted into an 'InterpolationFunction' object in Mathematica, and assigned as a function in the differential equation for R_e. Several boundary conditions will be tried until errors become minimal and the visualization of the environment quantum potential displays reasonably.

Figures will be produced for the state-dependent potentials G_e, G_s, Q_e, Q_s and Q_{es}. The time-development of the interaction between R_s and R_e will be plotted for the potential barrier with an incident packet whose energy is half the barrier height.

3.3 Computation of the Two-Dimensional Aharonov-Bohm Environment

The calculations for the AB-effect will be based on modifications of the Mathematica notebooks provided by Thaller[34] and Liebmann[35]. A snapshot will be taken at the seven hundredth iteration for a time step (dt) value of 0.002 ($t = 700(0.002) = 1.4$). To demonstrate the characteristic AB shift, an infinitely long solenoid will be placed at the center of the double-slit setup. The vector potential to be used is[35],

$$\boldsymbol{A}_{\psi} = \begin{cases} \frac{\alpha}{R^2}(-x_2, x_1), & |x| \leq R \\ \frac{\alpha}{x_1^2+x_2^2}, & |x| > R \end{cases} \tag{3.3.1}$$

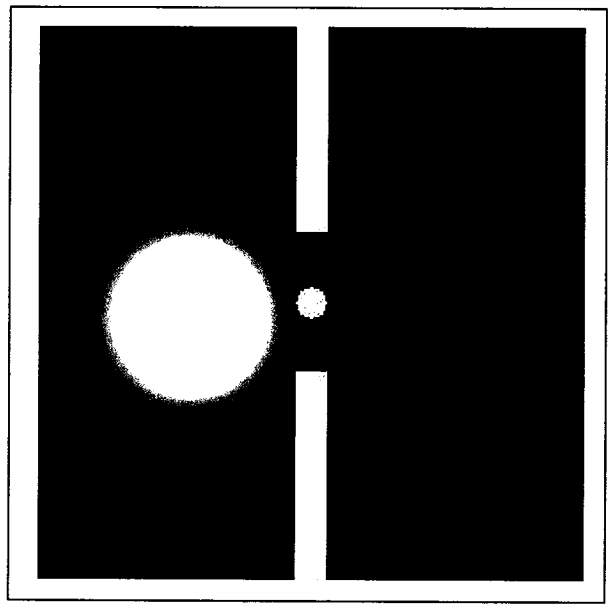

Figure 3.1: Setup of the two-dimensional double-slit and AB-effect setup. An infinitely long shielded solenoid is placed at the slit center.

where R is the radius of the solenoid and α is the magnetic flux of the magnetic field through the solenoid given by,

$$2\pi\alpha = \Phi = BR^2\pi. \tag{3.3.2}$$

Several values of α will be used. The double-slit experiment corresponds to $\alpha = 0$. A pattern shift to the right of the slit system is obtained for $\alpha = .25$ and to the left of the slit system for $\alpha = .75$. The effect of integral coil windings will be demonstrated for $\alpha = 1$. In all cases, the environment will be calculated by comparison with the CSE. Figures will be produced for the state-dependent potentials G_e, G_s, Q_e, Q_s and Q_{es}.

3.4 Computation of the Two-Dimensional Dirac Environment

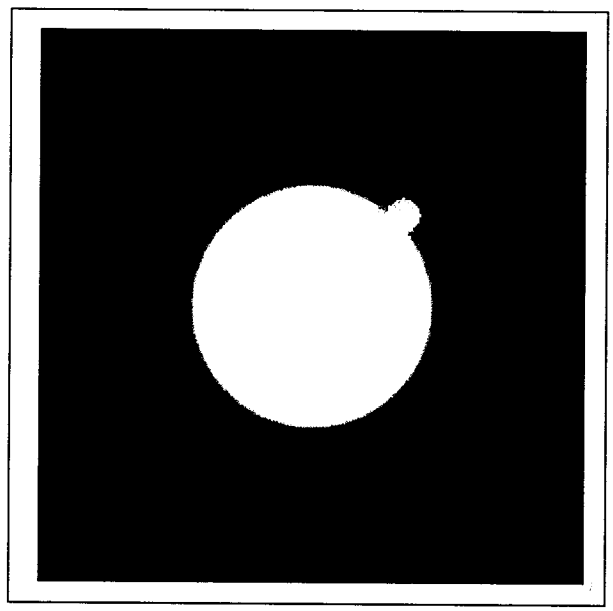

Figure 3.2: Setup of the two-dimensional Dirac spinor and an infinitely long shielded solenoid.

The calculations for the Dirac equation will also be based on modifications of the Mathematica notebooks provided by Liebmann[35]. The evolution of a single-particle and an environment wave will be calculated for a Dirac particle near a shielded vector potential of eq. (3.3.1), located at $\frac{2}{3}$ of the box length (fig. 3.2). Figures will be produced for the wave function spinor components ψ_1 and ψ_2, for the environment wave function ψ_e, as well as for the state-dependent vector potentials G_e, G_s. The environment will be calculated by comparison with the closed Dirac equation

$$\Big(i\gamma^u\partial_u - m\Big)\psi_s\psi_e = 0 \tag{3.4.1}$$

where ψ_s is a two-dimensional Dirac spinor, and ψ_e is a complex scalar function.

3.5 Results of One-Dimensional Scattering

Figure 3.3[36] summarizes the results of computations of the one-dimensional scattering. In the location of the barrier is placed a stationary wave packet. As time progresses, the wave packet becomes irregular in regions of overlap with the environment wave function. The inverse relationship between the particle wave function ψ_s and the environment ψ_e causes several peaks and troughs to appear. Wherever a peak occurs for one wave, a trough results in the opposite wave. It is further observed that all variations of peaks and troughs occur in regions left of the right-side of the barrier. This cut-off line presents a sort of turning point in the dynamics of the system. Also observed is a split in the particle wave packet. The split is attributed to the disturbance generated by the environment.

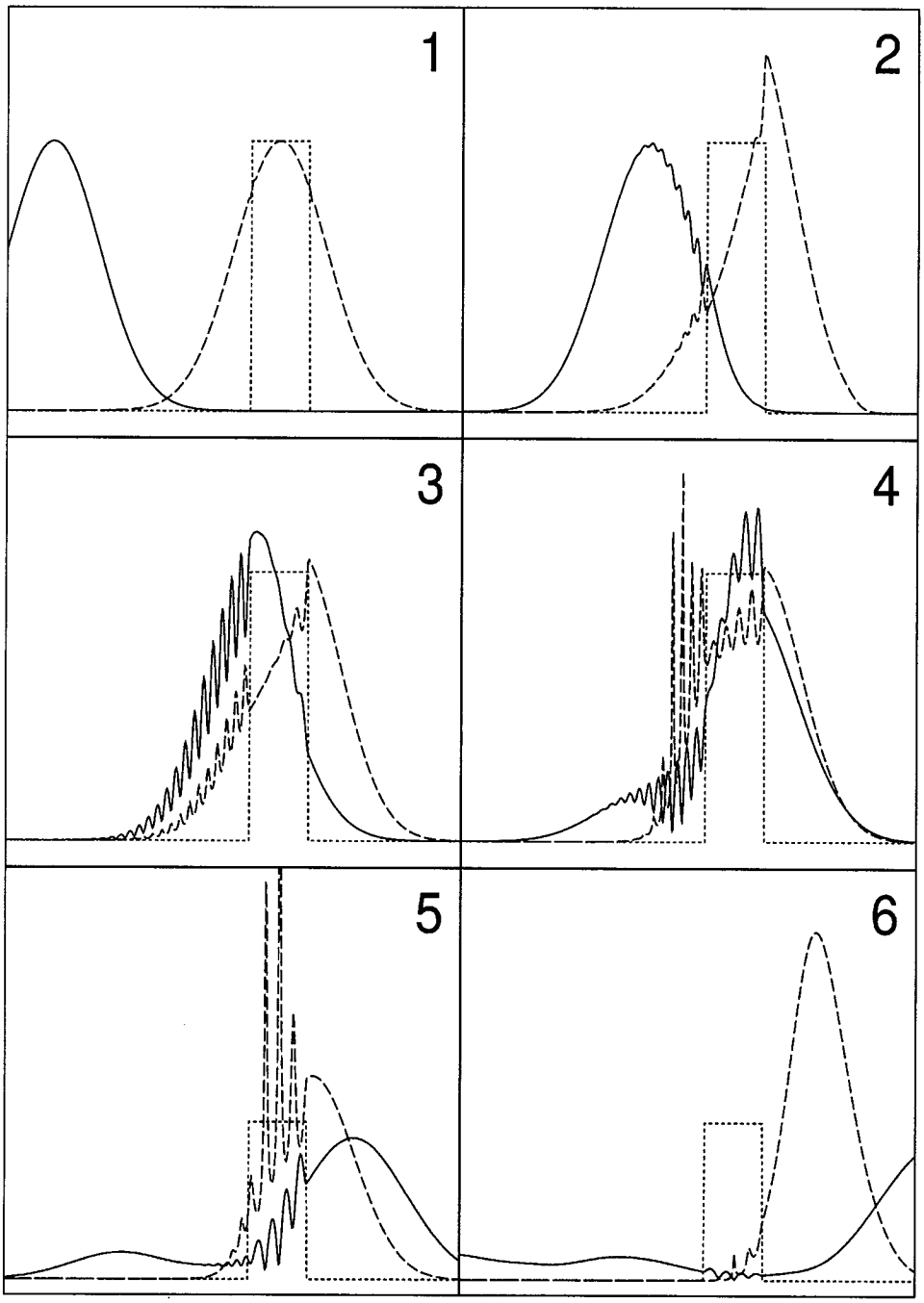

Figure 3.3: Time development of the interaction of the single-particle wave function ψ_s (*solid line*) and the environment wave function ψ_e (*long dashed line*) for one-dimensional particle and barrier system[36].

3.5.1 Environment of the Potential Barrier

Figures 3.4, 3.5, and 3.6 show the different SDPs for the system of a particle incident on a barrier. In the barrier region, the particle and environment SDPs behave very differently. The particle SDPs, $\boldsymbol{G_s}$ and Q_s, display a series of sharp needle-like spikes and holes, forming areas of strong repulsion and attraction. In front of the barrier, the SDVP $\boldsymbol{G_s}$ displays wide, flat, sail-type structures, whereas the SDP Q_s shows an equal number of spikes in the place of sails. The situation is reversed for the SDVP $\boldsymbol{G_e}$ and the SDP Q_e - the $\boldsymbol{G_e}$'s display spikes and the $\boldsymbol{Q_e}$'s display sail structures at the same locations. In the barrier region, both $\boldsymbol{G_e}$ and Q_e display flat, tall, and wavy walls. In general, an equal number of thin walls exist in both graphs.

As the energy of the incident wave packet is increased, two things happen. The peaks and sails become shifted towards the back of the graphs. This is expected since packets of higher energy are expected to arrive earlier at the barrier region than slower ones. The number of spikes and thin walls in the barrier region decreases. These results reflect the principle that more energetic packets have higher transmission ratios than the less energetic packets. Finally, on close inspection, the potentials $\boldsymbol{Q_e}$ and $\boldsymbol{Q_{es}}$ appear as nearly negative images of each other. This is expected by virtue of their relationship in eq. (3.2.1).

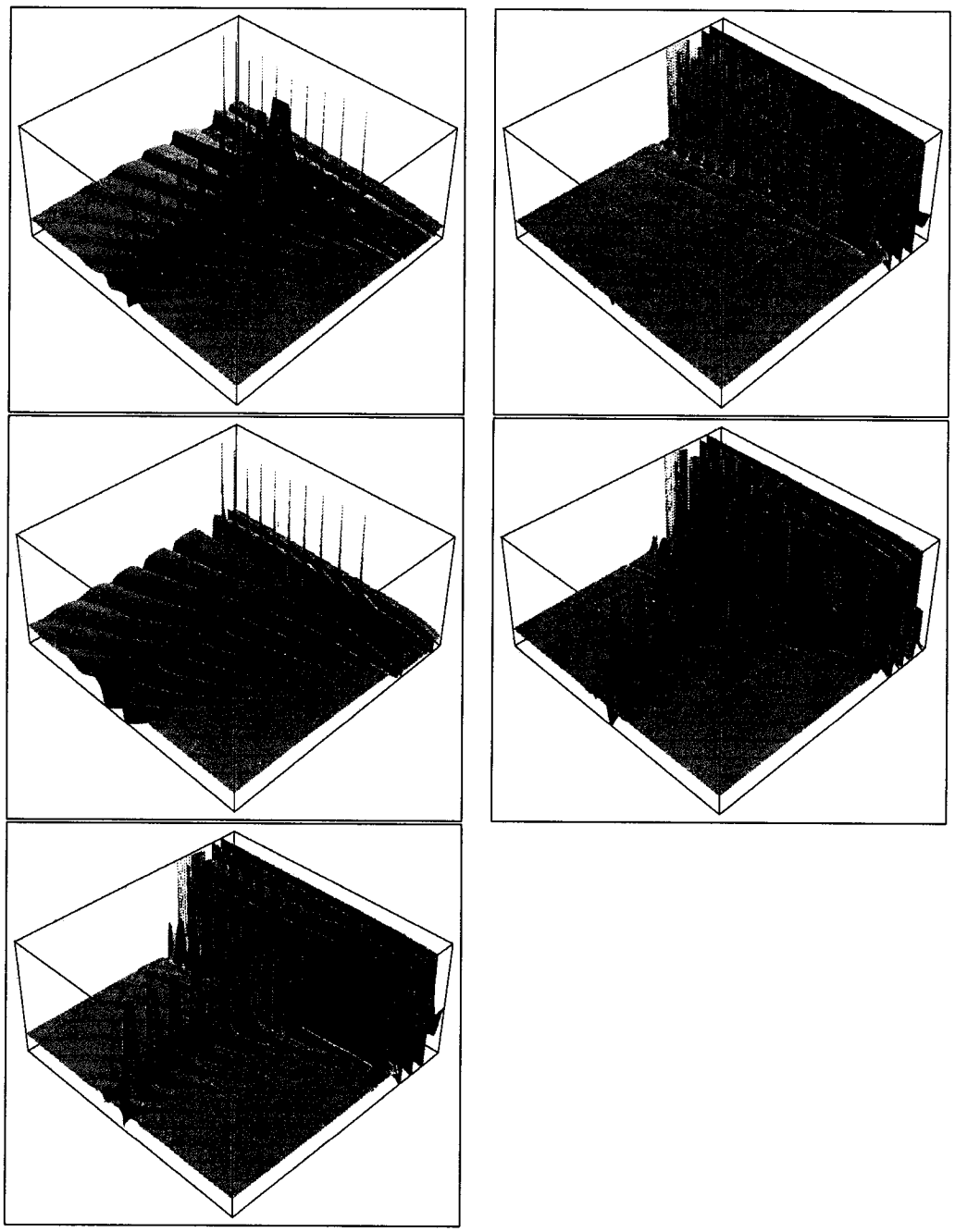

Figure 3.4: Left top to right bottom: State-dependent potentials $\boldsymbol{G}_s$, $\boldsymbol{G}_e$, $\boldsymbol{Q}_s$, $\boldsymbol{Q}_e$, and $\boldsymbol{G}_{es}$ for one-dimensional particle and barrier system. Energy of incident wave packet is half barrier height.

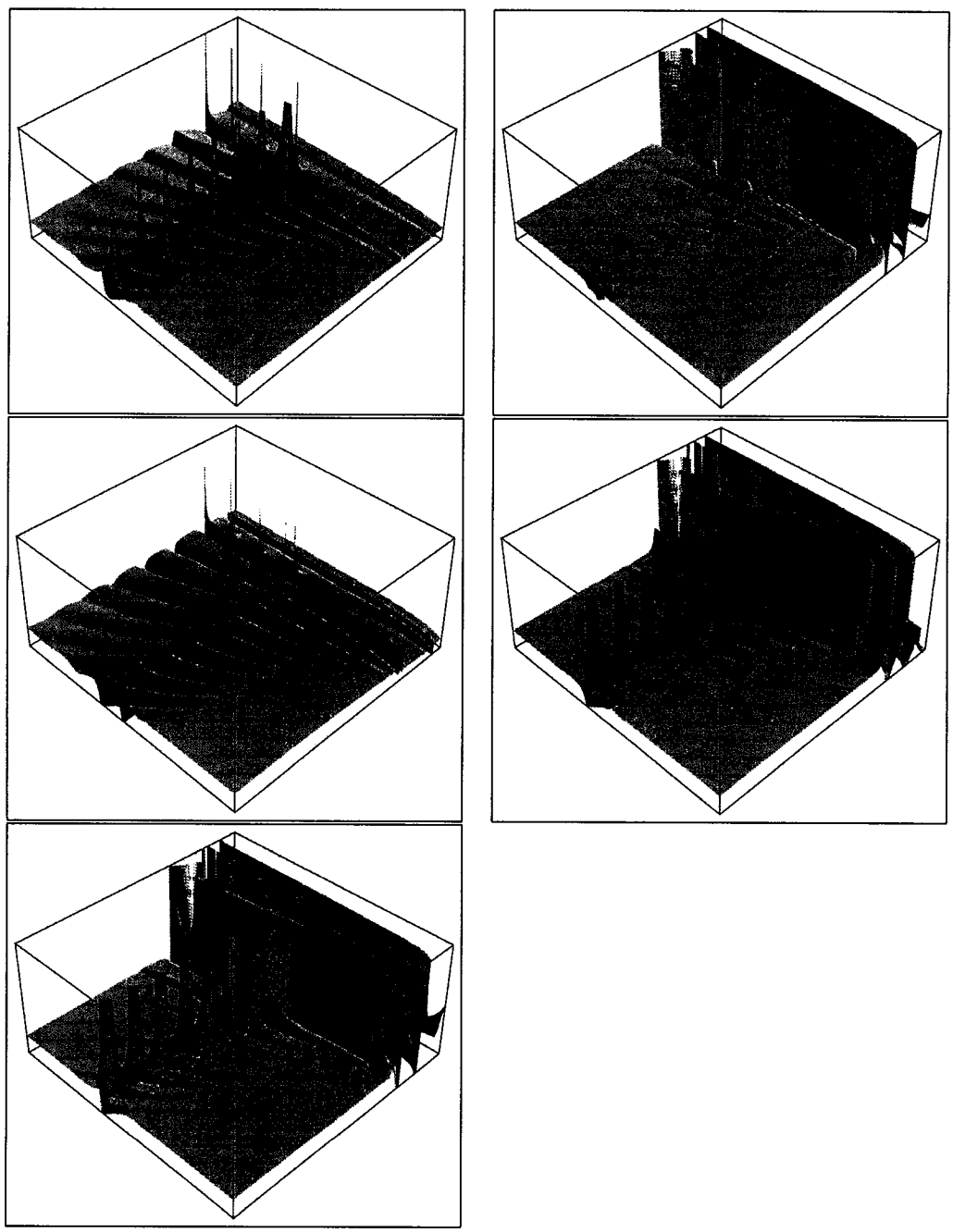

Figure 3.5: Left top to right bottom: State-dependent potentials $\boldsymbol{G_s}$, $\boldsymbol{G_e}$, $\boldsymbol{Q_s}$, $\boldsymbol{Q_e}$, and $\boldsymbol{G_{es}}$ for one-dimensional particle and barrier system. Energy of incident wave packet is equal to barrier height.

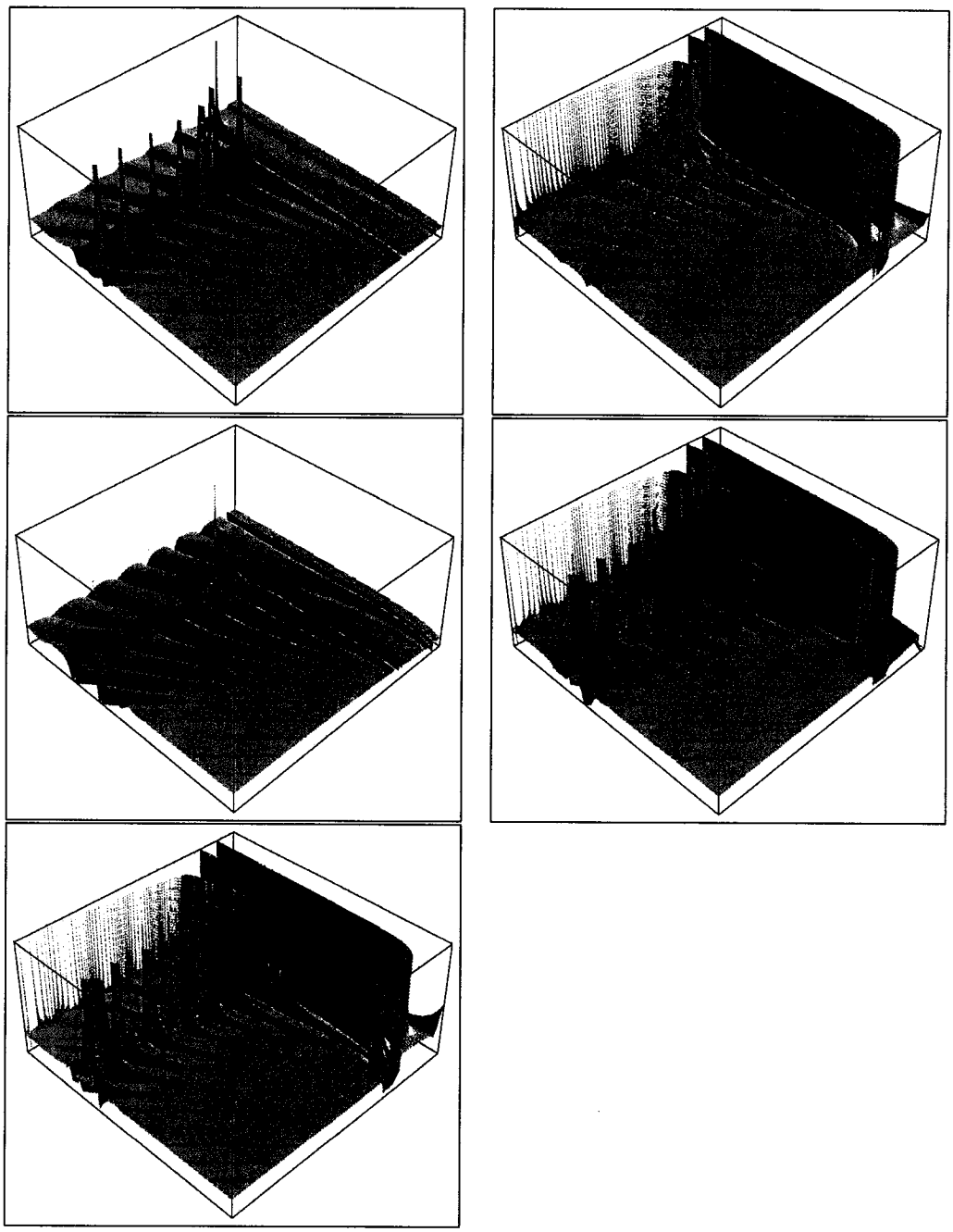

Figure 3.6: Left top to right bottom: State-dependent potentials $\boldsymbol{G_s}$, $\boldsymbol{G_e}$, $\boldsymbol{Q_s}$, $\boldsymbol{Q_e}$, and $\boldsymbol{G_{es}}$ for one-dimensional particle and barrier system. Energy of incident wave packet is twice barrier height.

3.5.2 Environment of the Potential Well

The figures for the potential well (figs. 3.7, 3.8, and 3.9) share similar properties as those of the potential barrier. The same alternating spikes and sails are displayed in regions front of the well. Similar effects are seen as the energy of the incident wave packet is increased. However, in the well region, the results are radically different. There instead, the well regions are characterized by several thin walls with increasing height as time progresses. The same behaviour is seen for all SDPs. As the energy of the incident wave packet increases, the number of walls decreases. Also, wall heights increase less substantially than do the lower energy packets. Finally, it is observed that the thickness of the walls increase for more energetic packets. These observations reflect how for more energetic packets, the well is less effective than for less energetic packets.

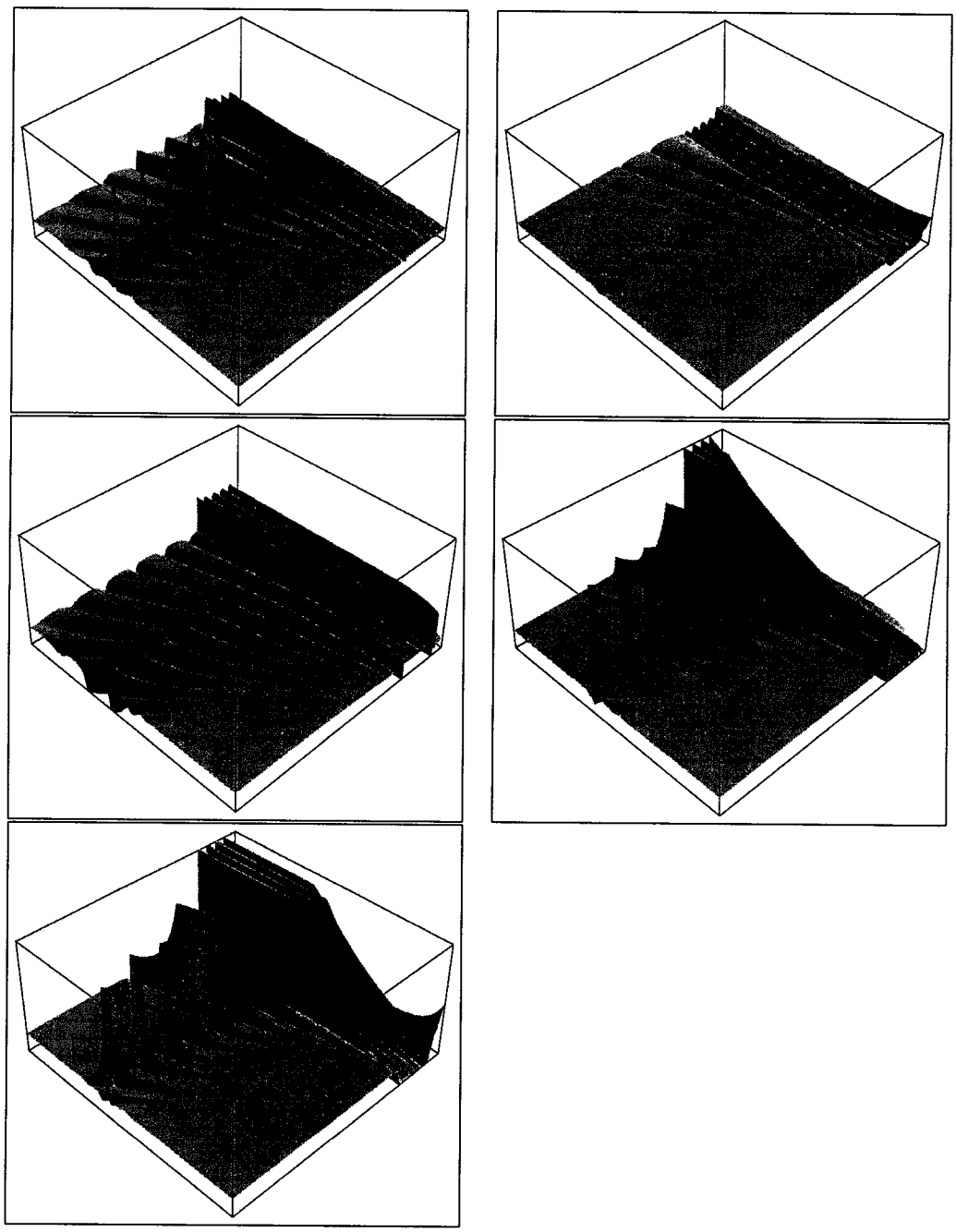

Figure 3.7: Left top to right bottom: State-dependent potentials $\boldsymbol{G_s}$, $\boldsymbol{G_e}$, $\boldsymbol{Q_s}$, $\boldsymbol{Q_e}$, and $\boldsymbol{G_{es}}$ for one-dimensional particle and well system. Energy of incident wave packet is half well depth.

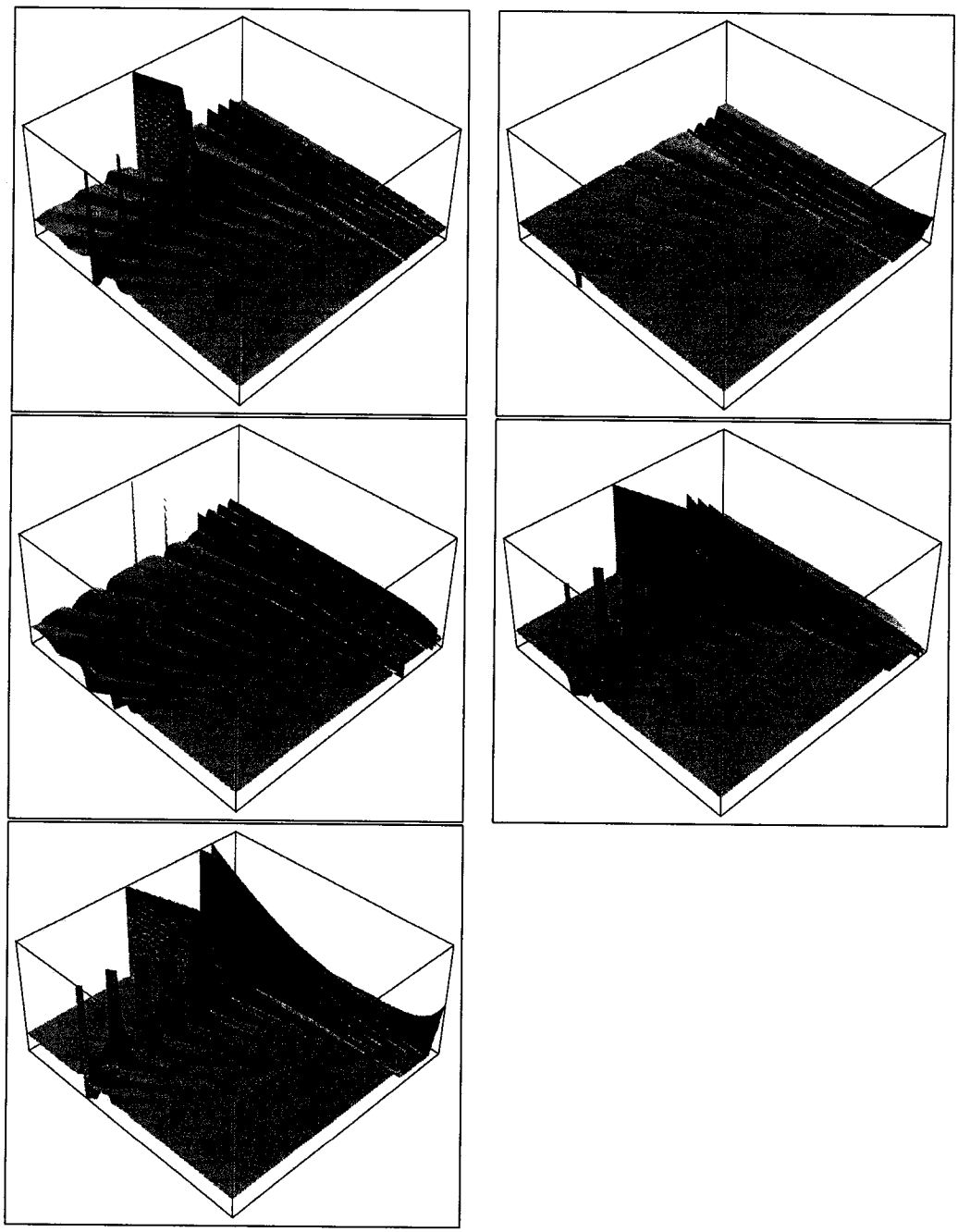

Figure 3.8: Left top to right bottom: State-dependent potentials $\boldsymbol{G_s}$, $\boldsymbol{G_e}$, $\boldsymbol{Q_s}$, $\boldsymbol{Q_e}$, and $\boldsymbol{G_{es}}$ for one-dimensional particle and well system. Energy of incident wave packet is equal to well depth.

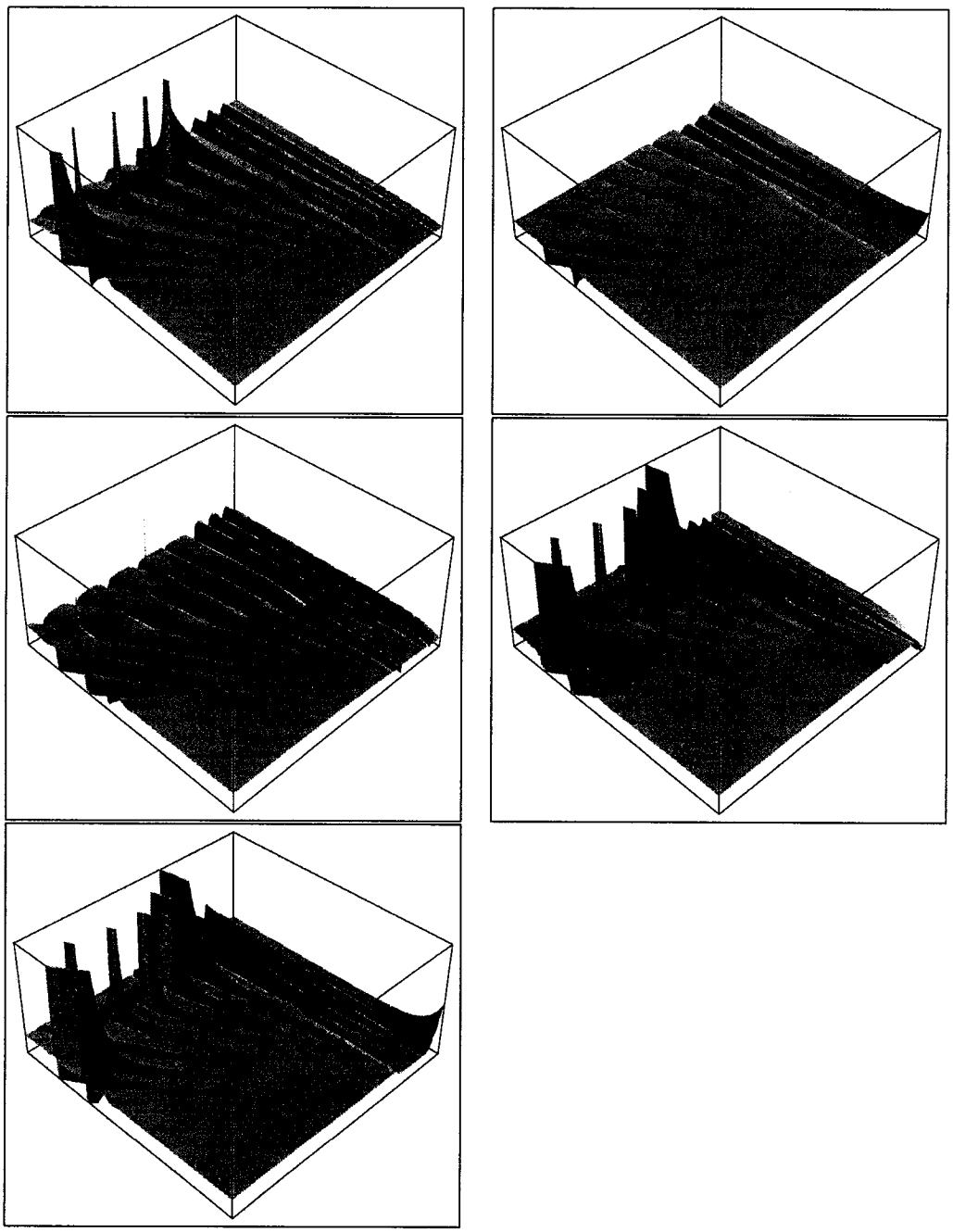

Figure 3.9: Left top to right bottom: State-dependent potentials $\boldsymbol{G_s}$, $\boldsymbol{G_e}$, $\boldsymbol{Q_s}$,$\boldsymbol{Q_e}$, and $\boldsymbol{G_{es}}$ for one-dimensional particle and well system. Energy of incident wave packet is twice well depth.

3.6 Results of the Two-Dimensional Interference

Figures 3.10 through 3.13 show SDPs $\boldsymbol{G}_e, \boldsymbol{G}_s, Q_e, Q_s$ and Q_{es} for a system of a gaussian wave packet incident on a double-slit wall. The graphs show areas of a small region behind the slit, near the scintillator screen. The probability amplitude R_s shows the expected interference pattern at the screen. The graphs are all symmetrical with respect to the center line from the back where the packet leaves, to the front at the scintillator location.

For a finite magnetic flux (fig. 3.11, $\alpha = 0.25$), the characteristic Aharonov-Bohm shift is evident. The vector potential has shifted the pattern to the right of the scintillator screen. The environment wave function, which represents the potential, is not only shifted, but also diminished to the right. The SDPs $\boldsymbol{G}_e$ and Q_e are polarized to the right, accompanied by an increase in potential strength to the left of the screen.

As the magnetic flux is further increased to $\alpha = 0.75$ (fig. 3.12), the same shift is evident, but in the reverse direction - to the left of the screen. The SDPs $\boldsymbol{G}_e$ and Q_e are this time polarized towards the left, accompanied by an increase in potential strength at the right of the screen. When the magnetic flux is brought to an integral value $\alpha = 1$ (fig. 3.13), the AB-shift disappears and the SDPs behave accordingly.

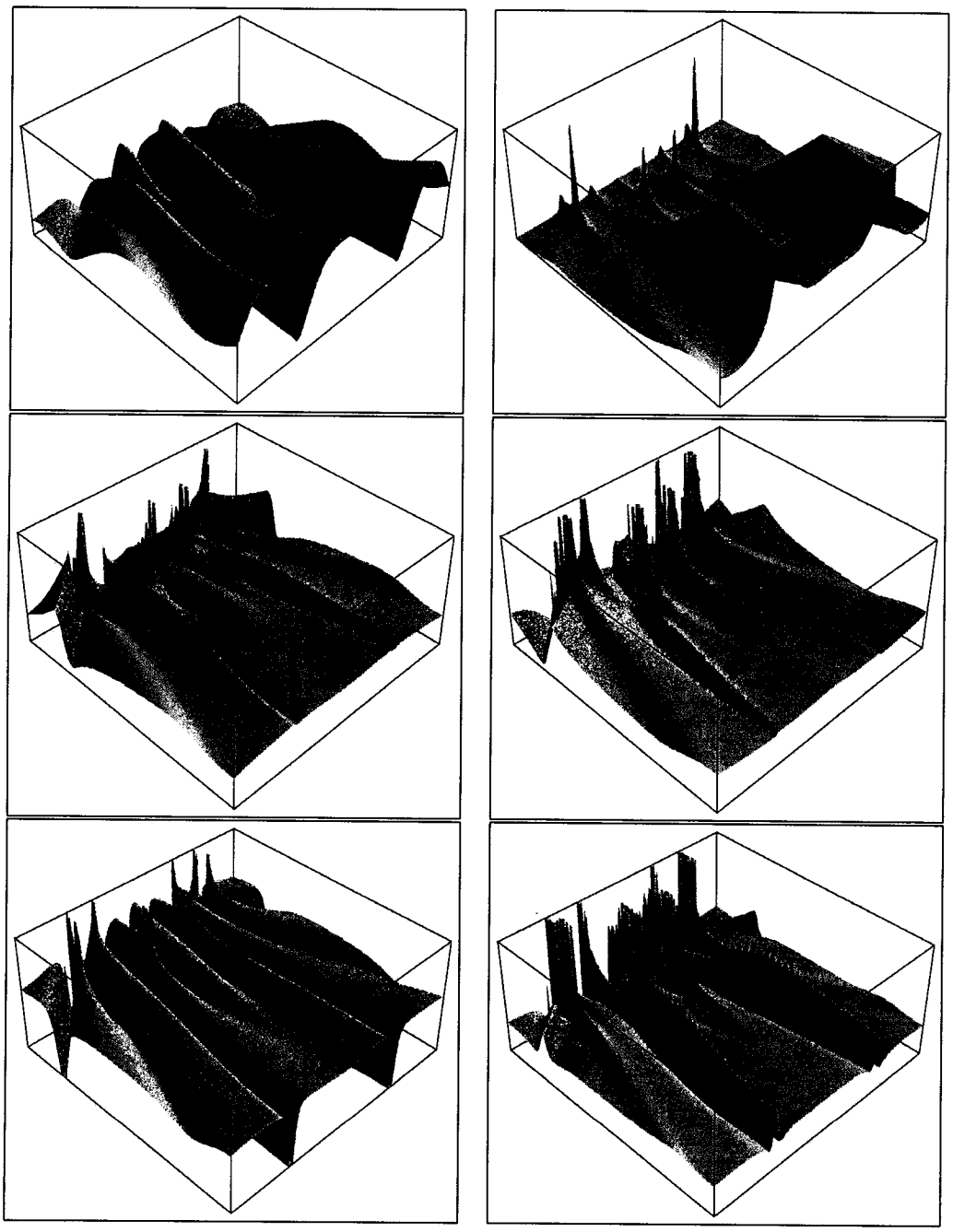

Figure 3.10: Left top to right bottom: Wave amplitudes R_s, R_e, state-dependent potentials $\boldsymbol{G}_s$, $\boldsymbol{G}_e$, $\boldsymbol{Q}_s$, and $\boldsymbol{Q}_e$, for two-dimensional particle and slit system at $t = 1.4$.

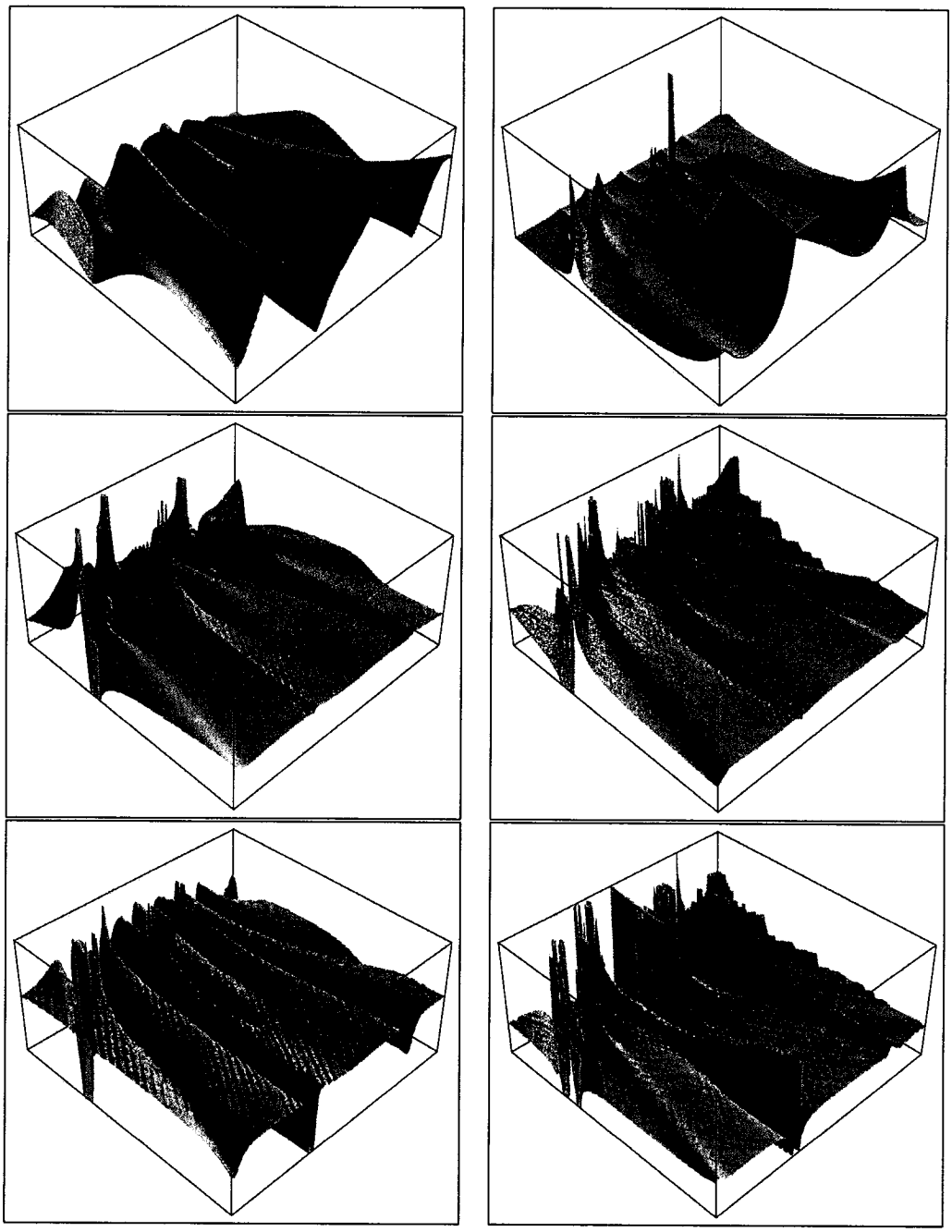

Figure 3.11: Left top to right bottom: Wave amplitudes R_s, R_e, state-dependent potentials $\boldsymbol{G}_s$, $\boldsymbol{G}_e$, $\boldsymbol{Q}_s$, and $\boldsymbol{Q}_e$ for two-dimensional Aharonov-Bohm setup at $t = 1.4$. Magnetic flux $\alpha = \frac{1}{4}$.

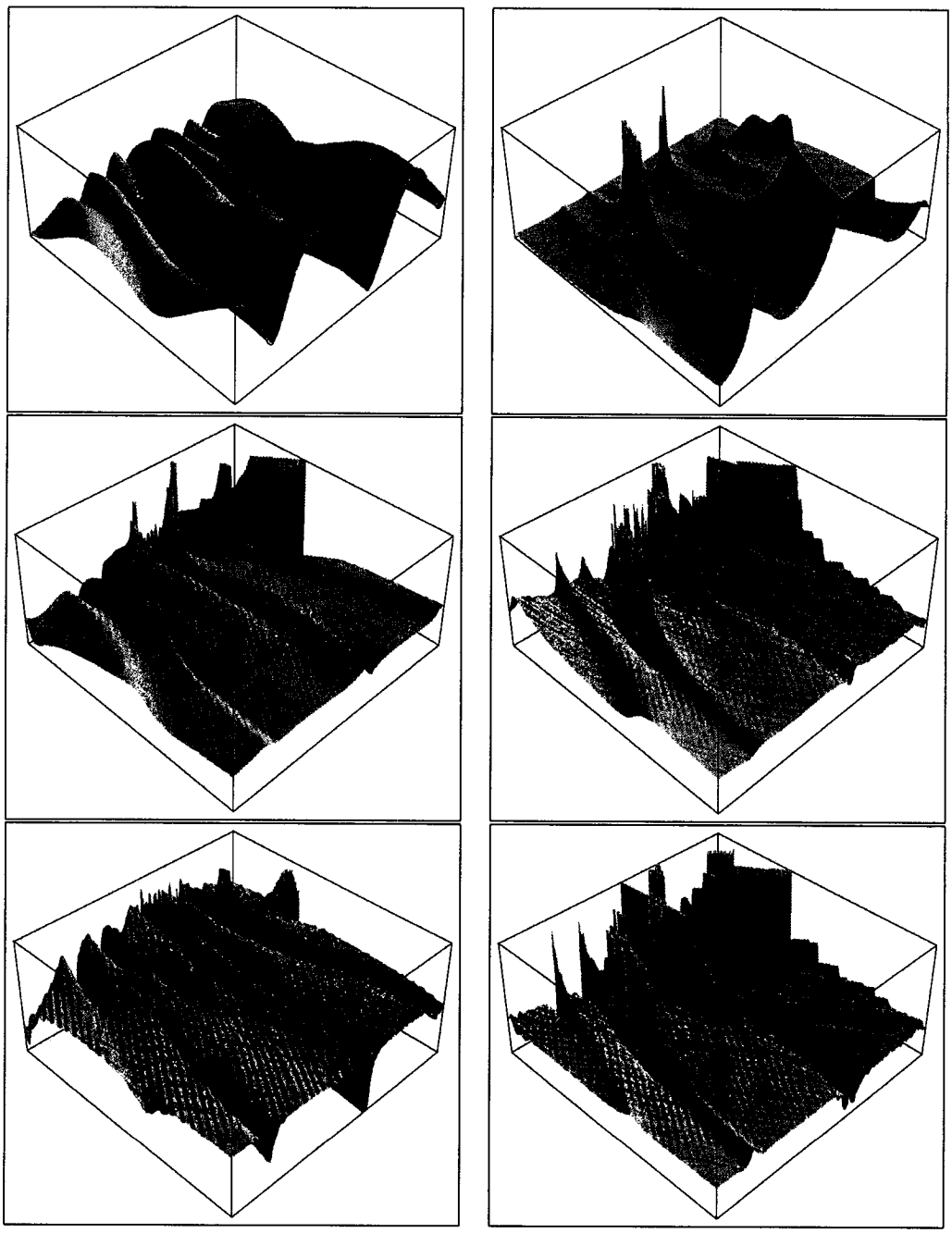

Figure 3.12: Left top to right bottom: Wave amplitudes R_s, R_e, state-dependent potentials $\boldsymbol{G}_s$, $\boldsymbol{G}_e$, $\boldsymbol{Q}_s$, and $\boldsymbol{Q}_e$ for two-dimensional Aharonov-Bohm setup at $t = 1.4$. Magnetic flux $\alpha = \frac{3}{4}$.

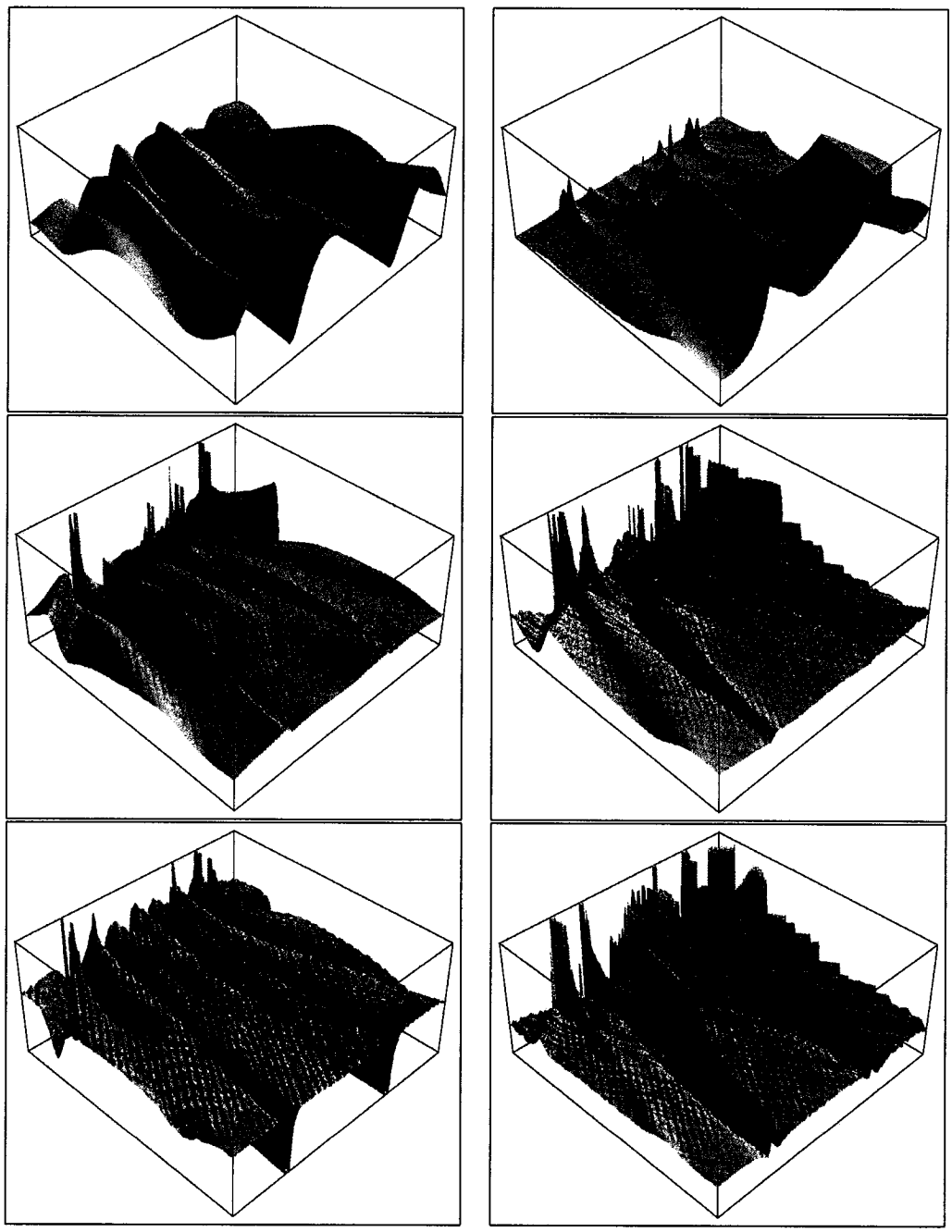

Figure 3.13: Left top to right bottom: Wave amplitudes R_s, R_e, state-dependent potentials $\boldsymbol{G}_s$, $\boldsymbol{G}_e$, $\boldsymbol{Q}_s$, and $\boldsymbol{Q}_e$ for two-dimensional Aharonov-Bohm setup at $t = 1.4$. Magnetic flux $\alpha = 1$.

3.7 Results of the Two-Dimensional Dirac Environment

The results of the Dirac computations, fig. 3.14, displays the circularly dispersing two components of a two-dimensional Dirac spinor. As the spinor expands towards the region where the shielded magnetic coil is placed, the spinor packet displays high irregularities. The environment wave amplitude R_e and the SDVP $\boldsymbol{G}_e$, reflect these fluctuations in the vicinity of the shielded coil. The irregularities dissipate further away from the center of the vector potential.

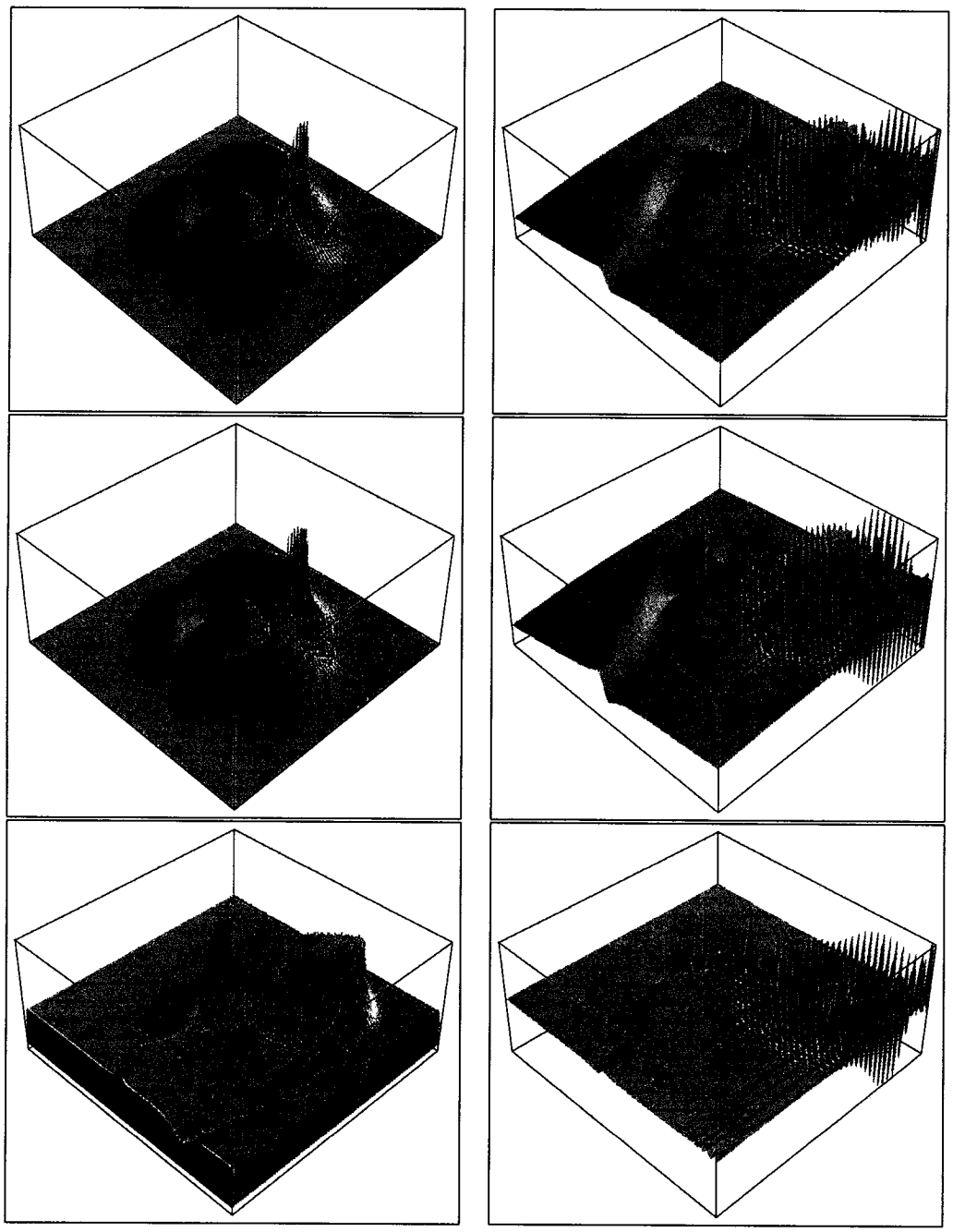

Figure 3.14: Left top to top bottom: Dirac wave amplitudes R_{s1}, R_{s2}, the environment amplitude R_e. Right top to right bottom: Dirac state-dependent potentials G_{s1}, G_{s2} and the state-dependent environment potential G_e.

3.8 Discussion of Results

The graphs displayed in this section underline two dominating factors in the relationship between the single particle and the environment. Since the initial conditions for the CSE used in most of the calculations involves the use of a gaussian packet equal to the initial condition for the single particle system, the initial environment is just a constant value. As time progresses, the environment amplitude takes on a more familiar oscillating structure. A trial of different initial conditions such as those employed in D'Amico[36], reveals that the evolution of ψ_e quickly progresses towards similar graphical forms as those studied here in the text. It must therefore be concluded that the form of ψ_e and the corresponding derived SDPs $\boldsymbol{G}_e$ and Q_e, are dominated by the single particle wave function ψ_s. More specifically, from a quick scan of the graphs, it is obvious that the dominating component of the figures is the state-dependent vector potential $\boldsymbol{G}_s$. All other SDPs take on some variation of this potential. However, this is to be expected since ψ_s is determined by the classical potentials, which are pre-defined functions in the calculations. The environment has little choice but to take on a form which reflects this initial selection - a form which is stored in the dynamics of ψ_s. In a more general case - one where SDR does not take place - the environment will be less constrained and only variably affected by ψ_s.

To conclude, it is remembered that initial conditions chosen are based on a trial and refinement process. Whether the environment graphs appear visually realistic or not, they represent only one of an infinite set of environments, some of which may present more visually stunning and intuitive displays.

Chapter 4

Interpretive Analysis

Symmetry principles are at the heart of modern physics. It is the reason why Einstein's theory of Relativity quickly became popular over the competing equally valid ether theory of Lorenz[37]. Today, a specific symmetry principle - gauge symmetry - has prompted a newly kindled and energetic debate. Like the numerous debates on the interpretation of quantum mechanics of the early and mid years of the 19th century[2], the reality and interpretation of gauge potentials proves to be the next topic from which a crop of new ideas will emerge. The gauge debate can be summarized by posing two questions: one, are gauge potentials real or simply express some freedom to choose internal space coordinates of a wave function; two, if they are real, how are we to understand the lack of correspondence between a particular potential A_μ and a physical situation? Richard Healey[12] writes,

> Different interference patterns corresponded to different 4-vector fields A_μ...Interference phenomena provide evidence that there is more to electromagnetism than is represented by the field $F_{\mu\nu}$, but there is nothing in these phenomena or in the theory that accounts for them to single out any particular A_μ as faithfully representing this additional physical

structure...

In this chapter, some observations will be made towards interpreting the need and usefulness of the environment wave function, the state-dependent classical potentials, and the CSE. Some issues to be addressed include the question of whether ψ_e violates current experimental data; a resolution to the BQM complication; the new version of the BQM classical limit; a suggestion on how ψ_e can be used to explain how A_μ may be made to faithfully represent additional physical structure; and the question of quantum coexistence and the ether concept. The chapter will conclude with a proposal on how Bohm's suggestion of extending quantum theory may be attained.

4.1 Experimental outcome and the environment wave function ψ_e

Throughout the derivations of chapter 2, special attention has been paid to ensure that the closed Schrödinger's equation reproduces the same results as SQM, and BQM. But upon further examination it is seen that the wave functions of SQM and BQM (ψ_s) differs from the total wave function of the CSE which is $\psi_s\psi_e$. At first sight, it appears that the addition of the extra environment wave function describes a different physical situation which can easily be tested experimentally. For example, ψ_s of SQM and BQM might describe a scattered wave packet, while $\psi_s\psi_e$ describes a free wave packet. Obviously, these describe two very different physical situations. There are two possibilities in resolving this problem. The first way deals strictly with SQM, the second way appeals to BQM.

One way to resolve the problem is to assume that ψ_e is not detectable in present-day experimental setups. The product structure of the CSE ensures that when ψ_s is very large, ψ_e will be very small. The two packets will not overlap on the average. But this is not a satisfactory explanation. What specifically about ψ_e is it that makes it undetectable? Why does ψ_s dominate the experimental outcomes?

Another way to resolve the question of experimental outcome is to argue that SQM does not allow for a full description of quantum mechanics, and appeal to BQM for the solution. To see if the use of the CSE represents a different physical situation, the trajectory of the single-particle $q_s(t)$ needs to be looked at. This is relevant because Bohm's theory explains interference patterns as the statistical accumulation of particle dots on a screen. Each particle leaves the electron gun with a slightly different initial condition than the other electrons. The density of electrons on the screen will produce a pattern equal to the probability density $R_s = \psi_s^* \psi_s$. If it can be shown that $q_s(t)$ of the system (ψ_s) equals $q_s(t)$ for the system (ψ_s, ψ_e) then the interference pattern will be identical for both systems and the experimental outcome of the two systems will be indistinguishable from each other.

To see that this is the case, the two particle equations of motion for system (ψ_s) and system (ψ_s, ψ_e) need to be compared. For (ψ_s) the equation reads,

$$m\frac{d^2 q_s}{dt} = -\nabla(V) - \nabla(Q_s). \tag{4.1.1}$$

The equation for (ψ_s, ψ_e) is,

$$m\frac{d^2 q_s}{dt} = -\nabla(Q_{es}) - \nabla(Q_e) - \nabla(Qs). \tag{4.1.2}$$

But the combined environment and interaction quantum potential is equal to the scalar potential $(\nabla(V_\psi) = \nabla(Q_{es}) + \nabla(Q_e))$. The trajectory of the particle s will be

equal in both descriptions (ψ_s) and (ψ_s, ψ_e). This also holds true if a vector potential is present. The resulting interference pattern will appear identical and experimental outcomes will not differ. The trajectory concept of BQM has come to the defense of the closed Schrödinger's equation.

4.2 Resolution of the BQM Complication

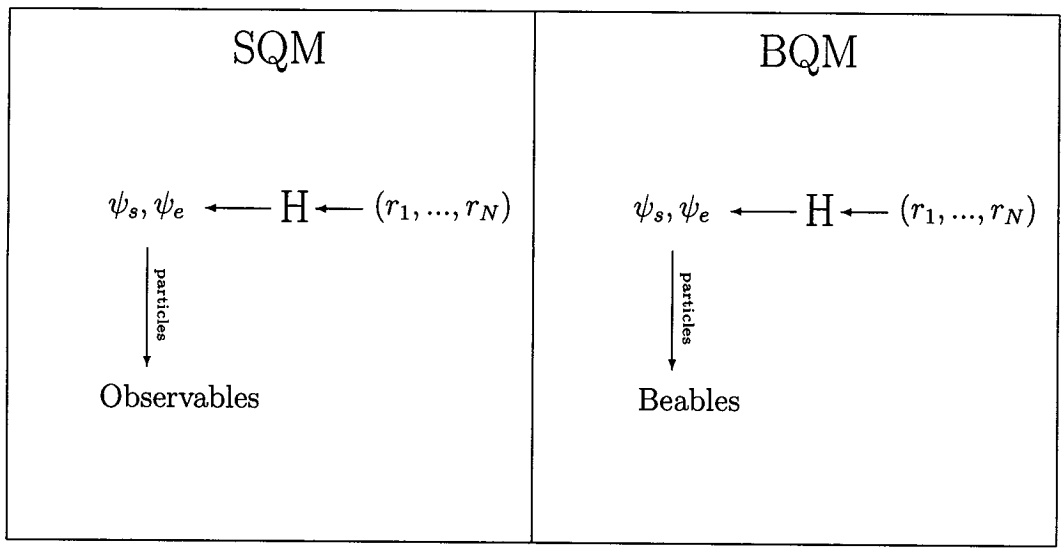

Figure 4.1: The relationship among objects of the formalism in non-relativistic SQM and BQM using state-dependent classical potentials

It was pointed out in chapter 1, that the use of the predefined functions $V, \boldsymbol{A}$ to represent classical potentials in quantum mechanics, created a rather distinct role for $V(x)$ from the quantum potential. It was mentioned that the dual role of $V(x)$ was a complication in BQM. The SDCP however, does not suffer from the same apparent complication. Since $V(x)$ is replaced by $Q_v = Q_e + Q_{es}$, and since Q_v is a part of the total quantum potential, it has been placed on equal footing with the Q_ψ (Q_s). The

new fig. 4.1 representing the relationship among objects of BQM and SQM shows not only how the complication in BQM is resolved, but also shows that NRQM and QFT share the same formalism with the exception of co-dependency (of particle and potential field) at the level of observables or beables.

A result of the changes introduced by the environment wave function is that the classical limit of BQM has changed from $Q_\psi = Q_s \to 0$ to the new condition $(V_\psi, \boldsymbol{A}_\psi) \xrightarrow{\text{SDR}} (V, \boldsymbol{A})$, where the set $(V_\psi, \boldsymbol{A}_\psi)$ contains the state-dependent potentials. What this shows is that the classical limit is approached not as the quantum potential vanishes, but rather as the total force becomes independent, or effectively independent of the quantum state. This simple result should seem obvious, since the passage to the classical world cannot be viewed as the elimination of quantum effects alone, but rather as the introduction of classical effects.

4.3 Gauge Potentials and the AB-Effect

The paper of Eynck, Lyre, and von Rummell[19] summarizes the AB-effect by highlighting three rival interpretations termed the A, B, and C-interpretation. In the A-interpretation, the gauge potential $\boldsymbol{A}_\mu$ is taken as the basic entity. In the B-interpretation, it is the magnetic field which is essential. And, in the C-interpretation, the closed loop or holonomy integral (the Dirac phase factor)

$$\exp\left(i \oint_C \boldsymbol{A} \cdot dx\right)$$

is taken as the basic physical object. Each interpretation offers some advantages and disadvantages. For example, the A and C -interpretation allow for local actions while the B-interpretation describes nonlocal behaviours[19]. The literature[12] indicates

a preference for the C-interpretation but not without some resistance. Healey[12] mentions one such objection,

> The objection is that holonomy properties cannot be nonseparable, since it is metaphysically unacceptable to suppose that space-time regions have global properties not determined by local properties at their constituent points. No scientific theory may postulate such "free-floating" global properties. If a gauge theory is to remain within the realm of science, rather than postulating miracles, it must provide some underlying local structure–novel gauge properties or objects–to provide the necessary metaphysical support for holonomy properties.

The response to this question, cited by Healey is,

> It seems to me that there is remarkably little to this metaphysical objection. It is reminiscent of Cartesian objections to Newtonian science. The response is straightforward: Nonseparable holonomy properties are no more "occult" or unscientific than Newtonian forces. In both cases, empirical success of the theory that postulates the allegedly problematic structures justifies belief in them, independently of whether or not further theorizing will turn out to provide a more familiar grounding for these structures.
>
> Epistemological objections may seem more promising. The idea here is that if the gauge theory is true, then there are striking facts that can satisfactorily be explained only by postulation of local theoretical structure that determines holonomy properties. Inference to the best explanation

therefore warrants that such structure indeed underlies these global properties.

The debate therefore is not leveled at the worth, beauty, or simplicity of the holonomy interpretation but rather that no explanation is given to the underlying physical structure resulting in holonomy properties. This is exactly the objection mentioned by Healey to the A-interpretation. It is concluded therefore that much of the gauge debate is the lack of clarity in the underlying structure, although the preferred holonomy does solve the problem of the surplus structure of the gauge potential. How then is gauge to be understood in the CSE interpretation?

The physical object of the CSE is the environment wave function ψ_e. It is related to the gauge potential by the equation,

$$\boldsymbol{G}_e = i\hbar \frac{\nabla \psi_e}{\psi_e}.$$

The functional dependence of ψ_e on $\boldsymbol{G}_e$ can be obtained by an integration yielding,

$$\psi_e = \frac{i}{\hbar} \oint_c G_{e\mu} dx^{\mu}.$$

This integral exists in loop-space and is just the holonomy mentioned above. The environment wave function can therefore be viewed as yet another interpretation of gauge, say the E-interpretation. It combines all three interpretations, removes the surplus structure arising with the gauge potential, and also provides an underlying physical structure by introducing the environment. Unfortunately, like all quantum potentials, it will necessarily describe nonlocal behaviours. The freedom to choose a gauge potential is hence related to the freedom to choose an environment which leaves ψ_s unchanged. As mentioned throughout this thesis, an infinity of different environments may lead to the same results.

4.4 Quantum Coexistence, the Ether, and Forces

State-dependent classical potentials and especially the CSE may be seen as a step backward towards the ether concept of the 1900's. When analyzing a free particle in SQM, the picture is that of a free wave packet evolving in time. The space around it is imagined to be empty. In BQM instead, the picture is that of a particle traveling under the influence of a quantum potential derived from the free wave packet. Although the particle is free classically, it is not free quantum mechanically - no classical potential is present but a quantum potential is nonetheless finite throughout space. The CSE takes this a step further. The total wave $\psi_s\psi_e$ is never completely free of any potential - classical or quantum. If the free Schrödinger's equation of SQM is compared with the CSE, it is observed that there are several ways for both systems to be equal. The environment wave function may simply be set to a constant C, throughout space for all time. In this case $\psi_s \rightarrow C\psi_s$ ($C = 1$ from normalization), and both waves evolve the same way through space and time. However, $\psi_e = C$ is only one of many possible choices acceptable by the CSE which creates an equivalent free system as in SQM. To see this, the constraint on the environment must be obtained by expanding eq. (2.3.1) as a free part and an interacting part,

$$i\hbar\frac{\partial\psi_s}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\psi_s = -\left(i\hbar\frac{\partial_t\psi_e}{\psi_e} + \frac{\hbar^2}{2m}\frac{\nabla^2\psi_e}{\psi_e} + \frac{\hbar^2}{m}\frac{\nabla\psi_e\nabla^2\psi_s}{\psi_e\psi_s}\right)\psi_s. \tag{4.4.1}$$

This equation is equal to the free Schrödinger's equation if the right-hand part vanishes, or

$$i\hbar\frac{\partial_t\psi_e}{\psi_e} + \frac{\hbar^2}{2m}\frac{\nabla^2\psi_e}{\psi_e} + \frac{\hbar^2}{m}\frac{\nabla\psi_e\nabla^2\psi_s}{\psi_e\psi_s} = 0. \tag{4.4.2}$$

The environment must therefore obey a Schrödinger-like equation with the environment coupled wave function dependent on the wave function of the single particle.

This complicated coupling will only yield a free-Schrödinger particle if the environment responds appropriately according to eq. (4.4.2).

Viewed this way, the environment resembles the ether explanation provided by Lorenz to explain the null results of the Michelson-Morley experiment[37]. Such an approach is criticized for two reasons, first because it is seen as a 'conspiracy' theory and second, because it has likewise increased the complexity of the description of nature. By conspiracy is meant that nature works in such a way that a compensating effect exists which is undetectable but which can be explained by simpler means. In the case of Lorenz's ether theory, the ether causes a nonmeasurable contraction of length of the arms in the Michelson-Morley experiment. But since the contraction cannot be measured, the ether cannot be discovered. Nature is therefore seen to conspire and to present us with results which are better explained by simpler terms. The special relativity theory provided another explanation but without the ether and with an additional simplifying benefit of symmetry. In Zahar's philosphical appraisal of Einsteins's contribution versus that of Lorenz, he writes[37],

> The ether programme did not collapse but was superseded by a programme of greater heuristic power.

It is therefore worth asking whether the CSE falls under the category of a conspiracy theory, and whether it has violated the Occam's razor by including yet another hidden variable (or hidden wave ψ_e) to the already hidden variables of BQM.

To address the first part of the question - conspiracy or not - the Feynman path integral will be recalled. As seen from chapter 2, the environment wave function originated from the Feynman path integral. The path integral was chosen because it possessed the special property which Feynman described as the main advantage of the

path integral approach. To recap, it will be remembered that a system q interacting with a second system Q can be written as a path integral without specific reference to Q - the effects of Q are summarized in an environment functional T_e. The path integral is,

$$K(b,a) = \int_{q_i}^{q_f} \left[\exp\left(\frac{i}{\hbar}S_s[q]\right)\right] T_e[q(t)]Dq(t). \tag{4.4.3}$$

This allows for the possibility that several distinct systems, say $Q_1, Q_2, ..., Q_n$ all have the same environment functional T_e. For example, if T_e can be expressed as

$$T_e[q(t)] = \exp\left(\frac{i}{\hbar}\int q(t)V(t)\right),$$

then the problem is equal to the solution of Schrödinger's equation for a scalar potential $V(q,t)$. But V may originate from an infinite set of possible environment functionals including the simplest possible case, the Langrangian of a scalar potential. This presents the same situation used to explain gauge symmetry and the AB-effect. Hence, if the environment wave function admits a conspiracy theory, it must be seen as originating from the Feynman path integral.

The second part of the question can be argued in different ways and is victim to personal taste. On the one hand, a new quantity is introduced ψ_e. On the other hand several quantities are removed, namely the classical potentials V and $\boldsymbol{A}$. Whether this constitutes agreement with or violation of Occam's razor is not clear. Either way, as mentioned in the previous answer, the concept of an environment wave function, or environment amplitude is already admitted by the Feynman path integral. What is clear however, is that the CSE replaces the classical potentials which appear asymmetrically in Schrödinger's equation with a product wave function $\psi_s\psi_e$ which appears symmetrically. The CSE therefore introduces further symmetries not admitted by SQM and Schrödinger's equation.

So then, how are forces to be interpreted according to the CSE. As seen from fig. 3.3, the usual picture of ψ_s bouncing off a potential wall is changed to a picture of the coexistence of two waves. The law of coexistence between wave components ψ_s and ψ_e is responsible for both barrier penetration and splitting of the particle self-wave packet. As mentioned in D'Amico[36], "this is a radically different picture in which ψ_e produces a disturbance, such as would occur in the presence of a wind or ether; it does not create a barrier".

Implications on forces, are that they are not the interaction of fields so much as they are the coexistence of components of the quantum wave function - an internal space. The usual way of dealing with forces is to include interactions terms obeying the required symmetries into the Langrangian for the combined system. The interaction is assumed beforehand. The CSE instead assumes a general form for the system; the forces come into play as constraints or complex boundary conditions which produce the same behaviour as would an assumed predefined form for the interaction. The constraint is effectively caused by the form of the environment which can take on infinite values for the same force. All forces are therefore fictitious and mere appearances from the coexistence of separate wave functions of a product wave function.

The difference between the two viewpoints is that in the former, a source is assumed such as an electromagnetic field. However, in the latter, the wave function is primary, whereas the presumed source field is an appearance or a specific aspect of the amplitudes. The electromagnetic field for example, is secondary - the wave function is primary. This resembles the geometric nature of general relativity. A particle appears to travel a force-constraining path provided by the curvature derived

from the mass density structure of the system. The gravitational force is an illusion created by the curved geometric intervals. The notion of curved space is primary, while the force is secondary.

4.5 Extension of SQM and BQM

It has been suggested by David Bohm[5] that a possible extension to the current quantum theory can come in the form of a nonlinear addition to the Schrödinger's equation. The nonlinearity is introduced to serve the same purpose as in the Ghirardi, Rimini, Weber[38] approach. For a large many-body system, the overall wave function would tend to collapse towards the particle positions. It is therefore worth asking whether the CSE admits a similar type of extension. The answer is that the CSE already has in it the beginnings of Bohm's suggested extension. It is noted that the SDR required to regain the results of SQM and BQM need not occur. In this case, the CSE is a function of two unknowns ψ_s and ψ_e. The condition of SDR provides the additional information necessary to make the CSE a well-posed problem. In situations where the potentials are non-classical and non-relativistic, neither QFT nor SDR is necessary. An additional equation would be needed to make the CSE a well-posed problem. What would the second equation look like? From the point of view of SQM, there is no indication of how to tackle such a program. From BQM however, the issue sounds more promising since what is missing is information on how the environment and particle interact. Clearly this depends on the positions of the particles within the environment system. When a classical potential is introduced to represent the environment, the particle paths are abstracted into the form of a classical potential $V(q)$. The second equation necessary to make the CSE solvable should therefore

contain particle paths. In this way, the suggestion of Bohm may be realized.

Chapter 5

Conclusion

The current thesis has proposed that the classical potentials of non-relativistic quantum mechanics be replaced by state-dependent quantum potentials in non-relativistic quantum theory. Justification for the proposal has come by appeal to observations derived from David Bohm's ontological interpretation of quantum mechanics, quantum field theory, and the Feynman path integral method. Through use of the notion of a quantum potential and by taking literally concepts such as the environment and influence functional of Feynman's path integral method, a closed Schrödinger's equation was derived.

The method has served to highlight several imprecisions with non-relativistic quantum theory - both for SQM and BQM. The picture of a free system - as one in which only a single system q is present - has shifted to one in which two systems coexist in an apparently disconnected and independent fashion. The problematic dual character ascribed to the classical potential of Bohm's ontological theory has been remedied by casting the potential in a form which has placed it on an equal footing with the quantum potential. Finally, the surplus structure of gauge potentials has been explained as a mapping of a specific class of vector potentials to a set of

environments which reproduce the same observable experimental outcomes.

The method however, has its limitations. The transformation applied to the Feynman path integral has removed magnetic effects. This does not pose a problem since the goal of the thesis has been to demonstrate the value of state-dependent potentials - a program which can be sufficiently demonstrated with only a non-vanishing vector potential. But a more rigorous approach could be developed by method I of sect. 1.5.1. However, the lack of progress in an ontological theory of quantum electrodynamics makes that program a limited one also.

At the heart of state-dependence has been the environment wave function ψ_e. In some ways the introduction of ψ_e is an inescapable return to ether concept of the 19th century. But on a deeper level, it lays testimony to Bohm's philosophy of order and wholeness[39] - that an apparent disconnected order ψ_s is never separate from an implicate order ψ_e from which it unfolds.

***

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Appendix A

Appendix - Mathematica Notebooks

A.1 One-Dimensional Scattering

```
(*/-------------------------------------------------\*)
(*| Portions based on Manfred Liebmann[35] and      |*)
(*|                   Berndt Thaller[34]            |*)
(*/-------------------------------------------------\*)

 << QuantumMechanics`QuantumKernel`;

(*/-------------------------------------------------\*)
(*| Initialize values                               |*)
(*\-------------------------------------------------/*)

qmInitialize[qmSystem_,qmStrength_] := Module[{},

    Off[General::"spell1"];
    Progress["Initializing"];

    reps = 8;
    T = 0;
    totreps = 0;
    borderleft = -35;
    borderright = 35;
    dx = 0.001;
    dt = 0.001;
    p0 = 6.;
    x0 = -7.;
    k0 = p0/2;
    qmPotential = qmSystem;
```

```
    qmTitle = {"1D_Barrier", "1D_Well","1D_Barrier_Closed"};
    qmEnergy = qmStrength;
    qmDataDirectory =
        StringJoin["T:\Data\\",
            qmTitle[[qmPotential]], "-",
            ToString[qmEnergy]];
    Off[CreateDirectory::"ioerr"];
    CreateDirectory[qmDataDirectory];
    SetDirectory[qmDataDirectory];

];

(*/-------------------------------------------------\*)
(*| Display progress                                |*)
(*\-------------------------------------------------/*)

Progress[str_]:=Module[{pstr=str},

    sTime=SessionTime[];
    Hours = Quotient[ sTime,3600];
    rSeconds =Mod[sTime,3600];
    Minutes = Quotient[rSeconds,60];
    Seconds = Mod[rSeconds,60];

    Print[pstr," ","Time=",Hours,":",Minutes,":",
        Seconds," Memory=",MemoryInUse[]];

];

(*/-------------------------------------------------\*)
(*| Define Potentials                               |*)
(*\-------------------------------------------------/*)

qmPotential[] := Module[{},

    Off[General::"spell1"];
    Off[NDSolve::"ndsz"];

    Progress["Defining Potential"];

    Vm = { 1, -1}; En  = {1/2, 1/4, 1/8};
    V0 =  En[[qmEnergy]] * p0^2 * Vm[[qmPotential]];
    V[x_] := If[Abs[x] > 1, 0, V0];
    H[x_] := Exp[I*k0*x];
    TblV = Table[V[x], {x, borderleft, borderright, dx}];
    QfnV = QNewFunction[Re[TblV], Im[TblV]];

];
```

```
(*/-------------------------------------------------\*)
(*| Define initial wave packet                     |*)
(*\-------------------------------------------------/*)

qmWavePacket[] := Module[{},

    Progress["Defining Wave Packet"];

    G[x_] := (1/Pi)^(1/4) Exp[-(x - x0)^2/2];
    G[x_] := (1/Pi)^(1/4) Exp[-(x - x0)^2/2];
    TblPsiS = Table[Module[{x = x1 - x0}, H[x]*G[x]],
        {x1, borderleft,borderright, dx}];
    QfnPsiS = QNewFunction[Re[TblPsiS], Im[TblPsiS]];
    Hs = QSchroedinger1D[QfnV, 1, dx];

];

(*/-------------------------------------------------\*)
(*| Store results to disk                          |*)
(*\-------------------------------------------------/*)

StoreData[RRe_,RRs_,GGe_,GGs_,GGe_,QQs_,QQe_,QQes_,T_]
    := Module[{},

    Progress["Storing Data"];"

    qmName = ToString[100000 +10000 * T];

    Export[StringJoin["Rs", qmName,
        ".lst"],TblRRs,"Table"];

    TblRRe = Table[RRe[x], {x, -20.0, 2.0, .1}];
    Export[StringJoin["Re", qmName,
        ".lst"], TblRRe,"Table"];

    TblGGs = Table[Evaluate[GGs[x]], {x, -10, 1.5, .0025}];
    Export[StringJoin["Gs", qmName,
        .lst "], TblGGs,"Table"];

    TblGGe = Table[GGe, {x, -10, 1.5, .0025}];
    Export[StringJoin["Ge", qmName,
        ".lst"], TblGGe, "Table"];

    TblQQs = Table[QQs, {x, -10., 1.5, .0025}];
    Export[StringJoin["Qs", qmName,
        ".lst"],TblQQs, "Table"];
```

```
    TblQQe = Table[QQe, {x, -10., 1.5, .0025}];
    Export[StringJoin["Qe", qmName,
        ".lst"], TblQQe,"Table"];

    TblQQes = Table[QQes, {x, -10., 1.5, .0025}];
    Export[StringJoin["Qes", qmName,
        ".lst"], TblQQes,"Table"];

    TblQQt = Table[QQt, {x, -10., 1.5, .0025}];
    Export[StringJoin["Qt", qmName,
        ".lst"], TblQQt,"Table"];

];

(*/-------------------------------------------------\*)
(*| Perform calculations                            |*)
(*\-------------------------------------------------/*)

Do[

    Do[

        qmInitialize[m,n];
        qmPotential[];
        qmWavePacket[];

        Progress[StringJoin["Evaluating",
                ToString[m],"-",ToString[n]];

        Do[

            totreps = totreps + reps;
            T = T +  dt * reps;

            QTimeEvolution[HS, QfnPsiS, dt, 6, reps];
            TblPsiS = QGetArray[QfnPsiS];

            TblRs = Abs[TblPsiS[[1]] + I TblPsiS[[2]]];

            RRs = ListInterpolation[ TblRs, {{borderleft, borderright}},
                InterpolationOrder ->6];

            GGs[x_] := (RRs'[x]/RRs[x]);
            QQs = -0.5*(RRs''[x])/RRs[x]);

            NSolution  = NDSolve[ { 0.5*Y''[x] + GGs[x]*
                Y'[x] == -V[x]*Y[x], Y[1] == 1, Y'[1] == 1}, Y,
                {x, borderleft,borderright}, MaxSteps ->Infinity];
```

```
            RRe = Y /. First[NSolution];
            GGe = RRe'[x]/RRe[x];
            QQes = -GGs[x]*RRe'[x]/RRe[x];
            QQe = V[x] - QQes;
            QQt = V[x] + QQs;

            TblRRs = Table[RRs[x], {x, -20.0, 2.0, .1}];

            StoreData[RRe,RRs,GGe,GGs,GGe,QQs,QQe,QQes,T_];

        ,{800}];
    ,{m,1,3}];
,{n,1,2}];

(*/-------------------------------------------------\*)
(*| Notebook End                                    |*)
(*\-------------------------------------------------/*)
```

A.2 Two-Dimensional Double-Slit

```
(*/-----------------------------------------------------\*)
(*| Portions based on Manfred Liebmann[35] and         |*)
(*|                   Berndt Thaller[34]               |*)
(*/-----------------------------------------------------\*)

<< QuantumMechanics`QuantumKernel`;

(*/-----------------------------------------------------\*)
(*| Initialize values                                  |*)
(*\-----------------------------------------------------/*)

qmInitialize[qmSystem_,qmStrength_]:=Module[{},

    Off[General::"spell1"];
    Off[CreateDirectory::"ioerr"];

    T = 0;
    totreps = 0;
    reps = 50;
    dt = 0.002;
    dx = 0.02;
    qmAlphas = {0, 1/4, 3/4, 1};
    qmTitles = {"2D_Double_Slit", "2D_AB_Effect"};
    qmAlpha = qmStrength;
    qmTitle = qmSystem;

    qmWorkDirectory =
        StringJoin["T:\Data\\", qmTitles[[qmTitle]], "-",
        ToString[qmSystem],"\dx=", ToString[dx]];

    CreateDirectory[qmWorkDirectory];
    SetDirectory[qmWorkDirectory];

    borderleft={-14.,-14.};
    borderright={14.,14.};
    dataleft = -4.;
    dataright= 4.;
    listleft = (dataleft - borderleft[[1]])/dx;
    listright = -1 + ( borderright[[1]]+ dataright)/dx ;
    plotleft=dataleft+dx/2;
    plotright=dataright-dx/2;
    qmPos={-1.,-1.};
    qmMomentum={6.,6.};
    Alpha = qmAlphas[[qmAlpha]];
```

```
];

(*/-----------------------------------------------------\*)
(*| Define Potentials                                   |*)
(*\-----------------------------------------------------/*)

qmPotential[]:=Module[{},

    If[qmTitle==2,

        phi[x1_,x2_] := ArcTan[x2/x1]-Pi;
        fnA1 = Compile[{x,y},-Alpha*y/(x^2+y^2)];
        fnA2 = Compile[{x,y},Alpha*x/(x^2+y^2)];
        tblA1 = Table[fnA1[x,y],{y,borderleft[[2]]+dx/2,
            borderright[[2]]-dx/2,dx},
            {x,borderleft[[1]]+dx/2,borderright[[1]]-dx/2,dx}];
        tblA2 = Table[fnA2[x,y],{y,borderleft[[2]]+dx/2,
            borderright[[2]]-dx/2,dx},
            {x,borderleft[[1]]+dx/2,borderright[[1]]-dx/2,dx}];
        vector = QNewFunction[tblA1,tblA2];
        scalar = None;
        Remove[tblA1,tblA2];
        ,
        phi[x1_,x2_] := 0;
        vector = None;
        scalar = None;

    ];
];

(*/-----------------------------------------------------\*)
(*| Define initial wave packet                          |*)
(*\-----------------------------------------------------/*)

qmWavePacket[]:=Module[{},

    Off[General::"spell1"];

    gauss[x_,t_,a_,x0_,p0_] :=
        Sqrt[1/(1+I t a)]*
        Exp[-((a/2) (x-x0)^2-I p0 (x-x0)+
            I t p0^2/2)/(1+I t a)];

    t0=-0.5;

    wave[x0_,y0_,kx_,ky_,a_]:=
        Compile@@{{x,y},
```

```
        Simplify[(a/Pi)^(1/2) gauss[x,t0,a,x0,kx]
            gauss[y,t0,a,y0,ky]*
            Exp[I*Alpha*phi[x,y]]]};

    f=wave[qmPos[[1]],qmPos[[2]],qmMomentum[[1]],qmMomentum[[2]],.5];

    psi0=Table[f[x,y],{x,borderleft[[1]]+dx/2,
        borderright[[1]]-dx/2,dx},
        {y,borderleft[[2]]+dx/2,
        borderright[[2]]-dx/2,dx}];

];

(*/-----------------------------------------------------\*)
(*| Store results to disk                               |*)
(*\-----------------------------------------------------/*)

StoreData[RRe_,RRs_,GGe_,GGs_,GGe_,QQs_,QQe_,QQes_,T_]:=
    Module[{},

    Off[General::"spell1"];

    qmName = ToString[100000 +10000 * T];

    Progress["Storing Rs"];
    TblRRs = Table[RRs[x,y],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Rs",qmName,
        ".lst"],TblRRs,"Table"];

    Progress["Storing Re"];
    TblRRe = Table[RRe[x,y],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Re",qmName,
        ".lst"],TblRRe,"Table"];

    Progress["Storing Gs"];
    TblGGs = Table[Evaluate[GGs[x,y]],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Gs",qmName,
        ".lst"],TblGGs,"Table"];

    Progress["Storing Ge"];
    TblGGe = Table[Evaluate[GGe[x,y]],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Ge",qmName,
        ".lst"],TblGGe,"Table"];
```

```
    Progress["Storing Qs"];
    TblQQs = Table[Evaluate[QQs[x,y]],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Qs",qmName,
        ".lst"],TblQQs,"Table"];

    Progress["Storing Qe"];
    TblQQe = Table[Evaluate[QQe[x,y]],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Qe",qmName,
        ".lst"],TblQQe,"Table"];

    Progress["Storing Qes"];
    TblQQes = Table[Evaluate[QQes[x,y]],{x,plotleft,plotright,.01},
        {y,plotleft,plotright,.01}];
    Export [StringJoin["Qes",qmName,
        ".lst"],TblQQes,"Table"];

];

(*/-------------------------------------------------\*)
(*| Remove invalid data from array                  |*)
(*\-------------------------------------------------/*)

CleanArray[]:=Module[{},

    aDim = Dimensions[arrRR];
    xDim = aDim[[1]];
    yDim = aDim[[2]];

    Progress["Cleaning Array "];

    For[i=1,i<=xDim,i++,
        For[j=1,j<=yDim, j++,
            If[ arrRR[[i,j]]=="ComplexInfinity",
                arrRR[[i,j]]=0
            ];
        ];
    ];
];

(*/-------------------------------------------------\*)
(*| Generate state-dependent potentials             |*)
(*\-------------------------------------------------/*)

StateDependentPotentials[] := Module[{},

    Progress[ "Importing Rs "];
```

```
    arrRR = Import["Rs.lst", "Table"];

    Progress["Interpolating Rs"];
    RRs = ListInterpolation[arrRR, {{plotleft, plotright},
        {plotleft,plotright}},InterpolationOrder -> 6];

    Progress["Importing Re "];
    arrRR = Import["Rc.lst","Table"]/arrRR;

    Progress["Interpolating Rs"];
    RRe=ListInterpolation[arrRR,{{plotleft,plotright},
        {plotleft,plotright}},InterpolationOrder->6];

    Progress[ "State-dependent potentials "];
    GGs[x_,y_]:=-(D[RRs,x] +D[RRs,y])/RRs[x,y];
    GGe[x_,y_]:=-(D[ RRe,x] +D[ RRe,y])/RRe[x,y];
    QQs[x_,y_]:= -0.5(D[RRs,{x,2}]) + D[RRs,{y,2}]/RRs[x,y];
    QQe[x_,y_]:= -0.5(D[RRe,x]) +D[RRe,{y,2}])/RRe[x,y];
    QQes[x_,y_]:= -(D[RRs,x] *D[RRe,x]  + D[
    RRs,y]*D[RRe,y])/(RRs[x,y]*RRe[x,y]);

    StoreData[RRe,RRs,GGe,GGs,GGe,QQs,QQe,QQes,T];

];

(*/-------------------------------------------------\*)
(*| Display progress                                |*)
(*\-------------------------------------------------/*)

Progress[str_]:=Module[{pstr=str},

    sTime=SessionTime[];
    Hours = Quotient[ sTime,3600];
    rSeconds =Mod[sTime,3600];
    Minutes = Quotient[rSeconds,60];
    Seconds = Mod[rSeconds,60];

    Print[pstr," ","Time=",Hours,":",Minutes,":",
        Seconds," Memory=",MemoryInUse[]];

];

(*/-------------------------------------------------\*)
(*| Perform calculations                            |*)
(*\-------------------------------------------------/*)

Off[General::"spell1"];
```

```
Do[

    qmInitialize[qmSystem];
    qmParameters[];
    qmPotential[];
    qmBoundary[];
    qmWavePacket[];

    Progress["Beginning calculations"];

    Do[

        If[m == 1,
            Ha = QSchroedinger2D[scalar, vector,
                domObj, 1., 1., dx ];
            psiI = QNewFunction[4. Re[psi0], 4. Im[psi0]];
            ,
            Ha = QSchroedinger2D[None, None,
                None, 1., 1., dx ];
            psiI = QNewFunction[4. Re[psi0], 4. Im[psi0]];

        ];

        Do[

            totreps = totreps + reps;
            T = totreps * dt;

            QTimeEvolution[Ha, psiI, dt, 6, reps ];

            If[m == 1,
                psi2 = QGetArray[psiI];
                arrRR = Take[
                    Abs[psi2[[1]] + I psi2[[2]]],
                        {listleft, listright},
                        {listleft,listright}];
                Clear[psi2];
                Export[StringJoin["Rs", ToString[totreps],
                    ".lst"],arrRR, "Table"];
                Clear[arrRR];
            ,

            psi2 = QGetArray[psiI];
            arrRR = Take[
                Abs[psi2[[1]] + I psi2[[2]]],
                    {listleft, listright},
                    {listleft,listright}];
            Clear[psi2];
```

```
            Export[StringJoin["Rc", ToString[totreps],
                ".lst"],arrRR, "Table"];
            Clear[arrRR];
            ];

            , {n, 1, 14}
        ];

        If[qmSystem > 1, QDisposeFunction[vector]];
        If[m == 1, QDisposeFunction[domObj]];
        QDisposeFunction[psiI]; QDisposeOperator[Ha];

    , {m, 1, 1}];

    StateDependentPotentials[];

,{qmSystem, 1, 4}];

(*/-------------------------------------------------\*)
(*| Notebook End                                    |*)
(*\-------------------------------------------------/*)
```

A.3 Two-Dimensional Dirac

```
(*/-------------------------------------------------\*)
(*| Portions based on Manfred Liebmann[35] and      |*)
(*|                   Berndt Thaller[34]            |*)
(*/-------------------------------------------------\*)

<< QuantumMechanics`QuantumKernel`;

(*/-------------------------------------------------\*)
(*| Initialize values                               |*)
(*\-------------------------------------------------/*)

qmInitialize[] := Module[{},

    Off[General::"spell1"];
    Progress["Initialize"];

    h = 1/127;
    Alpha = 1/4;
    n1 = 1/h + 1;
    n2 = 1/h + 1;
    c = 200;
    B = 256;
    a = 10;
    b = 200;
    e = 1;
    dt = 1.h;
    T = 0;
    reps = 8;
    totreps = 0;

    qmTitle = "2D_Dirac";
    qmDataDirectory = StringJoin["T:\Data\\", qmTitle];
    Off[CreateDirectory::"ioerr"];
    CreateDirectory[qmDataDirectory];
    SetDirectory[qmDataDirectory];

];

(*/-------------------------------------------------\*)
(*| Display progress                                |*)
(*\-------------------------------------------------/*)

Progress[str_]:=Module[{pstr=str},

    sTime=SessionTime[];
```

```
    Hours = Quotient[ sTime,3600];
    rSeconds =Mod[sTime,3600];
    Minutes = Quotient[rSeconds,60];
    Seconds = Mod[rSeconds,60];

    Print[pstr," ","Time=",Hours,":",Minutes,":",
        Seconds," Memory=",MemoryInUse[]];

];

(*/-------------------------------------------------\*)
(*| Define Potentials                               |*)
(*\-------------------------------------------------/*)

qmVectorPotential[] := Module[{},

    Progress["Vector Potential"];

    Vector2D[h_, Alpha_] :=
        Compile @@ {{y, x},
        With[{x1 = x h, x2 = y h},
            I Alpha / ((x1 - 2/3) - I(x2 - 2/3))]};

    TblAi = Array[Vector2D[h, Alpha], {n2, n1}, 0];
    QfnAe = QNewFunction[Re[TblAi], Im[TblAi], Re[0 TblAi]];

];

(*/-------------------------------------------------\*)
(*| Define initial wave packets                     |*)
(*\-------------------------------------------------/*)

qmWavePacket[] := Module[{},

    Progress["Wave Packet"];

    Gauss2D[h_, a_, b_] :=
        Compile @@ {{y, x},
        With[{x1 = x h, x2 = y h},
        a*Exp[-b((x1 - 1/2)^2 + (x2 - 1/2)^2)/2]]};

    Gauss2DC[h_, a_, b_, e_, Alpha_] :=
        Compile @@ {{y, x},
        With[{x1 = x h, x2 = y h},
        a*Exp[-b((x1 - 1/2)^2 + (x2 - 1/2)^2)/2]Exp[
            I e Alpha Arg[(x1 - 2/3) + I(x2 - 2/3)]]]};

    PsiiS = Array[Gauss2D[h, a, b(*, e, Alpha*)],
```

```
        {n2, n1}, 0];
    PsiiC = Array[Gauss2DC[h, a, b, e, Alpha],
        {n2, n1}, 0];

    PsiA = QNewFunction[Re[PsiiS], Im[ PsiiS],
        Re[PsiiS], Im[ PsiiS]];
    PsiF = QNewFunction[Re[PsiiC], Im[ PsiiC],
        Re[PsiiC], Im[ PsiiC]];

];

(*/-------------------------------------------------\*)
(*| Set domain of shielded coil                     |*)
(*\-------------------------------------------------/*)

qmBoundary[] := Module[{},

    Progress["Domain"];

    Domain2D[h_] :=
        Compile @@ {{x, y},
        With[{x1 = x h, x2 = y h},
        If[(x1 - 2/3)^2 + (x2 - 2/3)^2 <= 1/32^2, -1, 1]]};

    TblDom = Array[Domain2D[h], {n2, n1}, 0];
    QfnDom = QNewFunction[TblDom];

];

(*/-------------------------------------------------\*)
(*| Define Two-Dimensional Dirac Hamiltonians       |*)
(*\-------------------------------------------------/*)

qmHamiltonian[] := Module[{},

    Progress["Hamiltonian"];

    scalar = None; vector = QfnAe; domain = QfnDom;
    mass = 1.; charge = 1.; units = 1.h;
    Ha = QDirac2D[scalar, vector, domain, mass, charge, units];
    Hf = QDirac2D[None, None, None, mass, charge, units];

];

(*/-------------------------------------------------\*)
(*| Store results to disk                           |*)
(*\-------------------------------------------------/*)
```

```
StoreData[RRe1_,RRe2_,RRs1_,RRs2_,GGe_,GGs1_,GGs2_]:=
    Module[{},

    qmName = ToString[100000 +10000 * T];

    Export [StringJoin["Re1-",qmName,".lst"],
        RRe1, "Table"];

    Export [StringJoin["Re2-",qmName,".lst"],
        RRe2, "Table"];

    Export [StringJoin["Rs1",qmName,".lst"],
        Abs[psiA1], "Table"];

    Export [StringJoin["Rs2",qmName,".lst"],
        Abs[psiA2], "Table"];

    Export [StringJoin["Ge1\",qmName,".lst"],
        Table[Evaluate[GGe[x, y]],
            {x, n1/5, 4n1/5, 1},
            {y, n1/5, 4n1/5,1}],
            "Table"];

    Export [StringJoin["Gs1",qmName,".lst"],
        Table[Evaluate[GGs1[x, y]],
            {x, n1/5, 4n1/5, 1},
            {y, n1/5, 4n1/5,1}],
            "Table"];

    Export [StringJoin["Gs2",qmName,".lst"],
        Table[Evaluate[GGs2[x, y]],
            {x, n1/5, 4n1/5, 1},
            {y, n1/5, 4n1/5,1}],
            "Table"];

];

(*/-------------------------------------------------\*)
(*| Perform calculations                            |*)
(*\-------------------------------------------------/*)

qmInitialize[];
qmVectorPotential[];
qmWavePacket[];
qmBoundary[];
qmHamiltonian[];

Do[
```

```
    psiA = QGetArray[PsiA];
    psiA1 = psiA[[1]] + I psiA[[2]];
    psiA2 = psiA[[3]] + I psiA[[4]];

    gA1 = ListDensityPlot[Abs[psiA1], PlotRange -> All,

    psiF = QGetArray[PsiF];
    psiF1 = psiF[[1]] + I psiF[[2]];
    psiF2 = psiF[[3]] + I psiF[[4]];

    RRe1 = 50 * Abs[psiF1/psiA1];
    RRe2 = 50 * Abs[psiF2/psiA2];

    Ps1s = ListInterpolation[Abs[psiA1],
        InterpolationOrder -> 6];
    Ps2s = ListInterpolation[Abs[psiA2],
        InterpolationOrder -> 6];
    PsiE = ListInterpolation[Abs[RRe2],
        InterpolationOrder -> 6];

    GGs1[x_, y_] := -(D[Ps1s, x] + D[Ps1s, y])/Ps1s[x, y];
    GGs2[x_, y_] := -(D[ Ps2s, x] + D[Ps2s, y])/Ps2s[x, y];
    GGe[x_, y_] := -(D[PsiE, x] + D[PsiE, y])/PsiE[x, y];

    QTimeEvolution[Ha, PsiA, dt, 6, reps];
    QTimeEvolution[Hf, PsiF, dt, 6, reps];

    totreps = totreps + reps;
    T = dt * totreps;

    StoreData[RRe1,RRe2,Abs[psiA1],Abs[psiA2],
        GGe,GGs1,GGs2,T];

    ,{m, 1, 2}];
,{n,1,5}];

(*/-----------------------------------------------------\*)
(*| Notebook End                                        |*)
(*\-----------------------------------------------------/*)
```

A.4 Generation of Figures

```
(*/-------------------------------------------------\*)
(*| Initialize values                               |*)
(*\-------------------------------------------------/*)

qmTitle = {"1D_Barrier", "1D_Well", "1D_Barrier_Closed",
    "2D_Double_Slit","2D_AB_Effect", "2D_Dirac"};
qmFilesS1 = {"Ge1", "Gs1", "Qe1", "Qs1", "Qes1", "Qt1"};
qmFilesS2 = {"Rs1", "Re1", "Ge1", "Gs1", "Qe1", "Qs1",
    "Qes1", "Qt1"};
qmFilesS3 = {"Rs1", "Rs2", "Re2", "Gs1", "Gs2", "Ge1"};
qmRangeS1 = {{-10, 50}, {-10, 50}, {-10, 50}, {-10, 50},
    {-10, 50}, {-10,50}};
qmRangeS2 = {{0, .5}, {0, 2}, {-10, 20}, {-10, 20},
    {-100, 250}, {-50,50}, {-50, 250}, {-10, 50}};
qmRangeS3 = {{0, 8}, {0, 8}, {-10, 150}, {-1, 1.5},
    {-1, 1.5}, {-2, 2}};
qmViewPoints = {{2, 2, 2}, {-2, 2, 2}, {2, -2, 2},
    {-2, -2, 2}};
qmPathFigures = "T:\Figures\\";
qmPathData = "T:\Data\\";
qmWidth = 72 *7.0;
qmHeight = qmWidth/2;

qmCreateS1 = 1;
qmCreateS2 = 1;
qmCreateS3 = 1;

(*/-------------------------------------------------\*)
(*| Module for One-Dimensional Scattering Graphs    |*)
(*\-------------------------------------------------/*)

CreateFigureS1[idx_] := Module[{},

    Do[

        $EPSDisplay[pl_] :=
            Module[ {file =
                StringJoin[qmFilesS1[[idx]] , "-",
                    ToString[qmViews],
                    ".jpg"]
                },
                Display[file, pl, "JPEG",
                    ImageResolution -> 600,
                    ImageSize -> 144]; pl] ;
```

```
        ListPlot3D[Tbl[[Range[40, 750]]],
            ImageSize -> {qmWidth, qmHeight},
            DisplayFunction -> $EPSDisplay,
            Mesh -> False, Axes -> None,
            Ticks -> None,
            ViewPoint -> qmViewPoints[[qmViews]],
            PlotRange -> qmRangeS1[[idx]]];

    ,{qmViews, 1, 4}];
];

(*/-----------------------------------------------------\*)
(*| Module for Two-Dimensional Two-Slit Plots Graphs   |*)
(*\-----------------------------------------------------/*)

CreateFigureS2[idx_] := Module[{},

    On[SurfaceGraphics::"gmat"];

    Do[

        $EPSDisplay[pl_] :=
            Module[ {file =
            StringJoin[qmFilesS2[[idx]] , "-",
            ToString[qmViews], ".jpg"]},
            Display[file, pl, "JPEG",
            ImageResolution -> 600,
            ImageSize -> 144];
            pl] ;

         Plot3D[RR[x, y], {x, 2, 599}, {y, 2, 199},
            PlotPoints -> 800,
            ImageSize -> {qmWidth, qmHeight},
            DisplayFunction -> $EPSDisplay,
            Mesh -> False, Axes -> None,
            Ticks -> None,
            ViewPoint -> qmViewPoints[[qmViews]],
            PlotRange -> qmRangeS2[[idx]]];

    ,{qmViews, 1, 4}];
];

(*/-----------------------------------------------------\*)
(*| Module for Two-Dimensional Dirac Graphs            |*)
(*\-----------------------------------------------------/*)

CreateFigureS3[idx_] := Module[{},
```

```
  On[SurfaceGraphics::"gmat"];

  Do[

    $EPSDisplay[pl_] :=
      Module[ {file =
            StringJoin[qmFilesS3[[idx]] , "-",
            ToString[qmViews],".jpg"]},
            Display[file, pl, "JPEG",
            ImageResolution -> 600,
            ImageSize -> 144]; pl] ;

    xi = Dimensions[Tbl][[1]];
    yi = Dimensions[Tbl][[2]];

    Plot3D[RR[x, y], {x, 1, xi}, {y, 1, yi},
        PlotPoints -> 800,
        ImageSize -> {qmWidth, qmHeight},
        DisplayFunction -> $EPSDisplay,
        Mesh -> False, Axes -> None, Ticks -> None,
        ViewPoint -> qmViewPoints[[qmViews]],
        PlotRange -> qmRangeS3[[idx]]];

  ,{qmViews, 1, 4}];
];

(*/-------------------------------------------------\*)
(*| Import One-Dimensional Scattering Data          |*)
(*\-------------------------------------------------/*)

ProcessDataS1[] := Module[{},

        SetDirectory[qmDataDirectory];
        qmData = FileNames[StringJoin[qmFilesS1[[qmGraph]],
            "*.lst"]];
        NumFile = Dimensions[qmData];
        Inc = 0;
        Tbl = {};
        If[ NumFile[[1]] == 0,

                Progress["No Files!"];
                ,
                While[Inc < NumFile[[1]], Inc++;
                    AppendTo[Tbl,
                    Import[qmData[[Inc]], "List"] ];
                ];
                CreateDirectory[qmGraphDirectory];
```

```
                SetDirectory[qmGraphDirectory];

                CreateFigureS1[qmGraph];
                Clear[Tbl];
        ];
];

(*/-------------------------------------------------\*)
(*| Import Two-Slit Data                            |*)
(*\-------------------------------------------------/*)

ProcessDataS2[] := Module[{},

        SetDirectory[qmDataDirectory];
        qmData = FileNames[StringJoin[qmFilesS2[[qmGraph]],
            "*.lst"]];
        NumFile = Dimensions[qmData];
        Inc = 0;
        Tbl = {};

        If[ NumFile[[1]] == 0,
            Progress["No Files!"];
            ,
            Tbl =   Import[qmData[[1]], "Table"] ;
            CleanData[];
            CreateDirectory[qmGraphDirectory];
            SetDirectory[qmGraphDirectory];
            CreateFigureS2[qmGraph];
            Clear[Tbl];
        ];
];

(*/-------------------------------------------------\*)
(*| Import Dirac Data                               |*)
(*\-------------------------------------------------/*)

ProcessDataS3[] := Module[{},

        SetDirectory[qmDataDirectory];
        qmData = FileNames[StringJoin[qmFilesS3[[qmGraph]],
            "*.lst"]];
        NumFile = Dimensions[qmData];
        Inc = 0;
        Tbl = {};

        If[ NumFile[[1]] == 0,
            Progress["No Files!"];
            ,
```

```
            Tbl =   Import[qmData[[1]], "Table"] ;
            CleanDataS3[];
            CreateDirectory[qmGraphDirectory];
            SetDirectory[qmGraphDirectory];
            CreateFigureS3[qmGraph];
            Clear[Tbl];
        ];
];

(*/-------------------------------------------------\*)
(*| Remove Unwanted Data from Two-Slit Array       |*)
(*\-------------------------------------------------/*)

CleanDataS2[] := Module[{},

    aDim = Dimensions[Tbl];
    xDim = aDim[[1]];
    yDim = aDim[[2]];
    nTbl = Table[0, {i, 600}, {j, 400}];

    For[i = 1, i <= xDim, i++,
        For[j = 1, j <= yDim, j++,

            If[ (i + j >= 900) && (i + j <
                  1300) && (i - j >= -300)
                  && (i - j < 300),

                ni = i - j + 301;
                nj = i + j - 900;

                If[EvenQ[nj], nj = nj/2,
                    nj = (nj - 1)/2];

                    nTbl[[ni, nj + 1]] =
                        Tbl[[i, j]];

            ];
        ];
    ];

    RR = ListInterpolation[nTbl, InterpolationOrder -> 6];

];

(*/-------------------------------------------------\*)
(*| Remove Unwanted Data from Dirac Data          |*)
(*\-------------------------------------------------/*)
```

```
CleanDataS3[] := Module[{},

    aDim = Dimensions[Tbl];
    xDim = aDim[[1]];
    yDim = aDim[[2]];

    Progress["Cleaning Array ", xDim, " ", yDim];

    For[i = 1, i <= xDim, i++,
        For[j = 1, j <= yDim, j++,

            If[ (Tbl[[i, j]] == "Indeterminate") ||
                (Tbl[[i, j]] == "Infinity"),
                Tbl[[i, j]] = 0;
            ];
        ];
    ];

    RR = ListInterpolation[Tbl, InterpolationOrder -> 6];
];

(*/-------------------------------------------------\*)
(*| Create All One-Dimensional Scattering Graphs    |*)
(*\-------------------------------------------------/*)

If[qmCreateS1 == 1,

    Off[CreateDirectory::"ioerr"];

    Do[
        Do[

            qmDataDirectory =
                StringJoin[
                qmPathData, qmTitle[[qmPotential]],
                "_",ToString[qmEnergy]];
            qmGraphDirectory =
                StringJoin[qmPathFigures,
                qmTitle[[qmPotential]], "_",
                ToString[qmEnergy]];

            Do[

                EPSFileExists =
                    Dimensions[
                    FileNames[
                    StringJoin[qmGraphDirectory, "\\",
                        qmFilesS1[[qmGraph]],
```

```
                    "*.jpg"]]][[1]];

                If[EPSFileExists == 1,
                    Progress["All Figures completed!"];
                    ,
                    ProcessDataS1[];
                ];

            ,{qmGraph, 1, 6}];
        ,{qmEnergy, 1, 3}];
    ,{qmPotential, 1, 3}];
];

(*/-------------------------------------------------\*)
(*| Create All Two-Slit Graphs                     |*)
(*\-------------------------------------------------/*)

If[qmCreateS2 == 1,

    Off[CreateDirectory::"ioerr"];

    Do[
        Do[

            qmDataDirectory =
                StringJoin[qmPathData,
                qmTitle[[qmPotential]], "_",
                ToString[qmEnergy]];
            qmGraphDirectory =
                StringJoin[qmPathFigures,
                qmTitle[[qmPotential]], "_",
                ToString[qmEnergy]];

            Do[

                EPSFileExists =
                Dimensions[
                FileNames[
                StringJoin[qmGraphDirectory, "\\",
                    qmFilesS2[[qmGraph]],
                     "*.jpg"]]][[1]];

                If[EPSFileExists == 1,
                    Progress["All Figures completed!"];
                    ,
                    ProcessDataS2[];
                ];
```

```
            ,{qmGraph, 1, 8}];
        ,{qmEnergy, 1, 4}];
    ,{qmPotential, 4, 5}];
];

(*/-------------------------------------------------\*)
(*| Create All Dirac Graphs                         |*)
(*\-------------------------------------------------/*)

If[qmCreateS3 == 1,

    Off[CreateDirectory::"ioerr"];

    Do[

        qmDataDirectory =
            StringJoin[qmPathData, qmTitle[[qmPotential]]];
        qmGraphDirectory =
            StringJoin[qmPathFigures, qmTitle[[qmPotential]]];

        Do[
            EPSFileExists =
                Dimensions[
                    FileNames[
                        StringJoin[qmGraphDirectory, "\\",
                        qmFilesS3[[qmGraph]],"*.jpg"]]][[1]];
            If[EPSFileExists == 1,
                Progress["All Figures completed!"];
                ,
                ProcessDataS3[];
            ];

        ,{qmGraph, 1, 6}];
    ,{qmPotential, 6, 6}];
];

(*/-------------------------------------------------\*)
(*| Notebook End                                    |*)
(*\-------------------------------------------------/*)
```