Bohmian Quantum Mechanics and the Finite Square Potential Barrier

Matthew Gorski
Physics Department, The College of Wooster, Wooster, Ohio 44691, USA
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This project studies Bohmian quantum mechanics, a hidden variable theory of quantum mechanics that postulates definite particle trajectories. The Bohmian approach is applied to a finite square potential barrier. Using *Mathematica 6*, we compute the particle trajectories in a statistical ensemble for three different energies. It is shown that the probability for a particle to be reflected or transmitted by the barrier approaches the values predicted by the orthodox approach to quantum mechanics. This paper discusses the role of the quantum potential, a concept often associated with Bohmian quantum mechanics. A simulation created in *Mathematica 6* allows a comparison of the orthodox and Bohmian approach to quantum mechanics. The simulation also shows the time evolution of the quantum potential.

I. INTRODUCTION

Quantum mechanics uses a mathematical object called the wave function to describe the state of a physical system. The main issue in the interpretation of quantum mechanics is whether the wave function describes all the physical information about a system or whether it leaves something out. A theory that interprets the wave function as describing all information about the system says that the wave function is *complete* and is called an orthodox interpretation, since most physicists ascribe to this view. A theory that interprets the wave function as leaving something out says that the wave function is *incomplete* and is called a hidden variables theory after whatever it is that the wave function does not describe [1]. Under the broad rubrics of orthodox and hidden variable theories, there are further interpretations and refinements. The goal of this project is to compare orthodox theories in general to a specific hidden variable theory called Bohmian Quantum Mechanics, developed by David Bohm [2–4].

Perhaps the main reason for thinking that the wave function is incomplete is that it only describes the probability with which a measurement returns a specific value. Experience from statistical mechanics suggests that probabilities are only due to ignorance [2]. There exists an exact specification of a physical system which accounts for the probabilistic predictions, even if observers cannot know the exact specification. This is not the orthodox response to quantum mechanical probabilities. Most physicists interpret the probabilities given by the wave function as fundamental, i.e. there is no underlying exact specification. Prior to a position measurement, for example, the system does not have an exact position. All that is true of the system is its disposition to yield certain results of a position measurement. There are two main reasons for the orthodox response: experiments verifying quantum theory *force* us to regard the wave function as complete, or that whatever might specify the exact state of a physical system is theoretically cumbersome and/or does not lead to any new prediction.

The first reason, the impossibility of hidden variables, is often motivated by Bell's Theorem. What Bell's Theorem shows is that a theory which postulates spatiotemporally local interaction between particles, as well as hidden variables, cannot account for the same data that orthodox theories can [5]. However, Bohmian quantum mechanics postulates nonlocal interaction by particles, so Bell's Theorem does not rule it out. The second reason for preferring the orthodox response over Bohmian mechanics will be evaluated throughout the rest of this paper. Whether this is good reason for thinking the wave function is complete depends on the precise nature of the proposed hidden variables.

So what are these hidden variables? Bohmian mechanics postulates exact particle trajectories for all time, regardless of whether a measurement has been performed. Roughly, the wave function is determined by Schrödinger's equation, and the particle trajectories are guided by the wave function according to an additional "guiding" equation unique to Bohmian theory. Bohmian theory then postulates that in a statistical ensemble of systems with identical wave functions, the initial positions of the particles are distributed according to a certain probability density. Bohm's theory treats the wave function as an objectively real part of a system [6], rather than as a representation of the system itself. These postulates are enough to make the same predictions as orthodox quantum theory. One further issue arises within Bohmian mechanics: whether an additional "quantum potential" is required to accurately describe the particle trajectories.

Whether Bohm's theory is cumbersome, or leads to any new predictions, will be examined through simulation, and computation applied to a typical problem in quantum mechanics: the square barrier potential. In section 2, I outline Bohm's theory in general. In section 3, I explain the theoretical approach to the square barrier potential. In section 4, I explain how *Mathematica 6* was used to approach this problem with both simulation and computation. In section 5, I discuss the equivalence of the orthodox theory and Bohm's theory in the case of the square barrier, and examine the use of the quantum potential.

This paper concludes that the postulation of hidden variables is not pragmatically useful, since acquiring the orthodox results from Bohm's theory does not require the calculation of particle trajectories. Of course, this does not rule out other practical applications. However, there are several advantages of Bohm's theory. It can explain all the orthodox results of quantum theory without the notion of fundamental uncertainty, so it explains the probabilistic results in the same way statistical mechanics explains probabilistic results[2]. It also teaches us what quantum experiments do in fact imply; they do not force notions of indeterminism, superposition, or a special role for measurement into our theory. A main advantage of Bohm's theory is that measurement is a continuous, analyzable process: it does not restrict the validity of Schrödinger's equation to times before a measurement has been made[3]. Finally, I conclude that the quantum potential is not a useful construct for explaining behavior due to interaction with the square barrier potential.

II. THEORY I: BOHMIAN MECHANICS

This section explains the Bohmian theory of one particle of mass m under the influence of a potential $V[t,\vec{x}]$. Like, orthodox quantum mechanics, Bohmian mechanics uses the Schrödinger wave equation

$$\imath\hbar\frac{\partial\Psi[t,\vec{x}]}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi[t,\vec{x}] + V[t,\vec{x}]\Psi[t,\vec{x}], \quad (1)$$

where $\hbar$ is Planck's reduced constant. In addition, Bohmian mechanics postulates a guiding equation

$$\vec{v}[t] = \frac{\hbar}{m}\frac{\mathrm{Im}[\Psi^*\nabla\Psi]}{\Psi^*\Psi}, \quad (2)$$

which describes the velocity of a particle. Finally, Bohmian mechanics considers a statistical ensemble of systems with the same wave function and with the initial positions distributed according to the probability density

$$\rho[t_0,\vec{x}] = \Psi^*\Psi. \quad (3)$$

These three equations constitute the core of Bohmian theory.

To see the consequences of these equations, it is helpful to rewrite the assumptions of Bohmian mechanics with the wave function in polar form:

$$\Psi[t,\vec{x}] = R[t,\vec{x}]e^{\imath S[t,\vec{x}]/\hbar}. \quad (4)$$

Schrödinger's equation becomes two equations through the substitution of Eq. 4 into Eq. 1, and equating real and imaginary parts. This implies the following two equations :

$$-\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} + \frac{\nabla S\cdot\nabla S}{2m} + V \quad (5)$$

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}(2\nabla R\cdot\nabla S + R\nabla^2 S). \quad (6)$$

When Eq. 4, is substituted into the guiding equation (Eq. 2), the guiding equation becomes

$$\vec{v}[t] = \frac{\nabla S[t,\vec{x}]}{m}. \quad (7)$$

Writing the wave function in polar form also means that the probability density is simply

$$\rho[t,\vec{x}] = R[t,\vec{x}]^2. \quad (8)$$

Multiplying Eq. 6 by $2R$, and substituting Eq. 8 gives

$$\frac{\partial\rho}{\partial t} = -\frac{1}{m}(\nabla R^2\cdot\nabla S + R^2\nabla^2 S) = -\frac{1}{m}\nabla\cdot(\rho\nabla S). \quad (9)$$

Substituting Eq. 7 into Eq. 9 gives

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot(\rho\vec{v}). \quad (10)$$

Eq. 10 is the "classical continuity equation" [7]. It implies that if the positions $\vec{x}$ in a statistical ensemble at time t_0 are distributed according to $\rho[t_0,\vec{x}] = |\Psi[t_0,\vec{x}]|^2$, and the positions evolve according to the guiding equation (Eq. 7), then the positions at time t will be distributed according to $\rho[t,\vec{x}] = |\Psi[t,\vec{x}]|^2$. Orthodox quantum mechanics also utilizes Eq. 9, but the probability density is the probability of making a certain *measurement* of a position; Bohmian mechanics has said nothing about measurement. The probability in Bohmian mechanics concerns positions in a statistical ensemble. The probability in orthodox quantum mechanics concerns measurements on a statistical ensemble. Further, although orthodox quantum mechanics uses Eq. 9, it does not utilize Eq. 10, because the orthodox theory does not define particle trajectories.

To summarize, the structure of Bohmian mechanics is as follows. The classical potential $V[t,\vec{x}]$ and Schrödinger's wave equation determine the wave function $\Psi[t,\vec{x}]$. The wave function, through the guiding equation (Eq. 2 or 7), determines the velocity of a particle. Given an initial position, the guiding equation determines the trajectory of a particle for all time. Finally, in a statistical ensemble with positions initially distributed according to the probability density $|\Psi[t_0,\vec{x}]|^2$, the positions will always be distributed according to $|\Psi[t,\vec{x}]|^2$. This ensures that Bohmian mechanics makes the same predictions as the orthodox approach.

A. Quantum Potential

Notice that I have said nothing yet about the quantum potential, despite its prominent role in many explications of Bohm's theory. This is because the quantum potential does not need to play a fundamental role in Bohm's theory. Eqs. 1,2, and 3 are sufficient to specify the theory [5, 7]. However, Bohmian mechanics shares the existence of definite trajectories, and the role of probability with classical mechanics. To extend the analogy, we can look at the force $\vec{F} = md\vec{v}/dt$ acting on a particle. From Eq. 7, the force is

$$\vec{F} = \frac{d(\nabla S)}{dt}. \tag{11}$$

Eq. 11 implies

$$\vec{F} = -\nabla(V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}), \tag{12}$$

using Eq. 7, 5 and the identity $2(\nabla S \cdot \nabla)\nabla S = \nabla(\nabla S \cdot \nabla S)$. Eq. 12 implies that a Bohmian particle is acted on by a quantum potential

$$Q[t, \vec{x}] = -\frac{\hbar^2}{2m}\frac{\nabla^2 R[t, \vec{x}]}{R[t, \vec{x}]}, \tag{13}$$

in addition to the normal potential V.

There are several salient features of the quantum potential. First, it is time-dependent and often very complex (see Section 5.1). Second, it is not due to any fundamental force but is dependent on the wave function. Finally, it does not need to play any fundamental role in Bohmian theory. This is because Eqs. 1, 2, and 3 are sufficient to specify the theory. The notion of force which was used in the derivation of the quantum potential is not needed in Bohmian theory. Despite these objections to the inclusion of the quantum potential, it is useful in intuitive explanations of Bohmian mechanics, and in showing that Bohmian theory approaches Newtonian mechanics in the classical limit (let $\hbar \to 0$ in Eq. 12)[7].

III. THE FINITE POTENTIAL BARRIER

The goal of this paper is to compare the Bohmian and orthodox approach to the finite potential barrier defined by

$$V[x] = \begin{cases} V & \text{if } -a \le x \le a \text{ (Region II)} \\ 0 & \text{if } x < -a \text{ (Region I)} \\ 0 & \text{if } x > a \text{ (Region III).} \end{cases} \tag{14}$$

This potential is shown in Fig. 1. The time independent solution outside the well is

$$\psi[x] = \begin{cases} Ae^{\imath kx} + Be^{-\imath kx} & \text{if } x \le -a \text{ (Region I)} \\ Fe^{\imath kx} + Ge^{-\imath kx} & \text{if } x \ge a \text{ (Region III).} \end{cases} \tag{15}$$

The constant k is related to the energy by

$$k = \frac{\sqrt{2mE}}{\hbar}. \tag{16}$$

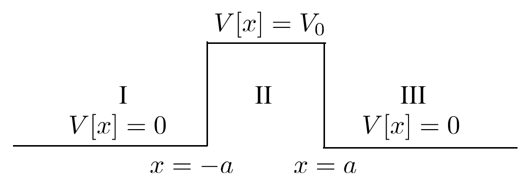

FIG. 1: The finite potential barrier is zero except between $x = -a$ and $x = a$.

The solutions outside the well are sinusoidal. When the time dependence is added, they represent plane waves traveling to the left or right. Since we will be considering only particles incident from the left, we do not need the solution representing a plane wave traveling to the left on the right of the well. In other words, we let $G \to 0$. Since the solution outside the well is a plane wave, it is not normalizable for a single energy. To study the physical situation, a continuous spread of energies is needed.

IV. COMPUTATION AND SIMULATION IN *MATHEMATICA*

The general outline of the implementation is as follows. First, we select parameters for the initial wave function and barrier. Then, using *Mathematica's NDSolve* command, we numerically integrate Schrödinger's equation for several energies that we are interested in. Next, the solution to Schrödinger's equation is used to compute the quantum potential, and for initial positions selected according to the appropriate probability density, the particle trajectories. With these data, we explore the trajectories and quantum potential in several directions: static images, transmission and reflection coefficients, and simulation. Simulation was achieved using *Mathematica's* *Manipulate* command.

V. RESULTS

A. Static Images

To begin to understand the behavior of a Bohmian particle encountering this potential, we can look at trajectories through the barrier for a variety of initial positions. The trajectories for 100 particles in a statistical ensemble are shown in Fig. 2 for the energy $E = V$. As the space-time plots in Fig. 2 show, as the energy increases, more particles are transmitted through the barrier. From these plots it also appears that the final position of the particles is a continuous function of their initial positions. The trajectories do not overlap. The closer a particle is to the well, the more likely it is to pass through the barrier. This is not expected classically

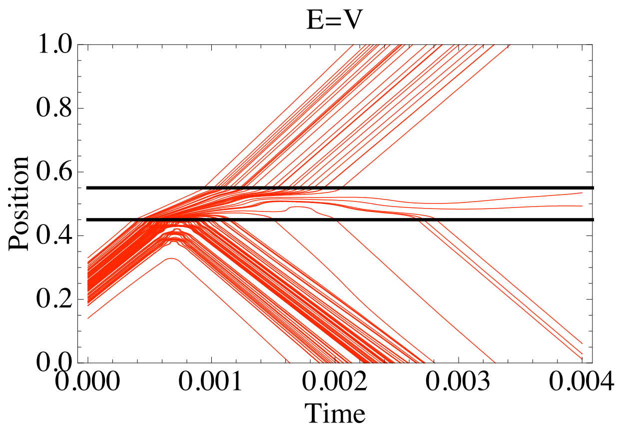

FIG. 2: Particle trajectories in a statistical ensemble. 100 initial positions are selected according to the initial probability density. The horizontal lines show the edge of a potential barrier of height V. The energy of the initial wave packet E is equal to the height of the potential barrier V. The times and positions are in generic units.

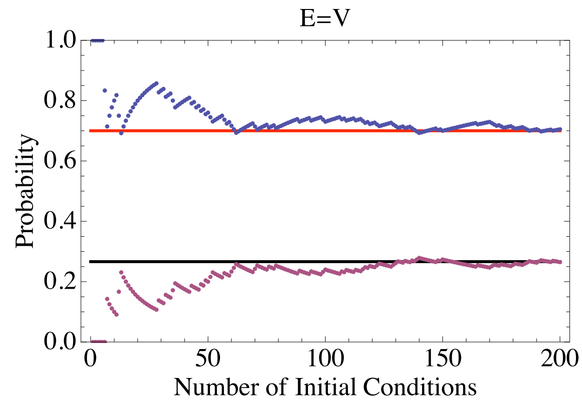

FIG. 4: Transmission and reflection coefficients in the Bohmian (points) and orthodox (lines) approaches. The expected transmission coefficient is shown in black and the expected reflection coefficient is shown in red. As the number of initial conditions is increased, the Bohmian prediction approaches the orthodox prediction. Shown here is the $E = V$ case.

because the potential barrier does not change through time. In the Bohmian picture, particles are guided by the wave function. The wave function evolves through time, so it is important when the particle interacts with the barrier. A further disanalogy with classical mechanics is that reflected particles change direction even when they are spatially separated from the potential.

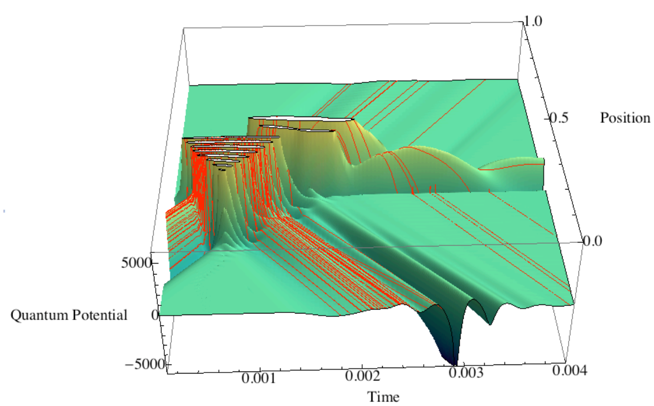

FIG. 3: The quantum potential and particle trajectories for a finite square barrier. Fifty trajectories from the Bohmian statistical ensemble are shown on top of the quantum potential. The energy of the initial wave function is $E = V$, where V is the height of the normal potential barrier. Quantities are in generic units.

The plot of the quantum potential $Q[t, x]$ shown in Fig. 3 is for a single energy $E = V$ with trajectories from the statistical ensemble plotted on top of the quantum potential. The quantum potential's relationship to the wave function is evident, since it undergoes rapid fluctuations when and where the wave function is also undergoing fluctuations. A plot of the quantum potential for the system has limited uses. Although the hills prior to the potential barrier indicate that particles will be reflected before interacting with the barrier, it does not provide useful information about which initial positions will pass through and which will not. Some features are also misleading. One might expect particles to be attracted to the valleys propagating in the negative position direction, but they are not. A space-time plot of the quantum potential is time intensive to produce, and gives limited information about the behavior of particles.

B. Equivalence to Orthodox Predictions

The percentages of transmitted and reflected particles should approach the values predicted by the orthodox approach as more systems in the statistical ensemble are considered. This is ensured in general by Eq. 8 and 9, but we would like to show it computationally in this particular case out of general interest and to ensure that our implementation is working correctly. The transmission and reflections coefficients were checked at the specific time $t = 0.004$. Shown in Fig. 4, the probability in a subset of the statistical ensemble approaches the values predicted by the orthodox integration of the wave function, as the number of initial conditions is increased.

C. Simulation

The simulation created using *Mathematica's Manipulate* command has a number of advantages and disadvantages. There are basically two display

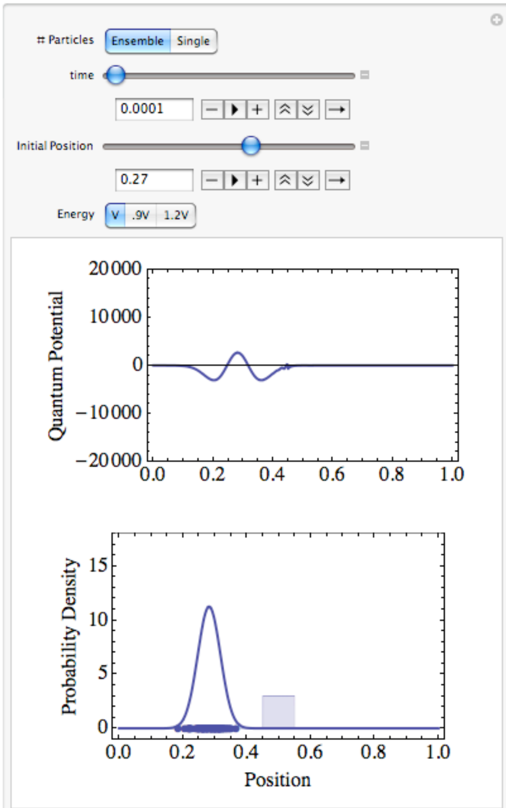

FIG. 5: The initial setting for the manipulator when it is displaying a statistical ensemble. The user can select from any of three energies, and scroll, enter, or play through time. In this setting, the initial position slider does nothing. Above the probability density, the quantum potential is shown. Below the probability density, 100 particles from the statistical ensemble are shown.

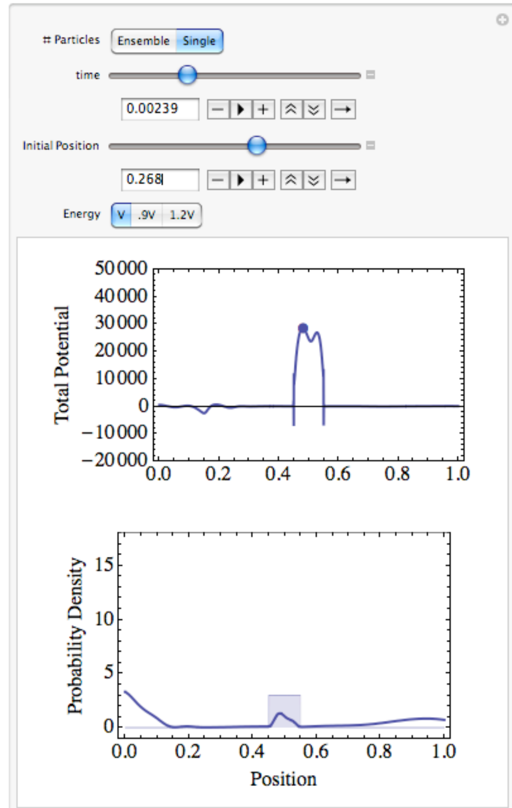

FIG. 6: A display of the manipulator for a single particle exhibiting interesting resonance behavior. The sharp spikes on the left and right of the normal potential barrier are not errors, but rather a very rapid change of the quantum potential.

options in which the user can select one of three energies. The user can view the quantum potential, and a statistical ensemble shown beneath the probability density. Fig. 5 shows the initial configuration of this option. With an example setting shown in Fig. 6, the other option is to view just a single particle plotted on top of the quantum potential and normal potential. This shows clearly how the two potentials combine to determine the behavior of a single particle. The two display options complement each other; the statistical ensemble obeys the probability density, but locally, the motion of a single particle is determined by the potential. The manipulator helps explain the role of the quantum potential more precisely than static images, since the dependence of the potential on the wave function is shown, and its effect on a particle can clearly be seen. However, the entire quantum potential cannot be shown without losing interesting detail on small orders of magnitude.

The current program contains generic units. In the code, variables for $\hbar$ and m are included, although they are set to $\hbar = 1$ and $m = 1/2$. The inclusion of these variables is intended to make the code transparent, and to allow the user to change these variables if desired. However, realistic values for these parameters cause long run times for the $NDSolve$ command. The install file allows easy extension to different energies, potentials, and initial wave functions.

VI. CONCLUSION

This project was successful in studying the approach of Bohmian quantum mechanics to the finite square barrier. It was shown that the probabilities associated transmission and reflection can be accounted for by considering a statistical ensemble with initial positions distributed according to an appropriate probability density. The concept of a quantum potential is often mentioned in the development of Bohm's theory. However, it is not a necessary feature of the Bohmian approach. This is because the Schrödinger's wave equation, the guiding equation, and an assumption about probability are sufficient for specifying the theory. The quantum potential does not provide "at a glance information" about behavior of the statistical ensemble and so is not useful for judging transmission and reflection. The quantum potential is useful for understanding the behavior of a single particle, since the quantum and normal potential act on a particle according to Newton's second law. The role of the quantum potential, and the transmission and reflection of Bohmian particles can be explored through the manipulator created in this project. An outstanding problem with the manipulator and this project in general is that it cannot handle or relate to realistic physical parameters.

An advantage of Bohmian mechanics over orthodox quantum mechanics is that the concept of measurement does not play a fundamental role in the theory. There is no collapse of the wave function in Bohmian mechanics, and probabilities are understood as arising from ignorance of a system's initial conditions. Thus, Bohmian mechanics is an antidote to the claim that a hidden variable theory is impossible. This project could easily be extended to simulating behavior in other types of potentials. First, however, this would involve resolving the issue of parameter dimensions. Investigating Bohmian mechanics further could involve applying it to areas in which it has an advantage over orthodox quantum mechanics such as dwell and tunneling times, escape times and positions, and quantum chaos [5].

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