BOHMIAN TRAJECTORIES OF INTERACTING PARTICLES TRAPPED IN A TWO-DIMENSIONAL HARMONIC WELL

by

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ABSTRACT

GREGORY KEITHLY. Bohmian Trajectories of Interacting Particles Trapped in a Two-dimensional Harmonic Well. (Under the direction of DR. DONALD JACOBS)

Bohmian mechanics is an alternate formalism of quantum mechanics that posits a particle is always existent, and furthermore there is a separate entity describing a wave-like disturbance in space and time, governed by the Schrodinger equation, that affects the motion of particles through a quantum potential energy. While conceptually palatable, in applications Bohmian mechanics presents notable problems of stability and feasibility when it comes to numerical modeling of multiple particles. After demonstrating basic properties of a Bohmian trajectory for a single particle from an exact model, the approximation scheme developed by Oriols and co-workers is generalized and implemented for two and three particles in a two-dimensional harmonic confining potential well. The original approximation scheme involves a set of coupled Schrodinger equations, one per particle associated with a conditional wavefunction. This separation approach tremendously reduces the computational complexity. Unlike mean field theory typically used in multiple particle systems, the lowest level of this approximation scheme retains space-time correlations between particle motions. Here, this separation approach is extended to generalized coordinates. Consequently, particle dynamics is described by a set of separate conditional wavefunctions, where each conditional wavefunction is associated with a generalized coordinate and its non-commuting conjugate momentum. Correlations in time and space are calculated through a set of p coupled one-dimensional Schrodinger equations for p degrees of freedom in the system. Bohmian trajectories are feasibly calculated with far more practicality as demonstrated with two and three interacting particles.

ACKNOWLEDGEMENTS

TABLE OF CONTENTS

LIST OF FIGURES

Chapter 1: An Introduction to Bohmian Mechanics

Bohmian Mechanics, and indeed all of quantum mechanics begins with the Schrodinger equation [1]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi, \tag{1.1}$$

where $\psi(x, t)$ represents the wave equations which gives us the information we are trying to determine about the system. Essentially any interpretation of quantum mechanics boils down to how one uses the wave equation, and how one interprets the results it provides.

As an example, the current most popular interpretation of quantum mechanics is the Copenhagen interpretation. In this interpretation the square of the absolute value of the wave equation defines the probability of finding a particle at that part of space and time, written as:

$$P(x, t) = |\psi(x, t)|^2. \tag{1.2}$$

In this interpretation the location of a particle is random, where the likelihood for finding the particle in a particular region of space is determined by a probability density function [2]. The precision of the theory is characterized by calculating the probability density after the Schrodinger equation is solved. In some ways the Copenhagen interpretation is quite simple; all one needs to do is solve the Schrodinger equation to determine all possible outcomes that can occur with their probabilities as a response to some sort of measurement. However, the Schrodinger equation is only applicable for an isolated system. As long as the system is not influenced by any external factors, the above prescription is valid. However, measuring the system will influence it in some way and the measurement process will have an effect on the possible outcome depending on the type of measurement, which will subsequently change the state of the system (usually stated as after the measurement is made). This process is referred to

as collapsing the wavefunction into a final state after the measurement process, which is a random selection of all possible outcomes. Conceptually, this line of interpretation is frustrating due to the underlying assumption that elements of a system are inherently random. The conceptual part about how measuring the system changes the system is easy to understand in terms of our everyday experience. For example, in the process of measuring the voltage across a resistor in a circuit using a voltmeter, the measured voltage is different than the actual voltage before the voltmeter was placed in the circuit because the voltmeter itself becomes part of the system. The concept about how a measuring procedure becomes part of the system, thereby causing the system to respond differently than it would have responded otherwise becomes more pronounced as the system size shrinks toward the molecular, atomic and sub-atomic scales. In addition, if one is not sure of what the exact state of the system is in a classical setting, there will be apparent randomness in what will be observed during the measurement process. Again, this apparent randomness increases as the system size becomes small due to the intrinsic sensitivity between noise and signal. These concepts are all well-rooted in measurement theory [3] applied to classical physics.

Unfortunately, the Copenhagen interpretation claims more than experimental evidence can support. It claims that the wavefunction of a system will collapse into a definite state only when it is observed. This would not be a problem if there was a single observer that everyone could agree on as an absolute reference. However, the theory does not define what an observer is, which means this aspect of the Copenhagen interpretation must be thrown out as a meaningless statement. Meaningless statements are not science, because by definition, a meaningless statement cannot be proven by any experiment. It is important to appreciate that the concept of an observer was introduced into the Copenhagen interpretation to deal with the

collapsing of the wavefunction, which is needed to be consistent with the apparent randomness and intrinsic uncertainties found in measurements, and for which the theory predicts correctly. Interestingly, one can remove the observer from quantum mechanics without difficulty. What cannot be removed, is how the measurement process affects the outcome of an experiment. The very process of measuring what state a system is in, actually changes the state in a non-local way. Perhaps, the concept of an observer has been elevated beyond the tangible concept of "measurement apparatus", which would serve as an observer. Regardless of why the observer concept has led to the Schrodinger cat paradox, and other philosophical conundrums, the Copenhagen interpretation has not only survived, but has become the standard view of quantum mechanics by many generations of physicists. The strength of the Copenhagen interpretation is in the calculational power of the Schrodinger equation, and the law of large numbers. Make enough experimental measurements with identical setups, and the average values predicted by quantum mechanics is in good agreement with the ensemble of experimental results.

An alternative view that eliminates the observer concept is the Bohmian interpretation. Physicist David Bohm first proposed this alternate interpretation of the Schrodinger equation in 1951 [4][5], and mathematically his framework boils down to writing the wave function in polar form:

$$\psi = Re^{\frac{iS}{\hbar}} \tag{1.3}$$

where both $R(x,t)$ and $S(x,t)$ are real functions of both position and time. These two functions then correspond to both the position and velocity via the equations

$$P = R^2 \tag{1.4}$$

$$v(x) = \frac{\nabla S}{m} \tag{1.5}$$

By plugging this polar form of the wavefunction into Schrodinger's equation, one can then derive two coupled partial differential equations to solve for both R and S given as:

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}[R\nabla^2 S + 2\nabla R * \nabla S] \tag{1.6}$$

$$\frac{\partial S}{\partial t} = -[\frac{(\nabla S)^2}{2m} + V(x) - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}] \tag{1.7}$$

The function $S(x, t)$ is the action, and the gradient of the action gives the momentum of the particle. Viewed in this way, the momentum and position of a particle are always defined at the same time, as long as the system is isolated. When one attempts to measure what the momentum and position of the particle is, one must couple some sort of measuring apparatus to the system, expanding the relevant degrees of freedom and having additional equations coupled. In Bohmian mechanics, one cannot ignore how one measures something. It must be modeled explicitly. In the process of measuring these properties, the position and momentum of the particles in the system will radically change relative to what they would have been if the measurement process was not performed. The outcome depends on the interactions between the system and its environment, which is dictated by the measurement apparatus and the experimental procedures used during the measurement process. [6][7]

The equations of Bohm map directly to the classical Hamilton-Jacobi equations. This means the equations for quantum mechanical systems are not much different than classical equations of motion in the sense that the equations of motion are deterministic. However, the equations of motion that derive directly from the Schrodinger equation have an additional force term that is not present in classical physics. When one converts the Hamilton-Jacobi equations in the form of Newton (e.g. F = ma), it becomes apparent that there is an extra force that is not accounted for in classical physics. This force derives from what is called the *quantum potential* given by: $-\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$. This potential depends on the configuration of all particles in a system,

which in this aspect alone is not different than any other kind of potential energy. The interesting

aspect that is present even for a 1 particle system, is that the quantum potential has a peculiar

form that does not appear in classical physics. Namely, the strength of the field, given by R, is in

the denominator. This means, no matter how small the field becomes, the influence on a particle

is long ranged (formally spanning across the universe). Thus, the quantum potential represents a

non-local field that affects the movements of particles. Mathematically, this force is calculated

using the wavefunction solution to the Schrodinger equation.

Conceptually Bohmian mechanics has many advantages over the Copenhagen

interpretation. For example, Bohmian mechanics has no wave/particle duality paradox. Under

Bohm's theory the particle is a physical object that exists at all points in time, and there is a wave

disturbance in space-time that affects particle motion manifested as a non-conservative force

derived from the quantum potential, which is associated with non-local effects. While models

within Bohmian mechanics make extensive use of time evolving probability densities, this is

because it is most convenient to consider what an ensemble of particles will do, so that one can

calculate average properties. In the same way one can map a classical set of trajectories in phase

space using Hamilton's equations of motion into a "fluid" flow problem, the Bohmian equations

of motion will work in the same way. Therefore, the randomness observed experimentally is

explained through the chaotic trajectories that appear in the ensemble of particles. Bohm showed

that independent of the initial conditions, the system will rapidly converge to an equilibrium

probability density that is the same probability density predicted by the Schrodinger equation.

Hence, there is no difference in the mathematical predictions. Said more simply, the randomness

found in the Copenhagen interpretation is explained under Bohm's interpretation as not knowing

the exact position and momentum of the particle before it is measured, as well as the influence of the measuring apparatus [8].

Within Bohmian Mechanics the inherent strangeness of quantum mechanics is reliant on additional factors that are not fully understood rather than quantum systems behaving inherently differently than classical. The quantum potential creates the apparent randomness that is measured due to volatile motions of particle trajectories. Moreover, the entangled states that are frequently invoked to demonstrate non-locality in quantum mechanics is retained in the Bohmian formalism through the quantum potential since the wavefunction has the entangled information. Non-local effects are fully associated with the wavefunction, and the collapse of the wavefunction becomes a continuous process as the particle configuration changes. Specifically, the collapse of the wavefunction is a deterministic process, which can be reversed in principle. In fact, recent experimentation has demonstrated that elements such as the transition of an electron to higher energy levels can be reversed while still in the process of occurring [13]. As another example, these wild chaotic motions are consistent with observations that indicate it is nearly impossible to predict which slit a particle goes through in a double slit experiment exhibiting quantum interference [9]. Additionally, experimentation in recent years has demonstrated that elements of the universe are not quite as spontaneous

Unfortunately, mathematically, and especially computationally, Bohmian mechanics has issues that prevents it from becoming widely adopted to calculate quantum effects. One source of difficulty is that the quantum potential features the $\frac{1}{R}$ term, which renders any attempts to simulate quantum trajectories as inherently unstable. A second source of difficulty is due to the coupled nature of Bohm's equations. As a back of the envelop calculation, naive brute force calculations of the Bohmian equations on a grid rapidly become practically impossible to carry

out on a super computer. To demonstrate the importance of this, if a system in 1 dimension requires M grid points (say M is 10^6), then to model N particles in 3 dimensions over the same span of physical space per dimension would require an array of size M^{3N}. For 10 particles, one would need 10^{180} grid points. Besides this large memory requirement, the time increment is in the sub-femtosecond range, meaning there might be 10^8 $calculations$ over the entire grid to simulate sufficient time of practical interest. Hence, simulating Bohmian equations of motion in a brute force way is completely unfeasible for our current computational abilities. However, if one can separate out the particles the array would then become size $N \times M^3$, and if the variables themselves are separated then the array's size reduces further to $3N \times M$. For 10 particles, this would require 10^8 $calculations$ over 3×10^7 grid points, which is feasible to carry out on a laptop.

In the ~70 years since Bohm initially proposed his theory, physicists have worked to mitigate these two problems. Bohm's equations can be adjusted to allow for better stability, and methods of separating particles with low levels of coupling have been determined. This thesis will focus on the second point, based upon a 2015 paper by Oriols et. al. [10] that models a N particle quantum system as N coupled Schrodinger equations. Inspired by the Oriols method of separation of particles with low levels of coupling, this thesis will attempt to take the decoupling approximation a step further and separate out to all conjugate variables. That is, given a generalized coordinate Q, and its conjugate momentum P, these conjugate variables will be tied to a 1D Schrodinger equation. The various (Q,P) conjugate pairs will be determined by classical physics. Then, a separate 1D Schrodinger equation for each conjugate pair of variables will be written. However, the 1D Schrodinger equations are not in a closed system. Rather, the other degrees of freedom from the same particle, or from other particles in the system, or from a

measuring apparatus, will affect each other. This means the potential energy is changing in time, as the particle configuration changes.

In essence, we are solving a $F = ma$ problem involving N particles, and everything follows along the same way as the classical equations of motion, except there is also a quantum potential, which is updated as the particles move, in the same way that all other potential energies are updated as particles move. In this thesis, one-, two- and three-particle systems embedded in two dimensions will be considered to test if the generalization of the method proposed by Oriols has merit. Modeling a closed three particle, 2D system will require six coupled Schrodinger equations to solve. Section 2 will discuss the general framework behind this separation of variables, section 3 will discuss an exact solution for a quantum harmonic oscillator to examine the motions expected from a single particle, and section 4 will demonstrate the trajectory of two and three particles utilizing separation of variables within a harmonic oscillator. Additionally, the same system modeled under the classical Hamilton's equations of motion (without the quantum potential) will be included to demonstrate the differences between Bohm's theory and the classical method as length scales and masses of the particles are modified.

Assuming this endeavor is successful, it will lend more feasibility towards the usage of Bohmian mechanics to model multi-particle interactions. While this thesis does not focus on the theoretical implications of Bohm's equations, instead focusing on the numerical side, having more modeling capabilities would render the theory far more workable going forwards, especially as recent experimentation begins to lend more credence to the Bohmian interpretation or other similar interpretations. A good example is a 2019 experiment that managed to track the movement of an electron from one energy state to the next [13]. This is something that should be impossible within the Copenhagen interpretation given that in that interpretation the travel from

one energy state to the next is supposed to be instantaneous. And while this one experiment

hardly disproves the entire interpretation, it does demonstrate the importance of considering

models of quantum mechanics beyond the one that is the most popular.

Chapter 2: Separation of Variables

The paper [10] that the majority of this thesis's theory is pulled from is admittedly more focused on trying to explain Bohmian mechanics in a simple three-dimensional system. This is as opposed to the more commonly used 3N dimensional configurational space that the wavefunction in quantum mechanics represents. Working with a time independent Schrodinger equation to find eigenfunctions is computationally simpler than trying to numerically directly evolve the wavefunction. It is worth noting that the configurational space used to describe the quantum state does not have a direct correspondence to the macroscopic world as we understand it. While this thesis will not attempt to explain everything in one three-dimensional setting, the methodology by which the paper separates out the particles is still beneficial for our purposes.

In the event you have a two-particle system, the wave function would take the form of $\psi(x_1, x_2, t)$, where x_1 and x_2 refer to trajectories $X_1(t)$ and $X_2(t)$. Thus, the Schrodinger equation for this system has the form:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_1} \nabla_1^2 \psi - \frac{\hbar^2}{2m_2} \nabla_2^2 \psi + V(x_1, x_2, t)\psi \tag{2.1}$$

While not as easily solvable as the single particle Schrodinger Equation, the Schrodinger Equation can be split apart. A key method that the 2015 paper presents is to separate out the two-particle equation into two conditional wave equations. The conditional wave equation is defined as the wave function for one particle defined at the positions for all other particles in the system. For our two-particle system the conditional wave equations become:

$$\psi_1(x, t) = \psi(x, x_2, t)|_{x_2 = X_2(t)} \tag{2.2}$$

$$\psi_2(x, t) = \psi(x_1, x, t)|_{x_1 = X_1(t)} \tag{2.3}$$

In the idealized case, where the potential energy of the system in fully noncoupled, i.e. when $V(x_1, x_2, t) = V(x_1, t) + V(x_2, t)$, we can follow the standard quantum mechanics method of separation of variables. Via this method, the wavefunction $\psi(x_1, x_2, t)$ can be rewritten to take the form of $\alpha(x_1, t)\beta(x_2, t)$, assuming of course that both α and β solve the 1D Schrodinger equation. In this idealized case, one can easily demonstrate that the conditional wave functions are proportional to the standard separation of variables.

$$\psi_1(x, t) = \psi(x, x_2, t)|_{x_2 = X_2(t)} = \alpha(x, t)\beta(x_2, t) \tag{2.4}$$

$$\psi_1(x, t) \sim \alpha(x, t)$$

The decoupling in the potential energy allows us to separate out by particle for any such situation. However, this is the idealized case, and generally the potential energy will involve coupling. For example, a potential energy of $V(x_1, x_2, t) = V_1(x_1) + V_2(x_2) + Cx_1x_2$ (where C is some constant that represents the amount of coupling) cannot be formally separated. While one cannot separate out the equation into two decoupled equations, for small enough levels of C the conditional wave equations can still be written in such a way that the final result is well approximated to the true value.

$$i\hbar \frac{\partial \psi_1(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_1(x,t)}{\partial x^2} + V(x, X_2(t))\psi_1(x, t) \tag{2.5}$$

$$i\hbar \frac{\partial \psi_2(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_2(x,t)}{\partial x^2} + V(X_1(t), x)\psi_2(x, t) \tag{2.6}$$

As such, assuming small levels of coupling, this approach is a powerful generalization to the method of separating out variables. The 2015 paper [10] works with conditional wavefunctions in terms of a hierarchical expansion to infinite orders, but derives the above equation as the lowest level approximation. For practical calculations, if greater accuracy is desired, there are next order correction terms that bring in additional coupled equations through a systematic set of hierarchical equations. For the exact solution, there will be an infinite set of coupled equations,

where each level involves higher powers of the coupling. This hierarchy of coupled equations can be truncated rapidly for weak coupling, and the above equations were shown to be quite accurate for the weak coupling case.

While the initial paper only separated out by particle, a postulate of this thesis is that if that much is possible, then separating by variable as well should also be feasible as a general approximation method. Considering the power of Lagrangian and Hamiltonian formulations of classical mechanics, it readily becomes clear that it is imperative to work with generalized coordinates and their conjugate momentums to maintain mathematical consistency. Trying to solve the wavefunction for the hydrogen atom lends itself as a good example of why stopping at the particle level for conditional wavefunctions is inadequate. A hydrogen atom consists of two particles (a proton and an electron), each of which has its own coordinates. By following the method detailed in the paper, one would essentially treat a hydrogen atom as two coupled 3D systems, involving a proton and an electron. However, as is well established in classical physics, a two-body problem can be reduced to a 1-body problem by using the center of mass coordinates and the relative position coordinate between the particles [11]. The center of mass coordinates of the hydrogen atom can be further separated in each dimension (e.g. Xcm, Ycm, Zcm), and for the discrete energy spectrum characteristic of the hydrogen atoms, the effective Hamiltonian can be further separated into three separate differential equations by using a spherical coordinate system. This example motivates why demanding validity for the quasi-separation process in terms of conditional wavefunctions is postulated to be applicable at the level of conjugate variables. From a different side of the argument, if this was not possible, then the parallel of Bohmian mechanics mapping to the Hamilton-Jacobi equations would be invalid, and hence Bohmian mechanics would have to be discarded in the form that Bohm derived (e.g. classical

equations of motion plus a quantum potential). This would imply the starting point is wrong, and thus the Schrodinger equation is wrong. The simplest thing to postulate is that all the machinery of classical mechanics carries over to quantum mechanics, except there is an additional force caused by the quantum potential that is non-local.

Chapter 3: Understanding Bohmian Trajectories: Exact Solution

This thesis is to be solved for a harmonic oscillator. As such the potential energy of the system will be $V = \frac{1}{2}kx^2$ where k is the spring constant and x is the distance from the origin, where the potential would be zero. While most quantum systems are too complex to solve the Schrodinger equation exactly, a harmonic oscillator presents numerous exact solutions. These solutions depend on the original conditions of the gaussian wavepacket. For this thesis, I will consider an exact solution (pulled from an online worksheet on quantum mechanics and later confirmed) and observe how it predicts the actions of the particle in this situation. The purpose for doing this is to familiarize ourselves with how quantum trajectories differ from classical trajectories where the quantum potential is absent.

To begin with we will use an initial, time independent wave function assuming no momentum:

$$\psi(x) = (\frac{m\omega}{\hbar\pi})^{\frac{1}{4}} * \exp\left(-\frac{m\omega}{2\hbar}(x - x_0)^2\right) \tag{3.1}$$

Where x_0 is the initial position of the wavepacket. Utilizing the Schrodinger equation one can expand this wave function out to its time dependent version. Performing these calculations will result in the wave function:

$$\psi(x,t) = (\frac{m\omega}{\hbar\pi})^{\frac{1}{4}} * \exp\left\{-\frac{m\omega}{2\hbar}(x - x_0\cos(\omega(t - t_0)))^2 - i\frac{m\omega}{\hbar}xx_0\sin(\omega(t - t_0)) + \right.$$

$$\left. i\frac{1}{4}\frac{m\omega}{\hbar}x_0^2\sin(2\omega(t - t_0)) - i\frac{\omega}{2}(t - t_0)\right\} \tag{3.2}$$

In this instance t_0 refers to when the time dependent wave equation simplifies down to the form of the time independent wave function, i.e.

$$\psi(x,t_0) = (\frac{m\omega}{\hbar\pi})^{\frac{1}{4}} * \exp\left(-\frac{m\omega}{2\hbar}(x - x_0)^2\right) \tag{3.3}$$

Which can be easily observed by plugging t_0 into the time dependent equation.

With this equation, one can then divide it up into the elements of Bohm's original

equation $\psi = Re^{\frac{iS}{\hbar}}$, such that:

$$R = \psi(x,t) = \pi^{-\frac{1}{4}} * \exp\left(-\frac{m\omega}{2\hbar}(x - x_0 \cos(\omega(t - t_0)))^2\right) \qquad (3.4)$$

$$S = -\hbar\left(\frac{m\omega}{\hbar}xx_0 \sin(\omega(t - t_0)) + \frac{1}{4}\frac{m\omega}{\hbar}x_0^2 \sin(2\omega(t - t_0)) - \frac{\omega}{2}(t - t_0)\right) \qquad (3.5)$$

And from the equations for quantum potential and velocity can be calculated given the equations

given above. From this we find that:

$$U = -\frac{\hbar^2}{2m}\left(\left(\frac{m\omega}{\hbar}\right)^2(x - x_0 \cos(\omega(t - t_0)))^2 - \frac{m\omega}{\hbar}\right) \qquad (3.6)$$

$$v = -\omega x_0 \sin(\omega(t - t_0)) \qquad (3.7)$$

Where U is the Quantum Potential Energy. Two elements immediately become apparent looking

at the S and velocity equation. First is that the velocity of the particle depends solely on the

nature of the wave packet, and not the actual position of the particle. As such any particle

associated with this wave packet will have the same oscillation regardless of if it is in the center

of the potential well or on the edge. Secondly, the time independent wave function has no

imaginary element. This means that S and therefor velocity will be 0, and thus under the

Bohmian interpretation t_0 can be thought of as the time when the particle is at rest. This setup

can be thought of as a pull and release initial condition, where assuming $t_0 = 0$, the particle
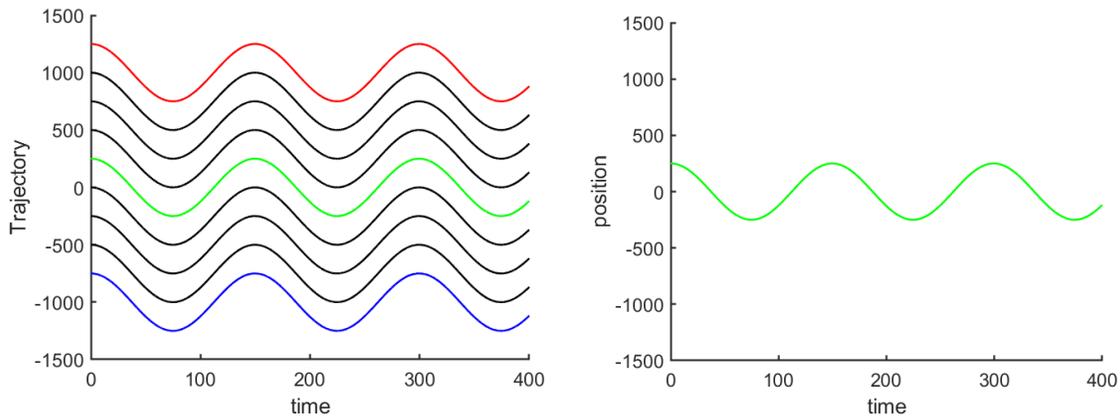
begins at rest but has a force acting upon it.

Figure 1: The trajectory of several particles for $x_0 = 250\ Ang$, $to = 0\ fs$, k=1e-4 $\frac{eV}{Ang^2}$, ranging in initial position from -750 to 1250 Ang (left). In all instances the particles follow the same oscillation pattern but with different positions. In this instance green corresponds to the trajectory closest to the classical case (right). These figures will have to be improved for the final thesis.

More interesting behaviors can be observed when one determines the equation for the trajectory of the particle by integrating the velocity equation. This leaves us with a trajectory equation of:

$$x = x_0 \cos\big(\omega(t - to)\big) + x_p - x_0 \tag{3.8}$$

Where x_p is defined as the position of the particle at time to. Plugging this equation into the Quantum Potential Energy equation leaves us with:

$$U = -\frac{\hbar^2}{2m}\left(\left(\frac{m\omega}{\hbar}\right)^2 (x_p - x_0)^2 - \frac{m\omega}{\hbar}\right) \tag{3.9}$$

Where Quantum Potential Energy becomes independent of time and instead depended only on the position of the particle and center of the wave packet at time to. Additionally, when one considers the situation where the particle's position is at the center of the wavepacket, i.e. where $x_p = x_0$ we are left with.

$$U = \frac{\hbar\omega}{2} \tag{3.10}$$

This essentially acts as the maximum possible value for the quantum potential, and farther away

a particle moves from x_0 in either direction the larger the negative magnitude of the quantum
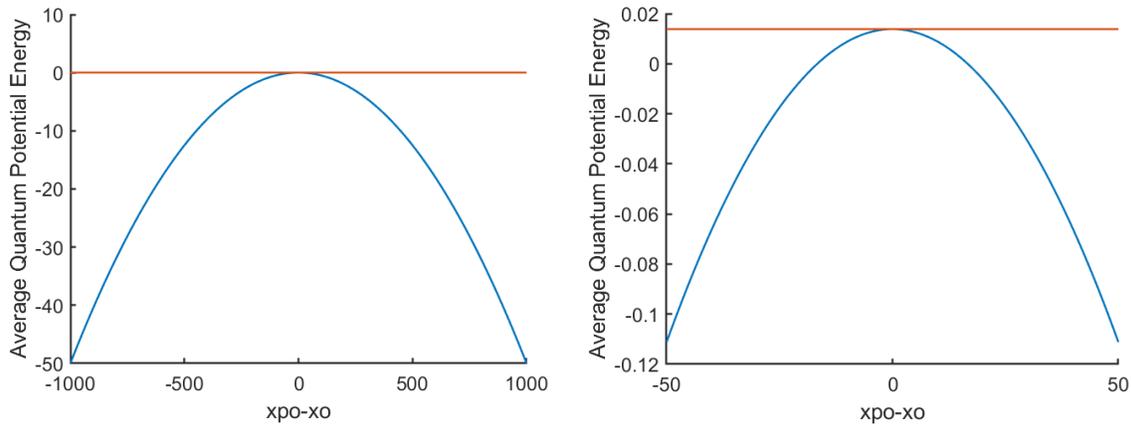
potential energy becomes.

Figure 2. The average quantum potential energy plotted vs $x_p - x_0$ for particles with the same

conditions as figure 1. The strait horizontal line represents the value of $\frac{\hbar\omega}{2}$.

One interesting dynamic of this exact solution is that the presence of quantum potential

energy causes the system to not follow conservation of energy. Energy is conserved per cycle, so

regardless of the amount of quantum potential energy the average energy for each oscillation the

average energy is conserved. However, the greater the negative magnitude of the quantum

potential, the more the total energy of the system will vary from moment to moment. Essentially,

the quantum potential can be thought of as an outside force acting upon the system. The greater

this outside force, the more the trajectories of the particle will stray from the actions one might
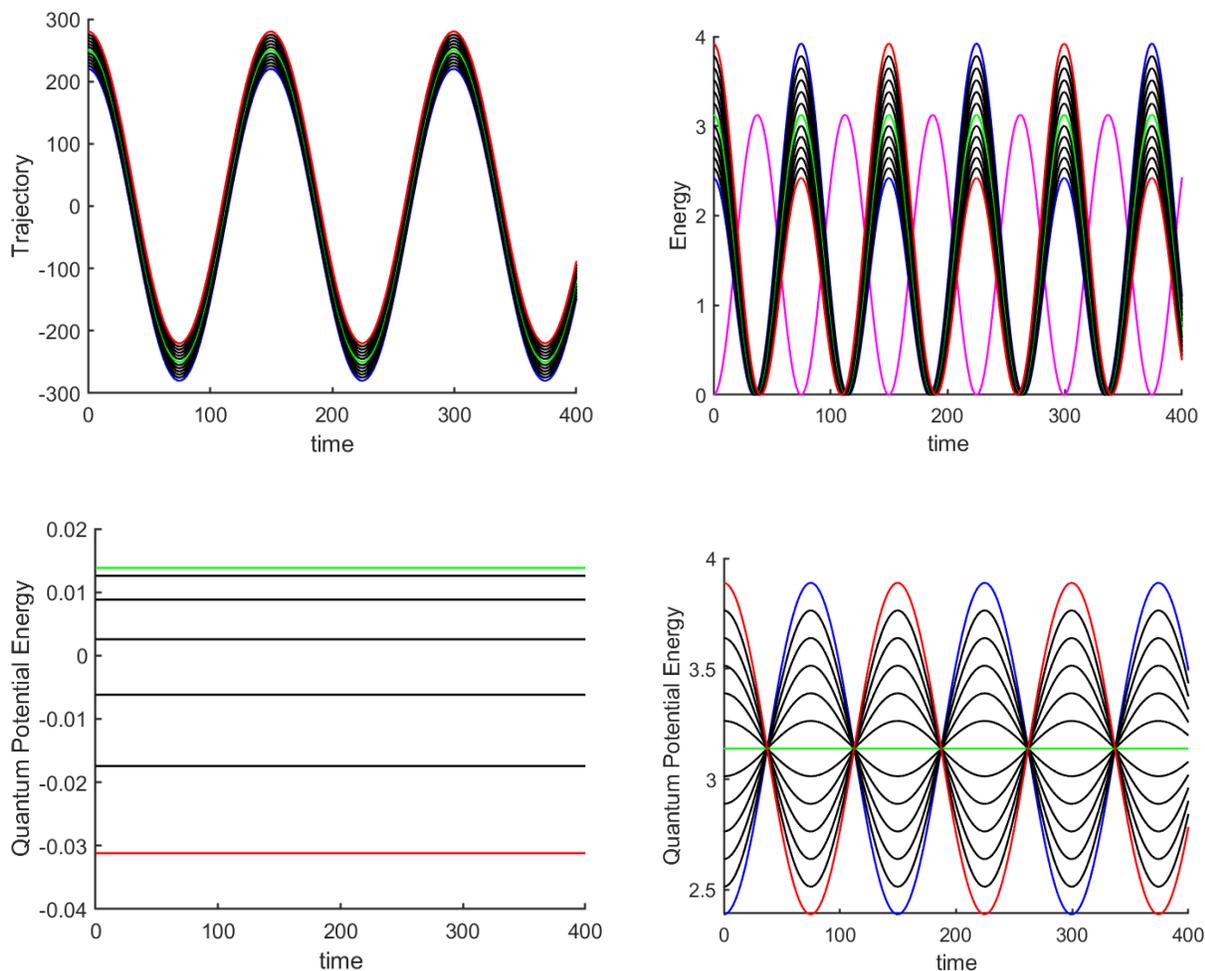
expect within classical mechanics.

Figure 3. The trajectory of several particles with the same conditions as figure one, ranging in initial position from 220 to 280 Ang, as well as various energies. In all plots, red, blue, and green correspond to the same particle, with green being the particle most closely matching the classical case. In the top right plot the magenta line corresponds to kinetic energy (which is constant for all particles), while the varied line is the standard potential energy. The bottom right plot represents total energy, which in this case is defined as the sum of kinetic, potential, and quantum potential energy.
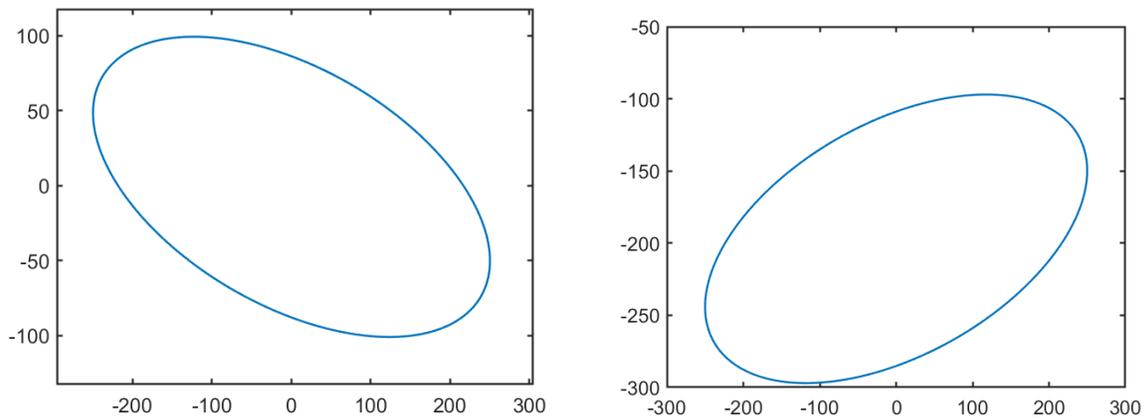
Figure 4. Two examples of this exact solution expanded out to two dimensions. The figure on the left represents the particle in the center of the wavepacket for both the x and y direction, resulting in an essentially classical trajectory. The figure on the left is a particle that is near the center of the wavepacket in the x direction, but far removed in the y direction. This results in its y oscillations occurring well away from the origin.

It is worth noting that this exact solution represents a somewhat idealized case of the wave function, hence its comparatively reasonable solution. However, given that two solutions to the Schrodinger equation will additionally solve the Schrodinger equation, we can use this to simulate the more complicated wave scenarios one might encounter in Quantum mechanics. Thus we define as new wavefunction ψ_{new} which would be equal to the following.

$$\psi_{new} = \frac{1}{\sqrt{2}}\psi|_{x_0=x_0} + \frac{1}{\sqrt{2}}\psi|_{x_0=-x_0} \tag{3.11}$$

We can then compare the actions of this equation for various values of x_0 and SigmaX, where SigmaX is defined as the uncertainty in the wave packet, and can be determined via the equation:

$$\sigma_X = \sqrt{\frac{\hbar}{m\omega}} \tag{3.12}$$

For situations where $\sigma_X \cong x_0$ we find that the two elements of the wave simply overlap without interfering. However, when $\sigma_X \ll x_0$ we instead see two separate peaks that, when they overlap,

create a notable interference pattern. It is this interference of wavepackets that produce the

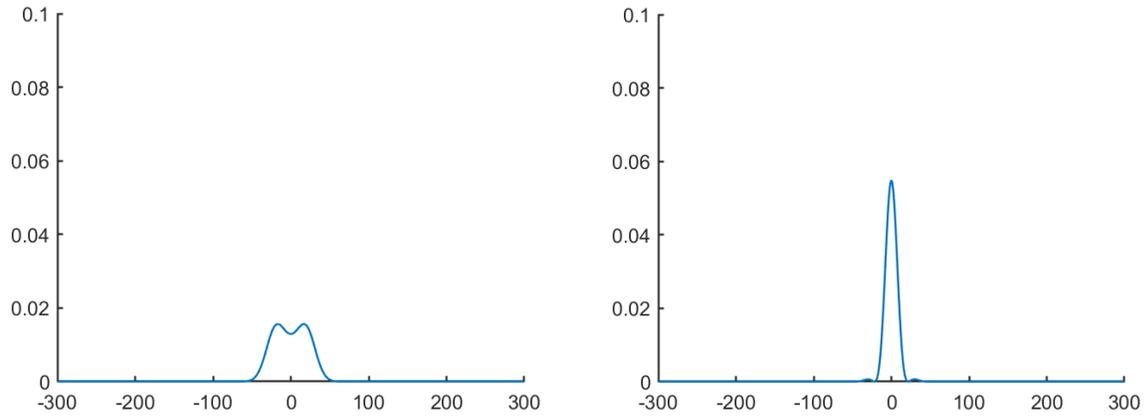quantum effects we see when multiple particles interact.

Figure 5. The overlap of the two elements of the wave function when $\sigma_X \cong x_0$ (σ_X=16.6291
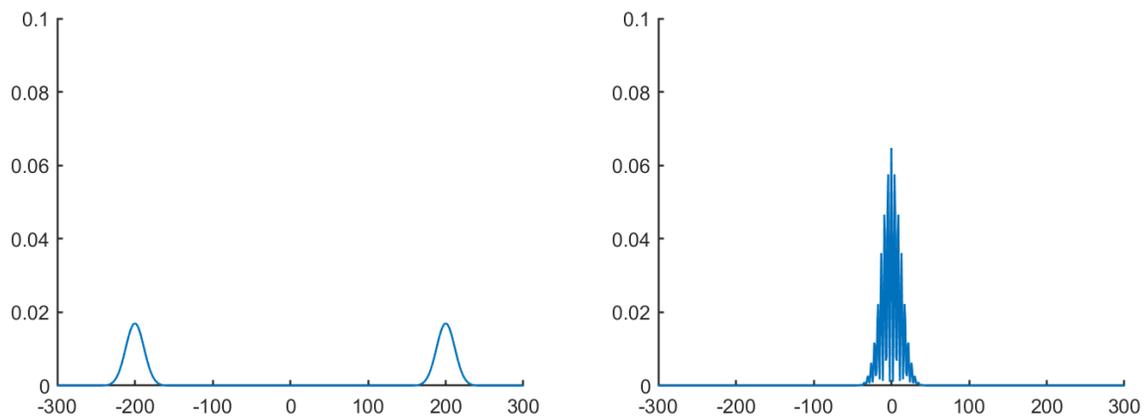
while $x_0 = 20$).

Figure 6. The interference pattern created from the overlap of the two elements of the

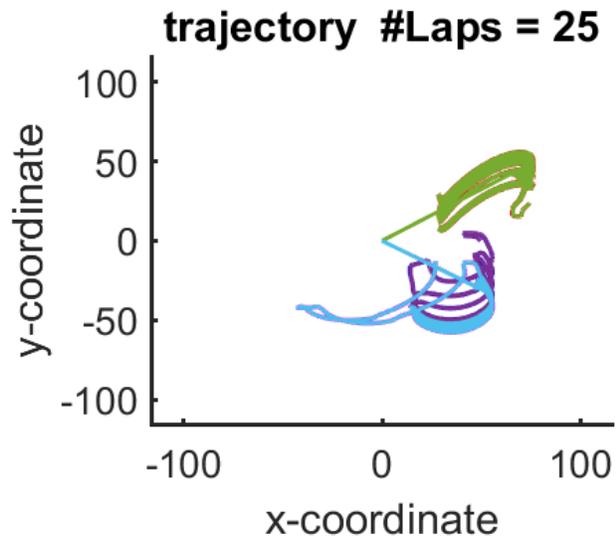wavefunction when $\sigma_X \ll x_0$ (SigmaX=16.6291 while $x_0 = 200$).

Figure 7. The trajectory of a particle in three separate positions under the effects of the of a wave interference pattern like the one from figure 6. As shown the particle behaves in a decidedly non-classical trajectory.

Chapter 4: Interacting Particles

In order to demonstrate the results found from separation of variables, we have created

models that replicate the actions of multiple particles in both the classical and quantum

trajectories of up to three particles in a two-dimensional system. For the classical case it was

decided to utilize a 4th order Runge-Kutta method to solve and maintain conservation of energy.

Meanwhile for the quantum solution it was decided to utilize a leapfrog method that alters

between a timestep of dt for the real elements of wave function and .5dt for the imaginary

details. It is worth mentioning that due to the numerical issues inherent in Bohm's original

equations, they were not utilized directly to solve for the particle trajectory. Instead, the wave

function of was solved directly using the Schrodinger equation and then the elements of R and S

were solved for via the equations

$$R = |\psi| \tag{4.1}$$

$$S = atan2(\psi_{imaginary}, \psi_{real}) \tag{4.2}$$

Admittedly this method of solving for Bohmian mechanics is one of the more derided elements of

current Bohmian mechanics, as using it essentially means adding extra steps onto an already solved

wave function. However, performing these additional steps allows us to actually see the trajectory

of the particle as opposed to standard quantum mechanics, so it is not much of a detriment.

To facilitate particle interaction, an extra potential energy term was added:

$$U_{interaction} = \frac{k_{int}}{2}(r - r_0)^2 \tag{4.3}$$

Where k_{int} is the spring constant for particle interaction (which can be set to a different value than

the k from the standard potential energy equation), r is the distance between two particles, and r_0

is defined as the resting length between the two particles. Every particle pair will have its own

value of U, resulting in only one for two particles and three for three particles. While this equation is utilized for both the classical and quantum cases, the definition of r changes between the two. In the classical case we only have a particle to worry about. Thus, r can be thought of simply as the distance between those particles, which can then be broken into x and y components to facilitate separation of variables. In the quantum case however, there is also a wave to account for. If we are working with the x variable, then solving for the r value must be a function in the x direction. In this case, we notice that the y value of each particle is a constant at each timestep, while x is describing a wave covering all possible x values. In this case r becomes a function of all values of x. In general, r between any two particles j and k takes the form of:

$$r_{jk} = \sqrt{(x - x_k)^2 + d_{jk}^2} \tag{4.4}$$

Where d_{jk} is the perpendicular distance between respective x axis of the two particles, with the equation being solvable for any x position along the axis of the particle r is being measured for.
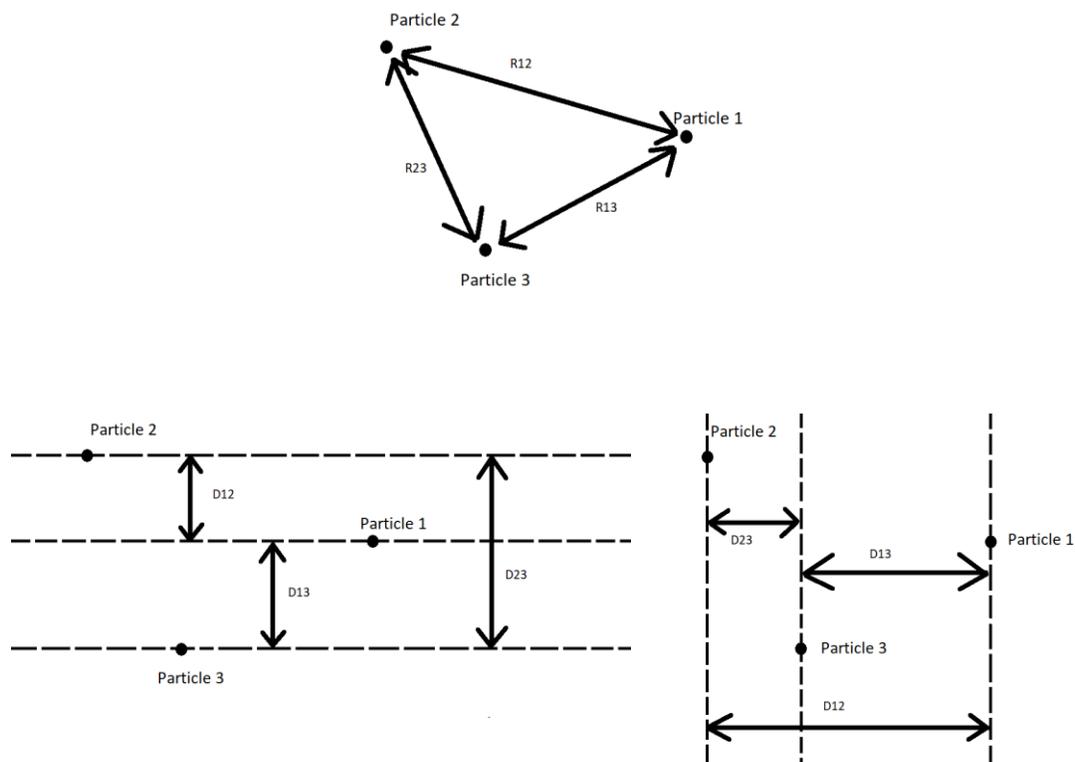
Figure 8. Visualization of the method for determining. the values of r in both the classical case (top) and quantum case (bottom two).

Through the methods discussed above, particle interaction for two and three particles could be consistently modeled, with CPU time being reasonable even for a non-dedicated computer. The rest of this section will demonstrate the more noteworthy elements found during the modeling process.
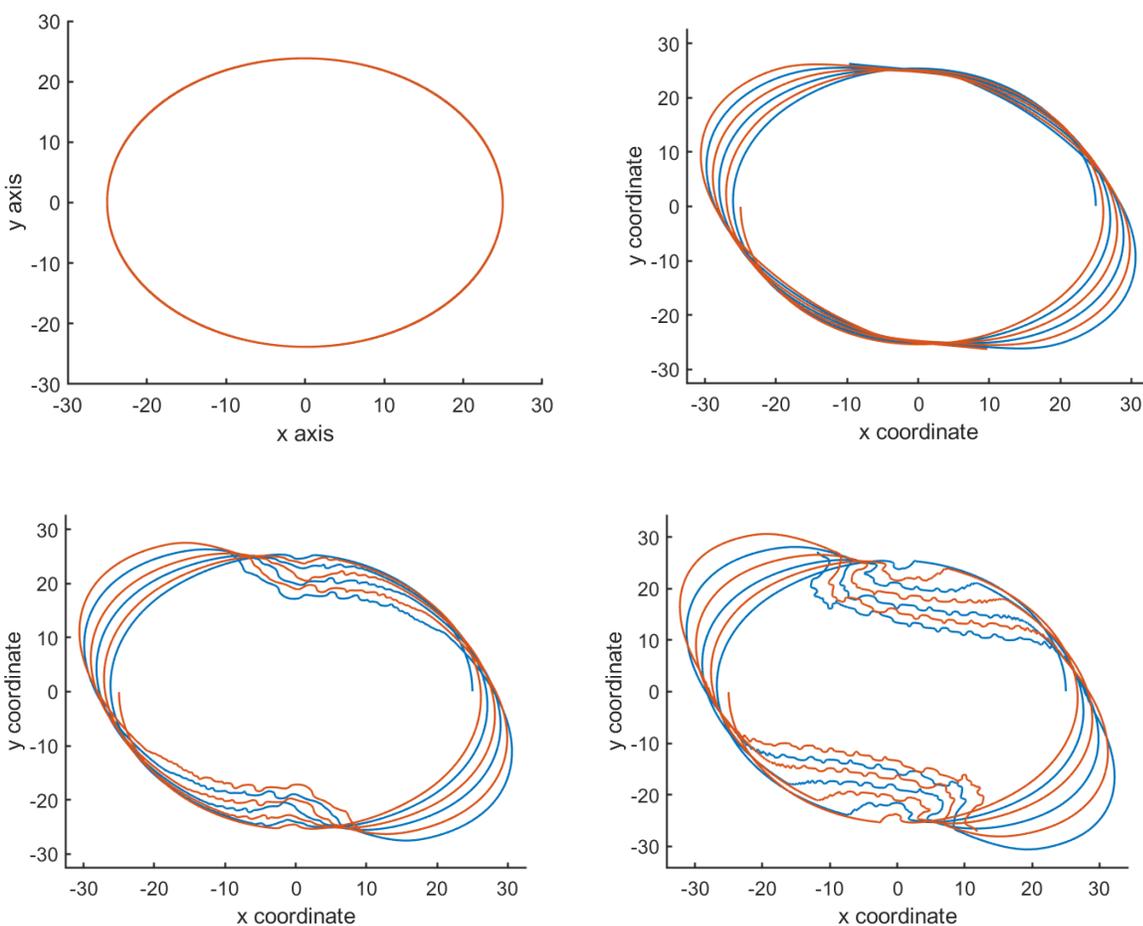
Figure 9. Two particles 25 Angstrom from the x axis, one on the positive side with a velocity of $10 \frac{Ang}{fs}$ in the positive y direction, the other with a velocity of $10 \frac{Ang}{fs}$ in the negative y direction. Spring constant of .01 $\frac{eV}{Ang^2}$ for both well and interaction. The plots represent the classical case (top left), σ_R=10 Ang (top right), σ_R=40 Ang (bottom left), σ_R=80 Ang (bottom right).

      As the uncertainty of the wave packet (and thus its width increases) the waves of the particles interact more and more, resulting in more quantum-like interactions for the particles. Meanwhile when σ_R is comparatively low the particles behave closer to their classical equivalent where they simply orbit each other. It's also worth mentioning that the wavering of lines in the

r_0=40 and 80 Ang cases could be a result of quantum effects, or numerical instability in the code. It is up to further refinement to determine if they are an inherent property of the system.
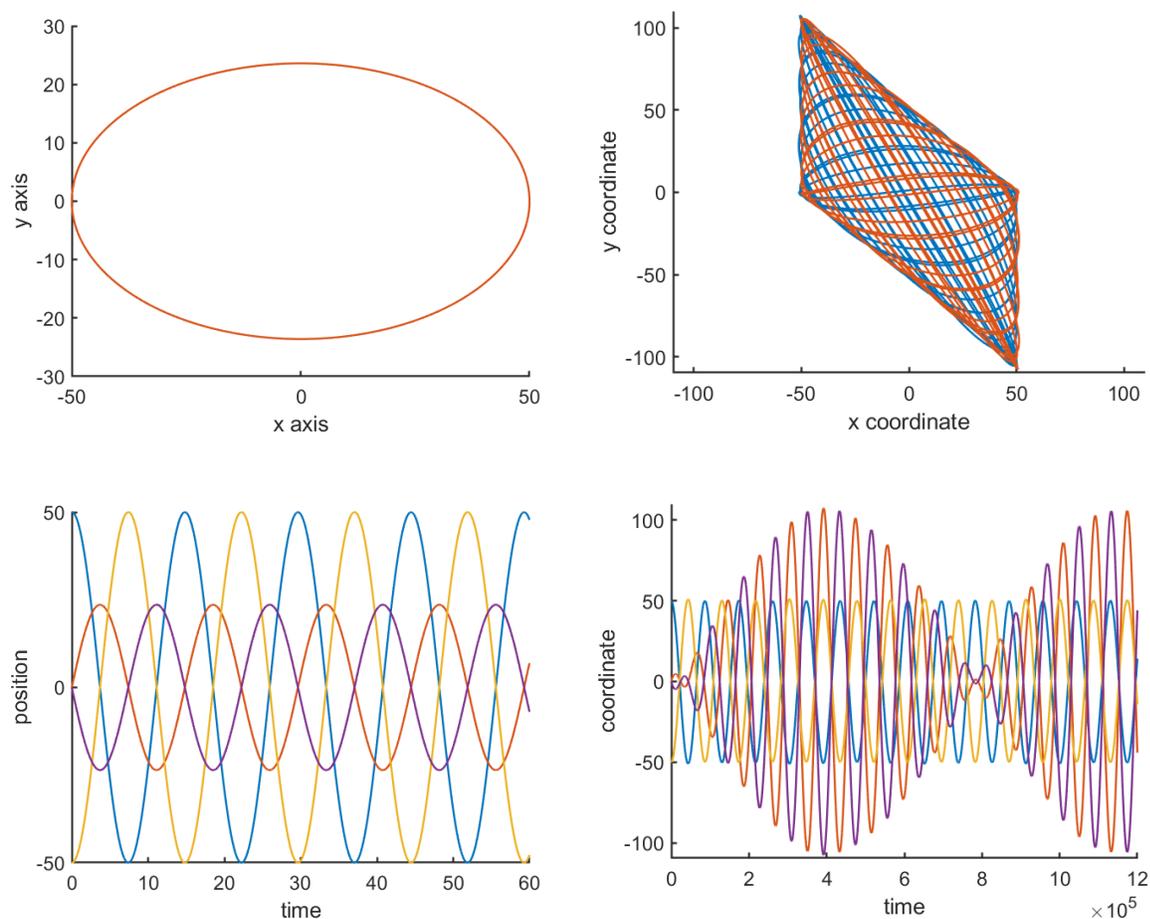

Figure 10. Trajectory of two particles in both the classical (left) and quantum (right) models. Two particles with initial positions of 50 and -50 Ang on the x axis, with initial velocities of 10 $\frac{Ang}{fs}$ in the positive and negative y direction respectively. r_0 =0 and σ_X=10 Ang. Spring constant of potential and interaction are both .01 $\frac{eV}{Ang^2}$.

Of note is how different the separate results are. In the classical case the two particles simply orbit around each other, while in the quantum case the particles travel to form a

parallelogram shape. At a low value of r_0, the trajectory of the particle becomes completely
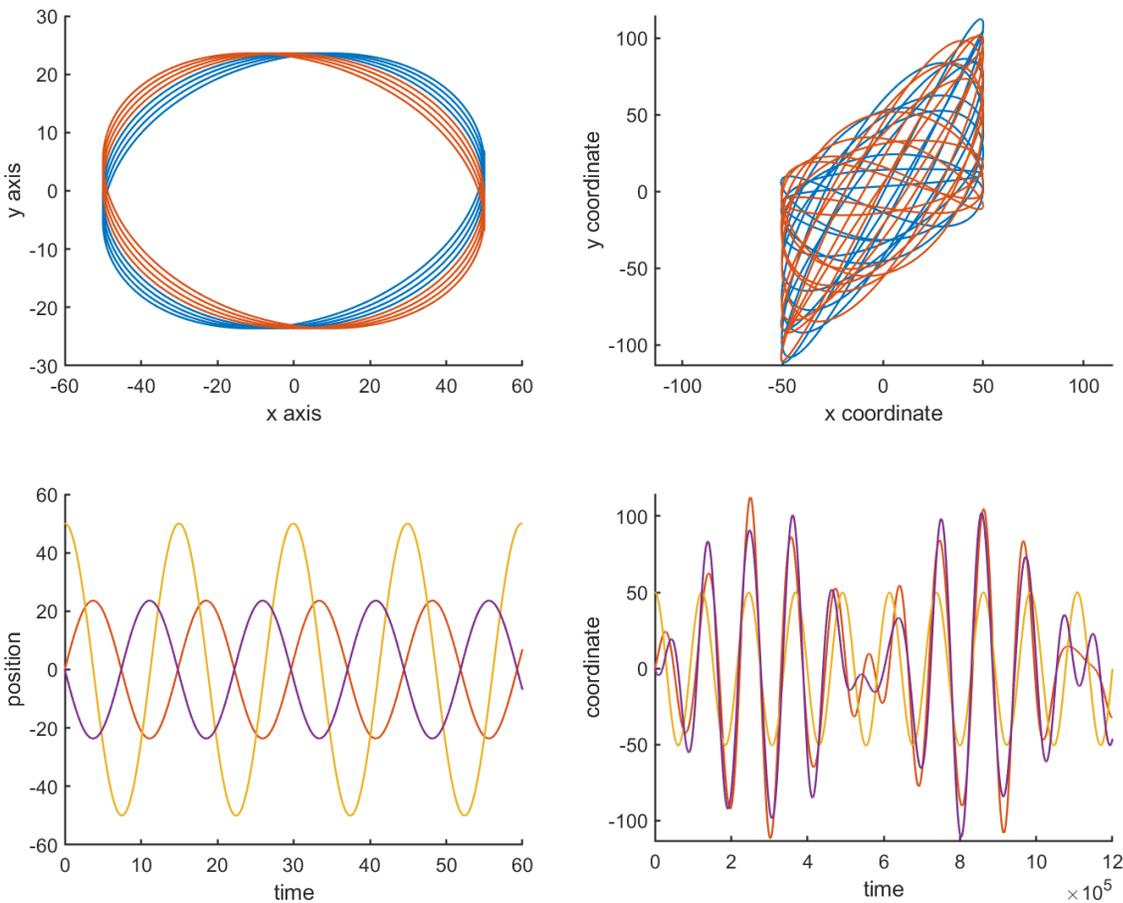
unrecognizable from the classical case.

Figure 11. Two particles of same initial position of 50 Ang on the x axis, with one having an

initial velocity of $10 \frac{Ang}{fs}$ positive y direction and the other having an initial velocity of $10 \frac{Ang}{fs}$ in

the negative y direction. Spring constant of potential and interaction are both $.01 \frac{eV}{Ang^2}$, and

σ_X=10 Ang, and r_0=0. Once again, a classical trajectory (left) and quantum trajectory (right).

Of note is that while the classical trajectory is symmetrical, this is not at all the case for

the quantum case. The particle with an initially positive velocity travels upwards, while the

particle with an initial downward velocity quickly changes directions to follow the first particle.

Interestingly this is completely unaffected by the order in which values are numerically

calculated, meaning that (at least within our system) this is an inherent property. There was no indication that these results are influenced by numerical error, but refinement of the code is needed and will allow a double check to verify these results are indeed correct.
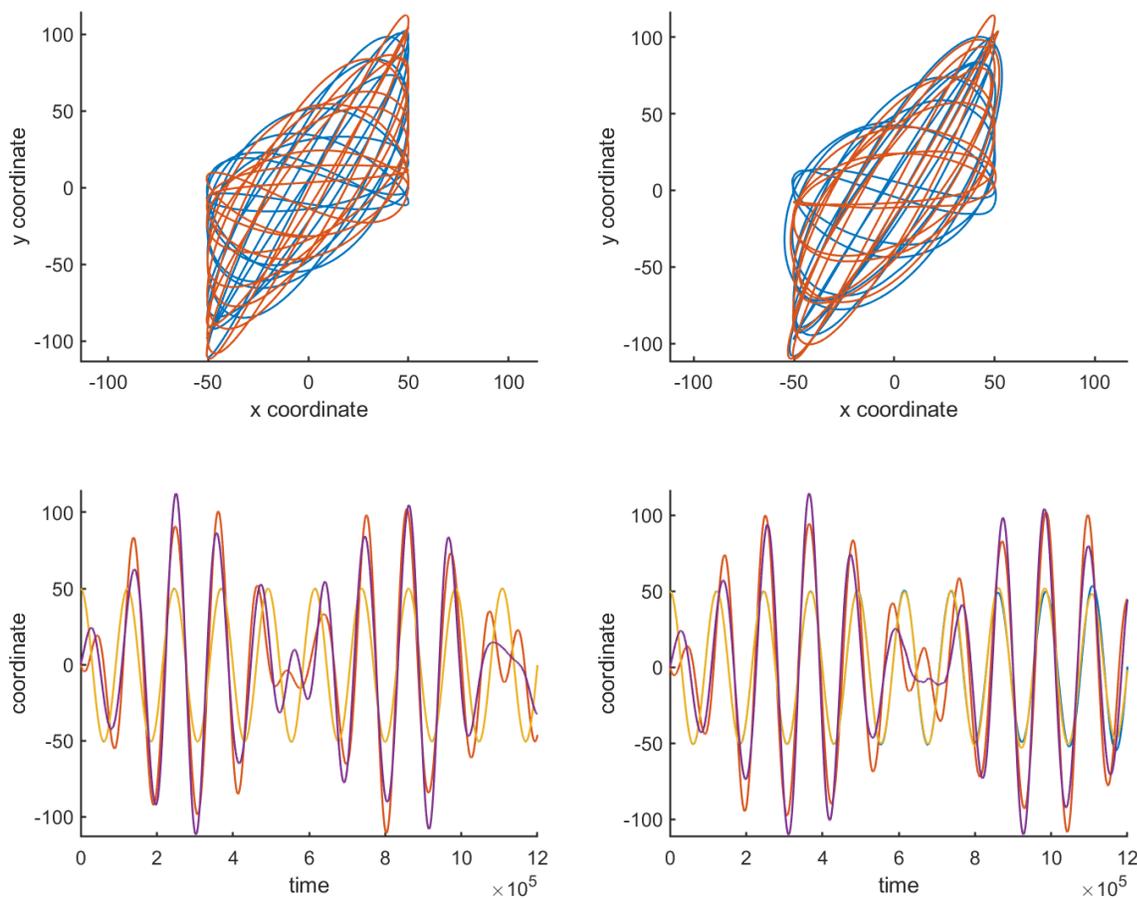

Figure 12. Same initial conditions as figure 9, except the two plots have an r_0 value of 0 (left) and 10 Ang (right).

The increased value of r_0 results in the trajectory of the particles being less relegated to the parallelogram shape. While still similar, the trajectory of the 10 Ang case becomes more curved, and with larger increases of r_0 it would likely more and more correspond to the classical case. Additionally, the 10 Ang plot demonstrates a bit of the interference pattern, though more

refinement should be performed to determine if this is quantum effects or simply numerical

instability. Also of note is that the left plot is the same as the right plot from Figure 9, but with

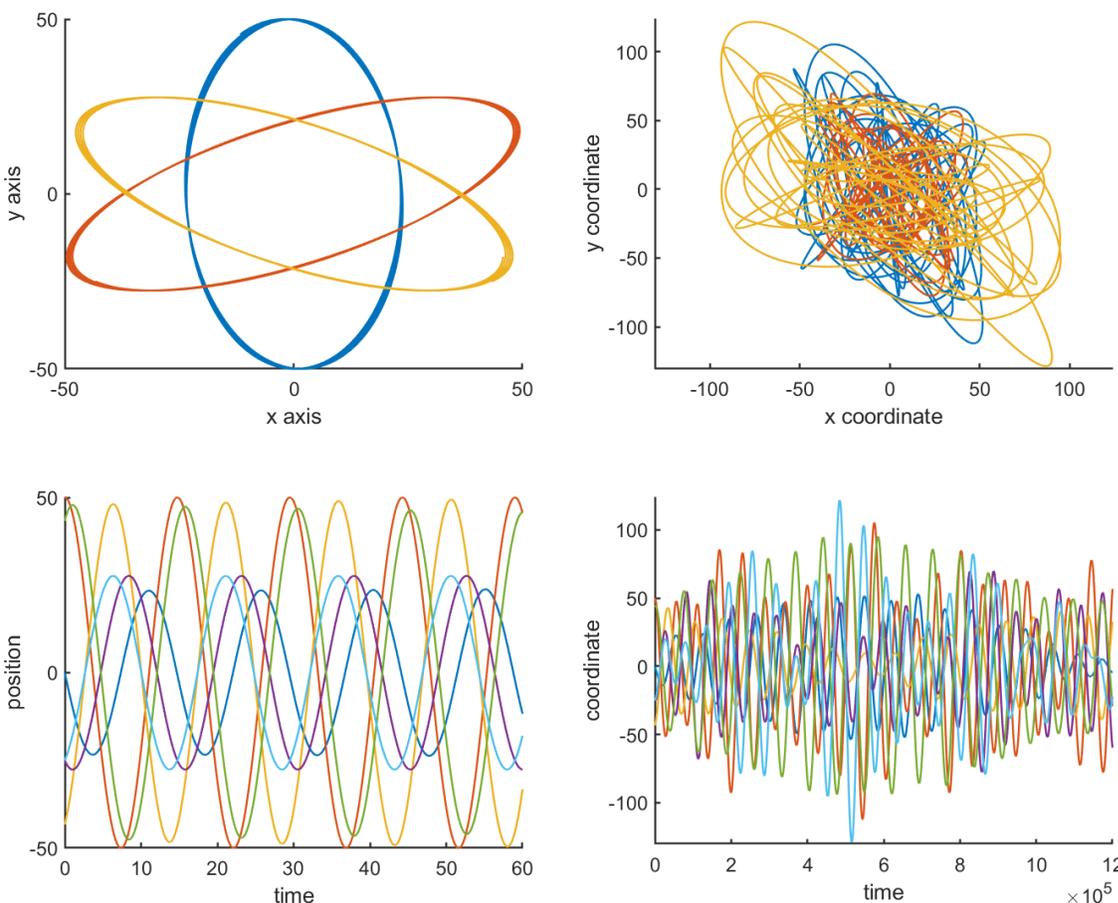the first particle numerically determined flipped.

Figure 13. Three particles calculated for the both the classical (left) and quantum (right) models.

Each particle has an initial radius from the origin of 50 Ang, and an initial velocity of $10 \frac{Ang}{fs}$

tangent to the circle in a counterclockwise direction. Spring constant of potential and interaction

are both $.01 \frac{eV}{Ang^2}$, and $\sigma_X = 10$ Ang, and $r_0 = 0$.

While the plot is capable of modeling three particles, the highly chaotic nature of such a

system makes it difficult to parse much information from this setup.

Through these trajectory plots several relationships can immediately become apparent. One such relationship is how the size of σ_R affects how the plot differs from that of the classical case. In a situation where σ_R is large the particle will take on a more quantum effect, whereas when σ_R is smaller the particle's trajectory begins to more resemble the classical trajectory. This makes sense given the discussion earlier about interference, given that the larger a wave packet is the more it can interfere with and be interfered with by other wave packets. Therefore, particles with large waves will undergo more quantum effects due to that interference. However even with small values of σ_R there is still some differentiation for the classical case, as even very thin waves can interact with each other. To have a truly classical effect we would require a σ_R of effectively 0, which would simply be point particles.

Another relationship present is the effect different values of r_0 has on the trajectory, as seen by comparing figures 9, 10, and 12. Smaller values of r_0 result in tighter trajectories far removed from the classical case, while larger values result in the trajectories beginning to match the classical case more closely. From a theoretical perspective this makes sense, as a quantum interaction will typically see two particles behaving as if they were one single particle. If the resting distance between particles is small, then the two particles are more intwined and more likely to interact with each other. Meanwhile if the rest distance is large, then the two particles are more likely to remain separate and behave as separate particles, which is what the classical model dictates.

The final point to make about the particle trajectories demonstrated in these models is likely the most obvious: even when modeling complete trajectories of particles rather than the probability fields of the Coppenhagen interpretation, Bohmian mechanics leads can lead to wildly different trajectories than what one would expect in classical physics. Even elements such

as the symmetry of particle motions may be present in the classical case but completely absent in the quantum trajectories. Quantum trajectories have an additional source of energy to the system outside of what is found in classical mechanics that can radically alter it.

Chapter 5: Conclusion

Through the process of separation of variables, we were able to simulate a multiparticle system with particle interactions with little computational stress compared to a direct approach or even a particle separation. The average run time for one of these models was typically around a few hours, compared to more than 10^6 hours needed to model three particles in three dimensions simultaneously using a direct approach, or more than 500 hours modeling three particles, each in two-dimensions. From these computational time gains, this endeavor was quite successful. The main efforts to be made in the future are to refine the code to ensure greater numerical stability. At present there is one place in the code that could produce error that could affect the long time dynamics of the quantum trajectories. In particular the Euler method was implemented to update the particle trajectories, but this should be replaced by a better, more accurate integrator approach, such as leapfrog or 4th order Runge-Kutta. Additionally, the current codes relies on small grid size to ensure stability, so increasing the effectiveness of the code would allow for a decrease in runtime for similar models. Beyond that, the other future developments would be to extend the code to more than three particles and in 3 dimensions, which would be straightforward as it would only require adding additional terms for $U_{interaction}$. Finally, tracking angular momentum would be interesting, since classically this should be conserved, and quantum mechanically the average over a cycle (or long-time average) should be conserved.

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