Introduction to Pilot Wave Theory

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Differential Equations

Probability Statistics

Linear Algebra II

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1 Abstract

Within the Copenhagen interpretation of quantum physics, the quantum observer generates conflicts such as the measurement problem or particle-wave duality, which leaves no room for trajectories. With the pilot-wave formulation of quantum mechanics, a probabilistic cluster of all possible trajectories can be modelled such that it provides a more intuitive understanding of the particle interactions at a quantum level. Two methods to simulate the possible trajectories are described in this paper. The first consist of extracting the trajectories from the reformulated quantum Newton equation in terms of position only. The second consists of solving the time-dependent Schrodinger equation numerically with the Crank-Nicolson scheme in order to extract a velocity field. No successful results have been achieved with the first method because the ordinary differential equation is extremely stiff and thus causes non-local effects and instability. The second method was more successful being that it generated the trajectories alongside different potentials for the ensemble of particles. The results conclude that the trajectories may be extracted from the time-dependent Schrodinger equation using numerical solvers and plotters. More work is to be done on the first method being that it is more efficient in computing multiple trajectories, which would save time should it be combined with machine learning.

2 Introduction

2.1 Motivation for Pilot-Wave Theory

An interest within Pilot-Wave theory is its formulation of Quantum Mechanics through its use of quantile quantum trajectories. This includes ensemble of particles with invariant probability distributions that are affected by phenomena such as the quantum potential, which would be negligible for particles whose mass are above a micro-magnitude.

The primary objective of this paper is to better understand the intermediate quantum trajectory of an ensemble of particles between its initial and final probability density positions, at an undergraduate level. An example best describing these conditions is the double-slit experiment, in which the particles are said to exhibit wave like properties that cause the familiar interference distribution pattern. Pilot-wave theory instead postulates each particle has a deterministic path that is guided by the wave function, which would allow us to perceive the precise trajectory of the particle between the initial and terminal positions.

The methods involved in this paper include 1. reformulating the quantum potential in terms of position and solving the quantum Newton equation to extract the probability density ρ and the action S, essentially reconstructing the wave function ψ entirely, and 2. solving the time-dependent Schrödinger equation normally to output the wave function ψ. From the wave function in the second method, the action is isolated. The spacial gradient and division by mass of the action provides the velocity field, and integrating the velocity field yields the trajectories given the initial and final conditions.

Before jumping straight into numerical methods for extracting trajectories, we must first derive the foundation on which the other variables such as the action and velocity field will be presented. This also includes derivations for equations describing the behaviour of the trajectories and the emergence of the quantum potential. Begin-

ning with classical mechanics, we will transition into the Copenhagen interpretation of quantum mechanics and finally, deBroglie-Bohm mechanics.

2.2 Preliminary Theory for Numerical Experimentation

2.2.1 Continuity Equation

An importance of continuum mechanics is the continuity equation, the implication of which is that within a local system energy cannot be destroyed nor created, nor even jump from one place to another, it must move in a continuous flow. The same principle is applied to mass and momentum. Its differential form can be expressed in the following way:

$$\partial_t \rho(r,t) + \nabla \cdot \vec{j}(r,t) = 0 \tag{1}$$

ρ is the particle density of a fixed volume W and $\vec{j}$ is the particle current density in W. Note the notation for partial differentiation will be the following: $\partial_j^i = \frac{\partial^i}{\partial j^i}$. In order to obtain this result let's consider an ensemble of particles with positions described by $r_i = (x_i(t),\ y_i(t),\ z_i(t))$ where i represents the i'th particle within the cluster of particles. The density of particles $\rho(r,t)$ can then be expressed as the summation of the Dirac delta function as such:

$$\rho(r,t) = \sum_{i=1}^{\infty} \delta(r - r_i(t)) \tag{2}$$

To understand the concept of the Dirac delta function, consider a standard Gaussian probability distribution of position of particles which is expressed by $P(x) = ke^{\frac{-x^2}{\sigma^2}}$ where σ is the standard deviation and k is equal to $\frac{1}{\sqrt{2\pi\sigma}}$.

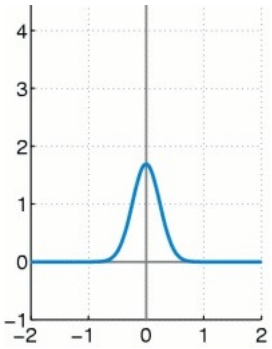

Figure 1: Delta Function

If there is no uncertainty in the position of the particle, that is to say the particle has been observed, the standard deviation collapses to zero and thus the probability distribution turns into a single spike. How the delta expression on the right side of the summation works, is that it takes some point r_i within W, and from that point moves to another point enclosed within W to check whether or not a particle is located there. The delta function outputs a 1 if there is a particle, and a 0 if there is no particle, hence the nature of having a spike where the probability of having a particle is near absolute. Summing up the values outputted by the delta function gives the amount of

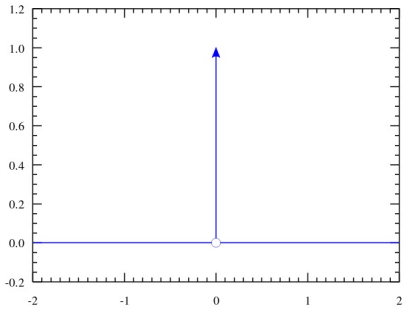

Figure 2: Delta Function

particles within W and thus with the volume of W, its particle density. Now, consider the particle current density of particles in and out of volume W through a small area dA on the skin of the volume given by:

$$\vec{j}(r,t) = \rho(r,t)\vec{V}(r,t) = \sum_{i=1}^{\infty} \delta(r - r_i(t))\vec{V}(r,t) \tag{3}$$

$\vec{V}(r,t)$ is the velocity vector field of the particles. At any instant t, the number of particles within W can be calculated by integrating the density of particles within W. From this, it follows that the rate of change of the number of particles in W is the following:

$$\frac{d}{dt}\iiint_W \rho(r,t)dV = \iiint_W \partial_t \rho(r,t)\ dV \tag{4}$$

Let ∂W be the surface area boundary of W and $\vec{n}$ be a unit vector normal to ∂W and pointing outside of the volume. The particle current density, moving chaotically through a small area dA within ∂W and not perfectly in the direction of $\vec{n}$, can be projected onto the normal by taking the dot product of $\vec{j}$ onto $\vec{n}$ which gives $\vec{j}(r,t)\cdot\vec{n} = \rho(r,t)\vec{V}(r,t)\cdot\vec{n}$. Because the particles cannot vanish nor be created during the flow, it follows that the rate of change of the number of particles within W is equal to the number of particles that are coming in and out of the surface of ∂W, which can be expressed by the following equation:

$$\frac{d}{dt}\iiint_W \rho(r,t)dV = -\iint_{\partial W} \rho(r,t)\vec{V}(r,t)\cdot\vec{n}\ dA \tag{5}$$

The relation expresses equivalency between the rate of change of particles within W and the amount of particles flowing through dA in the direction of $\vec{n}$. The negative sign on the right-hand side comes from the fact that the current density of particles has been projected onto $\vec{n}$, which has its direction pointing away from the volume. Additionally, $\vec{n}\cdot dA$ shall be rewritten as $d\vec{A}$ to represent the area with its normal vector being equal to the normal vector its section of ∂W.

By the Divergence Theorem, the outward flux of the velocity vector field passing through ∂W, a closed surface, is equivalent to the volume integral of the divergence of the field through the volume W:

$$-\iint_{\partial W} \rho(r,t)\vec{V}(r,t)\cdot d\vec{A} = -\iiint_W \nabla\cdot(\rho(r,t)\vec{V}(r,t))\ dV \tag{6}$$

By the subtraction of equation (6) by equation (7), the following expression is produced:

$$\iiint_W \left[\partial_t\rho(r,t) + \nabla\cdot(\rho(r,t)\vec{V}(r,t))\right]\ dV = 0 \tag{7}$$

Being that the volume integral equates to zero for all choices of volume W, the only way for the expression to equal zero is if the integrand is also equal to zero, giving the following:

$$\partial_t\rho(r,t) + \nabla\cdot(\rho(r,t)\vec{V}(r,t)) = 0 \tag{8}$$

Which can be rewritten into the more familiar form by substitution of particle current density, resulting in the continuity equation seen at the beginning of the section:

$$\partial_t\rho(r,t) + \nabla\cdot\vec{j}(r,t) = 0. \tag{9}$$

The continuity equation will be combined with the Hamilton-Jacobi equation to form the classical equivalent of the Schrödinger equation.

2.2.2 Derivation of the Euler-Lagrange equation

Another powerful equation is the Euler-Lagrange equation which has the ability the formulate the dynamics of a system easily.

Consider the classical Lagrangian, an equation describing the difference between the kinetic energy and potential of a particle:

$$\mathcal{L}(x, \dot{x}) = T(\dot{x}) - V(x) = \frac{m\dot{x}^2}{2} - V(x) \tag{10}$$

The action S, or the cost of the particle following some trajectory on the interval $[t_0, t_f]$, is written as the integral of the Lagrangian as such:

$$S(x(t), \dot{x}(t)) = \int_{t_0}^{t_f} \mathcal{L}(x(t), \dot{x}(t))\, dt \tag{11}$$

Notice the position x and velocity $\dot{x}$ are also functions of time as they vary through the trajectory. The significance of the action of a trajectory is observed within Hamilton's Principle, which states that out of all possible paths between positions $x_0 = x(t_0)$ and $x_f = x(t_f)$, a single one is distinguished among all by the requirement that is has the lowest action, meaning that it has the smallest difference between the kinetic energy and potential when integrated over t_0 and t_f. Let the distinguished physical trajectory,

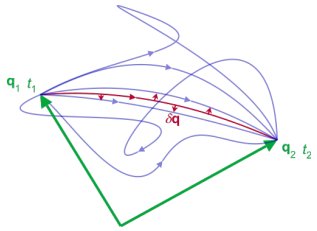

Figure 3: Principle of least action

the path with the lowest cost or action, be denoted as $x_p(t)$ and any variation from the physical path as $x(t)$. The path taken by the particle between the points t_0 and t_f is the one for which the action is stationary, therefore if we consider any change in action with respect to the change in variation, we get the following:

$$\left.\frac{\delta S(x_p(t))}{\delta x(t)}\right|_{x(t)=x_p(t)} = 0 \tag{12}$$

The derivative is noted with δs, since the action S is differentiated with respect to a function and not a variable. This expression is evaluated at the minimized action path $x_p(t)$, which will equate to zero. This is because the $x(t)$ represents any deviation from $x_p(t)$, and $x_p(t)$ is defined as the path that has no deviation from a path with minimal cost, therefore the deviation is equal to zero. This expression will repeat itself upon further derivations.

Now to continue the derivation of the Euler-Lagrange, consider a modified Lagrangian as a function of position, velocity, with some variation δ in both :

$$\mathcal{L}(x(t), \dot{x}(t)) = \mathcal{L}(x_p(t) + \delta x(t), \dot{x}_p(t) + \delta\dot{x}(t)) \tag{13}$$

To make this more tolerable to work with, a first order Taylor expansion is used to expand it into the following terms:

$$\mathcal{L}(x_p(t), \dot{x}_p(t)) + [(\partial_x \mathcal{L})\delta x(t) + (\partial_{\dot{x}} \mathcal{L})\delta \dot{x}(t)]_{\dot{x}(t)=\dot{x}_p(t)}^{x(t)=x_p(t)} + o(\delta x(t)) \tag{14}$$

First order is in reference to keeping the 0th and 1st order polynomials, any polynomial with an order higher than 1 will be considered as trivial as its values are much too small to consider, and will be known as the "tail" of the expansion. A brief reminder of this is:

$$e^x = e^0 + \left.\frac{de^x}{dx}\right|_0 x + \left.\frac{d^2e^x}{dx^2}\right|_0 \frac{x^2}{2} + ... = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \left.\sum_{n=0}^{\infty} \frac{f^n(a)(x-a)^n}{n!}\right|_{a=0} \tag{15}$$

This is simply a Taylor expansion centered at zero, otherwise known as a Maclaurin expansion or series. The action of the expanded and modified Lagrangian would of course be the integral from t_0 to t_f:

$$S(x_p(t)) = \int_{t_0}^{t_f} \mathcal{L}(x_p(t) + \delta x(t), \dot{x}_p(t) + \delta \dot{x}(t))\, dt \tag{16}$$

$$= \int_{t_0}^{t_f} \mathcal{L}(x_p(t), \dot{x}_p(t)) + \int_{t_0}^{t_f} [(\partial_x \mathcal{L})\delta x(t) + (\partial_{\dot{x}} \mathcal{L})\delta \dot{x}(t)]\, dt + 0(\delta x(t)) \tag{17}$$

The integral of the 0th order term is evaluated, and the second element within the 1st order term is evaluated via integration by parts:

$$S(x(t)) = S(x_p(t), \dot{x}_p(t)) + \int_{t_0}^{t_f} \left[(\partial_x \mathcal{L})\delta x(t) - \left(\frac{d}{dt}\right)(\partial_{\dot{x}} \mathcal{L})\delta \dot{x}(t)\right] dt \tag{18}$$

$$+ (\partial_{\dot{x}} \mathcal{L})\delta x(t)\Big|_{t_0}^{t_f} + o(\delta x(t)) \tag{19}$$

The difference between the left and right hand side is the variation of the action on the physical path $\delta S(x_p(t))$, which is 0 by the Hamilton principle of least action. The last term before the tail also vanishes as it is evaluating the variation at both the start and end points, which have zero variation. We are therefore left with the following:

$$S(x(t)) = \int_{t_0}^{t_f} \left[(\partial_x \mathcal{L})\delta x(t) - \left(\frac{d}{dt}\right)(\partial_{\dot{x}} \mathcal{L})\delta \dot{x}(t)\right] dt \tag{20}$$

Using the formal definition of a derivative, the derivative of this term will be equal to zero as stated in the description of equation (15), can be expressed using the following:

$$\lim_{\delta x(t)\to 0} \frac{\delta S}{\delta x(t)} = \frac{S(x_p(t) + \delta x(t), \dot{x}_p(t) + \delta \dot{x}(t)) - S(x_p(t), \dot{x}_p(t)}{\delta x} \tag{21}$$

$$= \frac{\delta}{\delta x(t)} \int_{t_0}^{t_f} \left[(\partial_x \mathcal{L}) - \left(\frac{d}{dt}\right)(\partial_{\dot{x}} \mathcal{L})\right] \cdot \delta x(t)\, dt = 0$$

Since this holds for any variation $\delta x(t)$, we are left with the following expression:

$$\left[(\partial_x \mathcal{L}) - \left(\frac{d}{dt}\right)(\partial_{\dot{x}} \mathcal{L})\right]_{\dot{x}(t)=\dot{x}_p(t)}^{x(t)=x_p(t)} = 0 \tag{22}$$

This is the Euler-Lagrange equation, which will be helpful in considering particle motion that satisfies the principal of minimal action and makes it easier to switch between Newtonian and Lagrangian representations of classical mechanics.

2.2.3 Derivation of the Hamilton-Jacobi equation

The Hamilton-Jacobi equation directly describes the dynamics of the particles and trajectories and will be useful in the future for extracting the trajectories. Now, for the derivation of the Hamilton-Jacobi, we begin by considering the Hamiltonian, which unlike the Lagrangian, is the addition of kinetic energy and potential of a particle:

$$H(x,p) = T(p) + V(x) \tag{23}$$

Next we consider the physical trajectory $x_p(t)$ once more, except now alongside a second physical trajectory $\tilde{x}_p(t)$ that shares the same end point although at a later time $t_f + \delta t$. This can be express by those two equations : $\tilde{x}_p(t) = x_0$, $\tilde{x}_p(t_f + \delta t) = x_f$. The second physical trajectory can then be rewritten like so

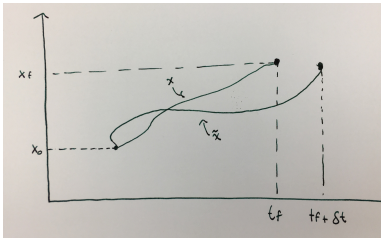

Figure 4: Trajectories

$$\tilde{x}_p(t) = x_p(t) + \delta x(t), t_0 \leqslant t \leqslant t_f$$

We can then define the position of a clump particles following the physical path with added time ϵ as the sum of its position at time t_f and the product of its velocity and the extra time ϵ

$$x_p(t_f + \epsilon) = x_p(t_f) + \dot{x}_p(t)\epsilon, 0 \leqslant \epsilon \leqslant \delta t$$

From that follows that the secondary trajectory can be express like so :

$$\tilde{x}_p(t_f + \delta t) = x_p(t_f + \delta t) + \delta x(t_f + \delta t)$$

$$\tilde{x}_p(t_f + \delta t) = x_p(t_f) + \dot{x}_p(t_f)\delta t + \delta x(t_f + \delta t)$$

Notice that $\tilde{x}_p(t_f + \delta t) = x_f$

$$-\dot{x}_p(t_f + \delta t) = \delta x(t_f + \delta t) \tag{24}$$

The action of the extended physical path can once again be rewritten in terms of the Lagrangian as such:

$$\begin{aligned} S(\tilde{x}_p(t), \dot{\tilde{x}}_p(t_f)) &= \int_{t_0}^{t_f+\delta t} \mathcal{L}(\tilde{x}_p(t), \dot{\tilde{x}}_p(t_f)(t))\ dt \\ &= \int_{t_0}^{t_f+\delta t} \mathcal{L}(x_p(t) + \delta x(t), \dot{x}_p(t) + \delta \dot{x}(t))\ dt \end{aligned} \tag{25}$$

Another Maclaurin expansion is used for the action of the modified physical path:

$$\int_{t_0}^{t_f+\delta t} [(\mathcal{L}(x_p(t), \dot{x}_p(t))\ dt) + ((\partial_x \mathcal{L})(x_p(t))\delta x(t) + (\partial_{\dot{x}} \mathcal{L})(\dot{x}_p(t))\delta \dot{x}(t))]\ dt + 0(\delta x(t)) \tag{26}$$

Once again, the element within the first order term within the expansion is evaluated via integration by parts giving the following:

$$\int_{t_0}^{t_f+\delta t} [\mathcal{L}(x_p(t), \dot{x}_p(t)\ dt] + [(\partial_{\dot{x}} \mathcal{L})\delta x(t)]\Big|_{t_0}^{t_f+\delta t} \tag{27}$$

$$+ \int_{t_0}^{t_f+\delta t} \left[(\partial_x \mathcal{L}) - \left(\frac{d}{dt}\right)(\partial_{\dot{x}} \mathcal{L})\right]^{\substack{x(t)=x_p(t) \\ \dot{x}(t)=\dot{x}_p(t)}} dt + o(\delta x(t)) \tag{28}$$

The first can be rewritten like so:

$$\begin{aligned} \int_{t_0}^{t_f+\delta t} [\mathcal{L}(x_p(t), \dot{x}_p(t)\ dt] &= \int_{t_0}^{t_f} [\mathcal{L}(x_p(t), \dot{x}_p(t)\ dt] + \int_{t_f}^{t_f+\delta t} [\mathcal{L}(x_p(t), \dot{x}_p(t)\ dt] \\ &= S(x_p(t), \dot{x}_p(t)) + \mathcal{L}(x_p(t), \dot{x}_p(t))\delta t \end{aligned} \tag{29}$$

Using the result in (25) and the definition of momentum the second term of the expansion can be rewritten like so:

$$[(\partial_{\dot{x}} \mathcal{L})\delta x(t)]\Big|_{t_0}^{t_f+\delta t} = (\partial_{\dot{x}} \mathcal{L})\delta x(t_f+\delta t) = -(\partial_{\dot{x}} \mathcal{L})(t_f+\delta t)\dot{x}(t) = \dot{x}_p(t_f+\delta t)\dot{x}(t_f)\delta t = -p(t_f+\delta t)\dot{x} \tag{30}$$

The third term, which resembles the Euler-Lagrange equation, vanishes because its value is insignificantly small, and is put into the tail. The three terms can then be substituted in the equation (28) which gives:

$$S(\tilde{x}_p(t), \dot{\tilde{x}}_p(t_f)(t)) = S(x_p(t), \dot{x}_p(t)) + \mathcal{L}(x_p(t), \dot{x}_p(t))\delta t - p(t_f + \delta t)\dot{x}(t_f)\delta t \tag{31}$$

Using the definition of a limit

$$(\partial_{t_f} S) = \lim_{\delta t \to 0} \frac{S(\tilde{x}_p(t_f), \dot{\tilde{x}}_p(t_f)) - S(x_p(t_f), \dot{x}_p(t_f))}{\delta t}$$

We conclude that

$$\partial_t S(x_p(t_f)) = -H(x_p(t_f), \dot{x}_p(t_f)) \tag{32}$$

This is the Hamilton-Jacobi equation, which states that an increase in time will di-

minish the action of the physical trajectory, as indicated by the negative Hamiltonian on the right hand side of the expression.

2.2.4 Derivation Canonical/Hamilton Equations

An alternative way to describe mechanical systems without the use of the Euler-Lagrange equation are the Hamilton equation. After derivation, we will use the result to come up with an expression for the action of the harmonic oscillator in the next subsection. The Hamilton equations themselves describe the change in momentum and position respectively. The derivation itself will make use of Cauchy's method of characteristics to solve a first order partial differential equation, whose idea is to find a characteristic curve solution such that the PDE reduces to multiple ODEs. We first begin by rewriting the Hamiltonian as a function of position, time, and momentum as such:

$$\begin{aligned} H(x,\dot{x},t) = \frac{m\dot{x}^2}{2} + V(x,t) = \frac{p^2}{2m} + V(x,t) = H(x,p,t) \\ -H(x,p,t) + \frac{p^2}{2m} + V(x,t) = 0 \end{aligned} \tag{33}$$

Using a derivation similar to that of the Hamilton-Jacobi, which would be trivial to transcribe, we conclude that the change in the action S with respect to a variation in the final position is equal to the momentum of the particle: $\partial_{x_f} S = p$. Therefore we can rewrite the Hamilton-Jacobi equation as:

$$\partial_t S + H(x, \partial_x S, t) = 0, \qquad S = S(x,t) \tag{34}$$

We continue by substituting the Hamiltonian from equation (31) into equation (32), and substituting the momentum p as $\partial_x S$, gives the following:

$$\partial_t S + \frac{1}{2m}\left(\partial_x S\right)^2 + V(x,t) = 0 \tag{35}$$

For convenience we can rewrite equation as some function F as a function of the gradient of the action S and the position:

$$\partial_t S + \frac{1}{2m}\left(\partial_x S\right)^2 + V(x,t) = F(\vec{x}, \nabla S(\vec{x})) = 0 \tag{36}$$

The gradient of the action ∇S has components that are partial derivatives with respect to x and x^o:

$$\nabla S = \begin{bmatrix} \partial_{x^o} S \\ \partial_x S \end{bmatrix} = \begin{bmatrix} p_o \\ p \end{bmatrix} \tag{37}$$

We rewrote time t as x^o so that we can represent the position as a vector of both time and position under the notation that both are physical coordinates. The position vector is therefore $\vec{x} = \begin{bmatrix} x^o \\ x \end{bmatrix}$, and the action $S = S(x, x^o)$.

Now, consider the condition of the solution of the PDE as $S(\vec{x}) = S_0(\vec{x})$ within a boundary Ω in $\mathbb{R}^2$, enclosed by a curve $\partial\Omega$. Within the curve $\partial\Omega$ are solution curves of a system of ODEs which can be denoted as $\vec{x}(r)$ where the vector for the actual position of the particle is parametrized smoothly by r. The concept behind method of characteristics is obtaining values of the action $S(r)$ along the curve starting at some

position on $\partial\Omega$. We select one point on $\partial\Omega$ of the possible differential curves with $\vec{x}(0) = y$.

We can denote the action and momentum along the curve r as $S(r) = S(\vec{x}(r))$ and $p(r) = p(\vec{x}(r)) = \nabla S\vec{x}(r))$. Therefore the change of the action S with respect to moving along the curve is denoted as:

$$\frac{dS}{dr} = \partial_{x^o} S\frac{dx^o}{dr} + \partial_x S\frac{dx}{dr} = \sum_{i=0}^{n} \partial_{x^i} S\frac{dx^i}{dr} \tag{38}$$

The action S, being a function of both x and x^o, will will have its partial derivatives added when totally differentiated, and in addition, since the variables themselves are changing with respect to r, by the chain rule they will be derivatives themselves, such as $\frac{dx^o}{dr}$. The expression can be collapsed into a summation for higher orders with more variables.

The change in momentum $p_j = \partial_{x^j} S$, with respect to moving along the curve can be therefore denoted as:

$$\frac{dp_j}{dr} = \frac{d}{dr}\left(\partial_{x^j} S(\vec{x})\right) = \sum_i \partial^2_{x^j x^i} S\frac{dx^i}{dr} \tag{39}$$

Notice the summation symbol now simply has an i under it, which is used to denote the same parameters as the summation before it. Finally, the function $F(\vec{x}, \nabla S(\vec{x})) = 0$ may be differentiated with respect to the curve $\vec{x}(r)$ which gives the following product and chain rule outcomes:

$$\frac{dF}{dr} = \partial_{x^j} F + \sum_i (\partial_{p_i} F)(\partial_{x^j} p_i) = \partial_{x^j} F + \sum_i (\partial_{p_i} F)(\partial^2_{x^i x^j} S) = 0 \tag{40}$$

Notice how equation (37) and (38) share the same $\partial^2_{x^j x^i} S$ term. We can actually make the summations equal on the condition that $\frac{dx^i}{dr} = \partial_{p_i} F$, which is in fact out condition to select the curves within Ω, with equations (36) to (38) being our system of ODEs from the original PDE F. With our new condition we can rewrite equation (38) as follows:

$$\partial_{x^j} F + \sum_i (\partial_{p_i} F)(\partial^2_{x^j x^i} S) = \partial_{x^j} F + \frac{dp_j}{dr} = 0 \tag{41}$$

Therefore we have our first canonical equation:

$$\frac{dp_j}{dr} = -\partial_{x^j} F \tag{42}$$

Our second canonical equation is the condition on which the curves are selected:

$$\frac{dx^i}{dr} = \partial_{p_i} F \tag{43}$$

Finally, our last canonical equation replaces $\partial_{x^i} S$ by p_i and $\frac{dx^i}{dr}$ by $\partial_{p_i} F$ in equation (40) to give the following:

$$\frac{dS}{dr} = \sum_i \partial_{p_i} F p_i \tag{44}$$

Equations (40) to (42) will be used to solve the Hamilton-Jacobi for the harmonic oscillator within the next subsection.

2.2.5 Derivation of Hamilton-Jacobi for the Harmonic Oscillator

Once again we will use the method of characteristics to solve a first order PDE, although now for a particle within the harmonic oscillator. Consider the Hamiltonian having a defined potential that isn't time-dependent:

$$H(x,p) = \frac{p^2}{2m} + \frac{kx^2}{2} \tag{45}$$

Substituting this expression within the Hamilton-Jacobi equation therefore gives:

$$\partial_t S + \frac{1}{2m}\left(\partial_x S\right)^2 + \frac{kx^2}{2} = 0 \tag{46}$$

We will denote $\partial_t S = \partial_{x^o} S$ as p_o and replace $\partial_x S$ by p in equation (47) to give a function of momentum, which gives the following:

$$p_o + \frac{p^2}{2m} + \frac{kx^2}{2} = 0 \tag{47}$$

We can once again write this as some function F, this time as a function of $\vec{x}$ and $\vec{p}$:

$$F(\vec{x},\vec{p}) = F\left(\begin{bmatrix} x^o \\ x \end{bmatrix}, \begin{bmatrix} p_0 \\ p \end{bmatrix}\right) = F(x^o, x, p_o, p) = p_o + \frac{p^2}{2m} + \frac{kx^2}{2} = 0 \tag{48}$$

Once again consider the solution space to be Ω, enclosed by $\partial\Omega$, which can be visually represented by the half plane where $t \geq t_i$ and the curve selected is at $x(t_i) = x_0$. The conditions to the PDE are $S(x_i) = S_i$, $p_i = \frac{d}{dx_i}S(x_i)$, and also we define $p_{oi} =$

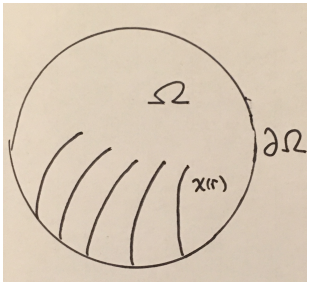

Figure 5: Boundary

$-H(p,x) = -\frac{p^2}{2m} - \frac{kx^2}{2}$.

Once again the curves are selected by the restriction $\frac{dx^i}{dr} = \partial_{p_i} F$, which gives the following system of 5 ODEs and their subsequent solutions:

$$\frac{dp_o}{dr} = -\partial_{x^o} F = 0 \tag{49}$$

$$\frac{dp}{dr} = -\partial_x F = -kx \tag{50}$$

$$\frac{dx^o}{dr} = \partial_{p_o} F = 1 \quad x^o = c + r, \quad r = t - t_i \tag{51}$$

$$\frac{dx}{dr} = \partial_p F = \frac{p}{m} \tag{52}$$

Notice that in equation (55), $\frac{dx}{dr} = \frac{p}{m}$, can be substituted into equation (53) to give:

$$\frac{d^2x}{dr^2} = \frac{1}{m}\frac{dp}{dr} = \frac{1}{m}(-kx) \tag{53}$$

We can bring the last term on the right hand side to the first term on the left hand side that also gives:

$$\frac{d^2x}{dr^2} + \frac{kx}{m} = 0 \tag{54}$$

We can rewrite the derivative using Newton's notation for differentiation, and replace $\frac{k}{m}$ by its equivalent ω^2:

$$\ddot{x} + \omega^2 x = 0 \qquad r = \pm\,\omega i \tag{55}$$

r is the roots of the complex characteristic equation of the second order homogeneous ODE. The general solution then takes the form:

$$x(r) = C_1 cos(\omega r) + C_2 sin(\omega r), \qquad x(0) = x_i, \quad p(0) = p_i \tag{56}$$

Solving for the coefficients by taking the derivative and substituting the initial conditions gives the following two equations:

$$x(t) = x_i cos(\omega(t - t_i)) + \frac{p_i}{m\omega} sin(\omega(t - t_i)) \tag{57}$$

$$p(t) = m\frac{dx}{dr} = -m\omega x_i sin(\omega(t - t_i)) + p_i cos(\omega(t - t_i)) \tag{58}$$

Now, the 5th ODE of the PDE or equation (48), is denoted by equation (46) of which we previously derived:

$$\frac{dS}{dr} = \sum_i (\partial_{p_i} F)p_i = p_o(\partial_{p_o} F) + p(\partial_p F) \tag{59}$$

From the solutions of the 3rd and 4th ODE for the PDE for the Hamilton-Jacobi for the harmonic oscillator, we know that $\partial_{p_o} F = 1$ and $\partial_p F = \frac{p}{m}$, and $p(t) = m\frac{dx}{dr} = -m\omega x_i sin(\omega(t - t_i)) + p_i cos(\omega(t - t_i))$, we have the following:

$$\frac{dS}{dr} = \frac{-p_i^2}{2m} - \frac{kx_i^2}{2} + \frac{1}{m}\left[-m\omega x_i sin(\omega r) + p_i cos(\omega r)\right]^2 \tag{60}$$

After integrating the expression, we get the action equal to:

$$S(t) = S_i + \left(\frac{p_i^2}{4m\omega} - \frac{m\omega^2 x_i^2}{4}\right) sin(2\omega(t - t_i)) + \frac{x_i p_i}{2}\left(cos[2\omega(t - t_i)] - 1\right)) \tag{61}$$

Notice within the trigonometric function we have the expression $2\omega(t - t_i)$ which when equal to π, the expression is equal to simply to the initial action S_i, which ultimately means any half period or full period travelled along the curve will lead to no change in the action, and will have the same action as started with.

In order to have the expression for the action evaluated at the final point (t_f, x_f), and select a proper initial momentum, which we begin by plugging t_f within equation

equation (60) to give the following:

$$x_f = cos(\omega(t_f - t_i)) + \frac{p_i}{m\omega} sin(\omega(t_f - t_i)) \tag{62}$$

Isolation for the initial momentum within this expression gives:

$$p_i = m\omega \frac{x_f - x_i cos(\omega(t_f - t_i))}{sin(\omega(t_f - t_i))} \tag{63}$$

Finally, substituting this expression within the equation for action (64), with the assumption that the initial action S_i is zero, gives the following:

$$S(t_i, x_i; t_f, x_f) = \frac{m\omega}{2sin(\omega(t_f - t_i))} \left[(x_f^2 + x_i^2)cos(\omega(t_f - t_i)) - 2x_f x_i\right] \tag{64}$$

In this case the parameters affecting the action are both the initial and final points. This expression is also known as the propagator for the harmonic oscillator.

2.2.6 Brief Formulation of the Classical Schrödinger equation

Now, we may use the previously derived equation to formulate a classical expression of the Schrödinger wave equation. Recall the previously derived equations:

$$\partial_t S + H = 0, \qquad \partial_x S = p, \qquad \partial_t \rho + \nabla \cdot (\rho \vec{V}) = 0 \tag{65}$$

We first consider the polar form of the wave function, denoted as:

$$\psi(x,t) = R(x,t) e^{\frac{iS(x,t)}{\hbar}} \tag{66}$$

The expression for R is define as the square root of the density:

$$\rho(x,t) = R^2(x,t), \qquad R = \sqrt{\rho(x,t)} \tag{67}$$

The expression for density can be substituted within the continuity equation in equation (68), where $\vec{V} = \frac{p}{m} = \frac{1}{m}\partial_x S$, which gives the following:

$$\partial_t R^2 + \nabla \left(R^2(x,t) \frac{1}{m} \partial_x S(x,t) \right) = 0 \tag{68}$$

The pair of the Hamilton-Jacobi and the continuity equation equates to the classical equivalent of the wave equation of which the proof will be skipped over:

$$i\hbar \left(\partial_t \psi(x,t)\right) = -\frac{\hbar^2}{2m} \nabla^2 \psi(x,t) + V(x,t)\psi(x,t) + \frac{\hbar^2}{2m} \frac{\nabla^2 \mid \psi(x,t) \mid \psi(x,t)}{\mid \psi(x,t) \mid} \tag{69}$$

Note that the absolute value brackets around the ψ denote the modulus of the complex function. Being that we now know how to consider the formulation of the classical equivalent of the wave equation, for the sake of extracting quantum trajectories and representing the velocity field using Pilot-Wave theory, we will consider the quantum mechanical Schrödinger equation in the last subsection of the preliminaries, which does not contain the last term for its classical equivalent.

2.2.7 deBroglie-Bohmian Manipulation of the Quantum Mechanical Schrödinger equation

We will now formulate a way to describe the probability density, as well the desired velocity vector field of the quantum particles. Consider the quantum mechanical Schrödinger equation:

$$i\hbar(\partial_t\psi(x,t)) = \frac{-\hbar^2}{2m}\nabla^2\psi(x,t) + V(x,t)\psi(x,t) \tag{70}$$

Multiplying both sides by the complex conjugate of the wave function $\psi^*(x,t)$ results in the following expression:

$$i\hbar\psi^*(x,t)(\partial_t\psi(x,t)) = \frac{-\hbar^2}{2m}\psi^*(x,t)\nabla^2\psi(x,t) + \psi^*(x,t)V(x,t)\psi(x,t) \tag{71}$$

We then take the complex conjugate on both sides of the equation, resulting in:

$$-i\hbar\psi(x,t)(\partial_t\psi^*(x,t)) = \frac{-\hbar^2}{2m}\psi(x,t)\nabla^2\psi^*(x,t) + \psi(x,t)V(x,t)\psi^*(x,t) \tag{72}$$

We then subtract equation (74) by equation (75) to give the following result:

$$\begin{aligned} &i\hbar\left[\psi^*(x,t)(\partial_t\psi(x,t)) + \psi(x,t)(\partial_t\psi^*(x,t))\right] \\ &= \frac{-\hbar^2}{2m}\left[\psi^*(x,t)\nabla^2\psi(x,t) - \psi(x,t)\nabla^2\psi^*(x,t)\right] \end{aligned} \tag{73}$$

Notice the term with the potential $V(x,t)$ vanishes as it cancels with its complex conjugate. The expression within the square brackets on the left can then be collapsed into the total derivative, resulting in the identity that a function multiplied by its complex conjugate is simply the modulus of the function squared. This gives the following:

$$\begin{aligned} \partial_t\left[\psi^*(x,t)\psi(x,t)\right] &= \partial_t \mid\psi(x,t)\mid^2 \\ &= \frac{-\hbar^2}{2m}\left[\psi^*(x,t)\nabla^2\psi(x,t) - \psi(x,t)\nabla^2\psi^*(x,t)\right] \end{aligned} \tag{74}$$

The modulus squared of the wave function $\mid\psi(x,t)\mid^2$ is commonly known as the probability density of the particles, and therefore the expression equates to:

$$\partial_t \mid\psi(x,t)\mid^2 = \partial_t\rho(x,t) \tag{75}$$

Recall by the continuity equation, for the one-dimensional case it follows:

$$\partial_t\rho(x,t) = -\nabla\cdot(\rho(x,t)\vec{V}(x,t)) = -\partial_x(\rho(x,t)\vec{V}(x,t)) = -\partial_x\vec{j}(x,t) \tag{76}$$

This therefore results in the particle current density equating to:

$$\vec{j}(x,t) = -\frac{i\hbar}{2m}\left[\psi^*(x,t)\partial_x\psi(x,t) - \psi(x,t)\partial_x\psi^*(x,t)\right] = \rho(x,t)\vec{V}(x,t) \tag{77}$$

The velocity field may finally be extracted when isolating for it to give the final ex-

pression that depends only on initial conditions:

$$\vec{v}(x,t) = \frac{\vec{j}(x,t)}{\mid \psi(x,t) \mid^2} \tag{78}$$

Notice we are finally describing the velocities of the particles in terms of the wave function! Using this expression we can determine the velocities of the particles varying on initial conditions. Note however since we are missing the last term from the classical equivalent of the Schrödinger equation, we must derive them from the quantum mechanical version that will come with a few adjustments.

Once again consider the Schrödinger equation with the following expression substituted within it:

$$\psi(x,t) = R(x,t)e^{\frac{iS(x,t)}{\hbar}} \tag{79}$$

The imaginary part of the the Schrödinger equation gives the continuity equation:

$$Im : \partial_t \rho(x,t) - \partial_x \left(\frac{1}{m} \partial_x S(x,t) \rho(x,t) \right) = 0 \tag{80}$$

Furthermore, the real part gives the Hamilton-Jacobi equation, although now with an extra term:

$$Re : \partial_t S(x,t) + \frac{1}{2m} \left(\partial_x S(x,t) \right)^2 + V(x,t) + Q(x,t) = 0 \tag{81}$$

The expression $Q(x,t)$ refers to the quantum potential of the system, which when isolated for and undergone the proper substitution, gives the following expression:

$$Q(x,t) = -\frac{\hbar^2}{2m} \frac{1}{R(x,t)} \partial_x^2 R(x,t) \tag{82}$$

Now that we have our quantum mechanical versions of the Hamilton-Jacobi, continuity, and Schrödinger equation, we require but one last way to understand the way the particles move. That is, a way to directly put Newton's second law of motion into quantum mechanics.

Consider the following equivalency:

$$\vec{v}(t) = \frac{\vec{j}(x,t)}{\mid \psi(x,t) \mid^2} = \left(\frac{1}{m} \partial_x S(x,t) \right) \tag{83}$$

This expression is subsequently substituted into Newton's second law to give the following:

$$m \frac{d}{dt} \vec{v}(x,t) = m \frac{d}{dt} \left[\frac{1}{m} \partial_x S(x,t) \right] = \frac{d}{dt} \left(\partial_x S(x,t) \right) = \left[\partial_x^2 S(x,t) \frac{dx}{dt} + \partial_{xt}^2 S(x,t) \right] \tag{84}$$

A partial derivative ∂_x may be factored out to comprise:

$$\partial_x \left(\frac{1}{2m} \left(\partial_x S(x,t) \right)^2 + \partial_t S(x,t) \right)_{x=x(t)} \tag{85}$$

From the real part of the Schrödinger equation we know that the expression within the brackets is equal to negative potential $-V(x,t)$ and negative quantum potential $-Q(x,t)$, which along with changing the partial derivative into a one-dimensional

gradient, can be substituted to give the final result:

$$m\frac{d}{dt}\vec{v}(x(t),t) = -\nabla[V(x,t) + Q(x,t)]_{\,x=x(t)} \tag{86}$$

This represents the direct correlation between Newton's classical second law of motion, and the way particles behave at a quantum physical level, also known as "The Quantum Newton equation".

3 Method of Reformulating the Quantum Potential

This section is stand alone in this paper. It covers the material necessary for a possible way to get rid of the wave function and express the particles trajectories only in the form of an ordinary differential equation. Due to the non-locality and instability on the DE we failed to put that approach in practice. In some sense it is an invitation to consider this approach in future research.

Recall the imaginary part of the Schrödinger equation, otherwise known as the continuity equation:

$$Im : \partial_t \rho(x,t) - \nabla \cdot \left(\frac{1}{m}\partial_x S(x,t)\rho(x,t)\right) = 0 \tag{87}$$

Notice the $\partial_x S(x,t)$ can be replaced by momentum p, and dividing it by m gives the velocity field $V(x,t)$ of the particles. We redefine the velocity field or flow velocity to be specific to the trajectories by evaluating the change in the position of the particle with respect to moving along the path. We now define it as the material derivative along the path as such:

$$\frac{dx}{dt} = \vec{V}(t), \quad x(0) = x_0 \tag{88}$$

To better define what this means, we transform our coordinate system into curvilinear coordinates who's coordinate basis is defined with respect to the distinct trajectories that don't intersect. We move from $(x,t) \to (x_0,t)$ where x_0 is the initial position of the trajectory. The material time derivative itself can be expanded using chain rule:

$$\frac{d}{dt} = \partial_t + (\partial_t x)(\partial_x) = \partial_t + \vec{V}(t)\partial_x \tag{89}$$

It will be customary however to change the notation of the total derivative. We will say that a total time derivative is equivalent to a partial derivative where the position is held constant:

$$\frac{d}{dt} = \partial_t|_{x_0} \tag{90}$$

And with such we can combine the two previous expressions into our definition of the material time derivative:

$$\partial_t|_{x_0} \equiv \partial_t|_x + \vec{V}\partial_x|_t \tag{91}$$

In the case of the continuity equation, the partial time derivatives can be rewritten as

holding the position constant, and the divergence of the particle current density can be expanded using product rule:

$$\partial_t \rho|_x + (\nabla \cdot \vec{V})\rho + \vec{V}(\nabla \cdot \rho)\Big|_t = \partial_t \rho(x,t)|_x + (\nabla \cdot \vec{V})\rho + \vec{V}\partial_x \rho|_t = 0 \tag{92}$$

Notice the first and last term are what comprise of the defined material time derivative, and thus can be compressed into the following expression:

$$\partial_t \rho(x,t)|_{x_0} + (\nabla \cdot \vec{V})\rho = \frac{d\rho}{dt} + (\nabla \cdot \vec{V})\rho = 0 \tag{93}$$

The question now is, what exactly is meant by the divergence of the velocity field? One way to think about it is in the context of fluid flow within a system. The divergence measures the outward flux of mass flowing through an infinitesimal volume at a given point within the fluid velocity field.

We can also think in terms of probability. A particle has a certain probability of being located on a region between the points $a = (x,t)$ and $b = (x + \delta x, t)$, which will be called as leftmost and rightmost points respectively. At some time later $t + \delta t$, the leftmost point would have moved some displacement because of its velocity resulting in $c = (x + \vec{V}(x,t)\delta t, t + \delta t)$ and the same would happen for the rightmost, where it becomes $d = (x + \delta x + \vec{V}(x + \delta x)\delta t, t + \delta t)$. What happens is that the probability

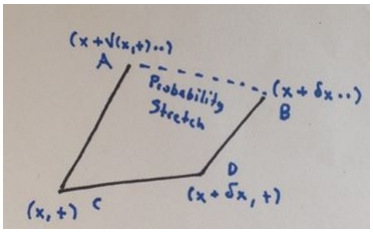

Figure 6: Probability Stretch

density is stretched with the passage of time and flow of the trajectories. The rate of this stretching is characterized by the following expression:

$$\frac{1}{\delta t}\left[\vec{V}(x + \delta x, t) - \vec{V}(x,t)\right]\delta t = \vec{V}(x + \delta x, t) - \vec{V}(x,t) \tag{94}$$

Dividing it by some infinitesimal length gives the rate of stretch relative to the original length:

$$\frac{1}{\delta x}\left[\vec{V}(x + \delta x, t) - \vec{V}(x,t)\right] \to \frac{\delta \vec{V}}{\delta x} \tag{95}$$

As $\delta x \to 0$, we are given an expression for the one dimensional case of the divergence of the velocity field. It is therefore defined as the relative rate of change of small x-intervals ℓ with respect to time:

$$\nabla \cdot \vec{V}(\vec{r}, t) = \frac{1}{\ell}\frac{d\ell}{dt} \tag{96}$$

We can now rewrite the continuity equation in equation (23) by substituting this

expression and multiplying both sides by ℓ. We notice that we can also compress it into its total derivative form and give the following:

$$\ell \frac{d\rho}{dt} + \frac{d\ell}{dt}\rho = 0, \rightarrow \frac{d}{dt}(\rho\ell) = 0 \tag{97}$$

We can rewrite $\ell \equiv dx$ being that it is an infinitesimal of length and result in the final expression:

$$\frac{d}{dt}\left[\rho(x,t)dx\right] = 0 \tag{98}$$

What we end up within the expression being differentiated is the probability density multiplied by a volume element, which gives the probability. What the expression is therefore saying is that over time, the probability does not change. The probability referring to the initial probability of the particles and their separation density from one another. If there is no change of probability throughout the velocity field, then we say that the divergence of the vector field, that is the amount of matter moving away from an infinitesimal volume, is zero.

Now, what does this mean for the trajectories? Well the initial probability between the particles is conserved meaning that each trajectory stays with its specific quantile within the probability distribution. The particle trajectories therefore travel with a

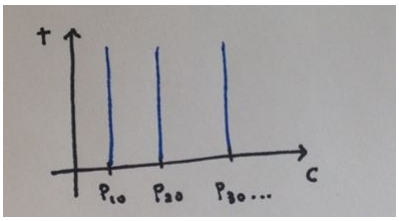

Figure 7: Evolution of quantiles over time

constant probability even with expansion or contraction of the position of the particles, they are all shifted equally to preserve probability. Furthermore, this also means that the trajectories of the particles will never cross. Now, if the probability in conserved,

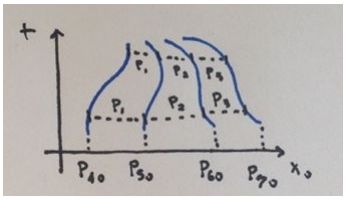

Figure 8: Evolution of percentiles over time

then for any time t it will be equivalent to its initial magnitude:

$$\rho(x_0, 0)dx_0 = \rho(x(x_0, t), t)dx \tag{99}$$

Notice how the change in position is dependent on the deviation from the starting

position x_0 after some time t. We can divide both sides by the infinitesimal dx_0 to get the following expression:

$$\rho(x(x_0,t),t)\frac{dx}{dx_0} = \rho(x_0,0) \tag{100}$$

The change of position with respect to the change of the initial position can be rewritten as the partial derivative holding time constant:

$$\partial_{x_0} x|_t = x' \tag{101}$$

We can also notice that:

$$\partial_x|_t = (\partial_{x_0}|_t)(\partial_x x_0|_t) = \frac{1}{x'}(\partial_{x_0}|_t) \tag{102}$$

Substituting this and isolating for the probability density results in:

$$\rho(x(x_0,t),t) = \frac{\rho(x_0,0)}{x'} = \frac{\rho(x_0)}{x'} \tag{103}$$

This means that the probability density is equivalent to the initial density after dividing by the change in position with respect to the change in initial position at a fixed time t. Now this expression will be used to reformulate the quantum Newton differential equation, beginning with the quantum potential which is the following:

$$Q = \frac{-\hbar^2}{2m}\frac{\partial_x^2 R}{R} \tag{104}$$

To begin this reformulation, we will begin by defining the probability density and its partial derivatives. Using equation (37) we rewrite $R(x,t)$ as the following:

$$R(x,t) = R(x(x_0,t),t) = \sqrt{\rho}(x(x_0,t),t) = \rho_0(x_0)^{\frac{1}{2}}(x')^{\frac{-1}{2}} = R_0(x_0)x'^{\frac{-1}{2}} \tag{105}$$

Taking the first partial derivative gives:

$$\partial_x R = \frac{1}{x'}\partial_{x_0}\left(R_0(x_0)x'^{\frac{-1}{2}}\right) = R_0'(x_0)(x')^{\frac{-3}{2}} + R_0(x_0)\left(\frac{-1}{2}\right)(x')^{\frac{-5}{2}}x'' \tag{106}$$

$$= R_0' x'^{\frac{-3}{2}} - \frac{1}{2}R_0 x'^{\frac{-5}{2}}x'' \tag{107}$$

Taking the second partial derivative with the established identity in equation (36) gives:

$$\partial_x^2 R = \frac{1}{x'}\partial_{x_0}\left(\partial_x R\right) = \frac{1}{x'}\partial_{x_0}\left(R_0' x'^{\frac{-3}{2}} - \frac{1}{2}x'^{\frac{-5}{2}}x''\right) \tag{108}$$

This expression allows us to have our final equation for the quantum potential as follows:

$$Q(x(x_0,t),t) = \frac{-\hbar^2}{2m}\frac{\partial_x^2 R}{R} = \frac{-\hbar^2}{2m}\left[\frac{R_0''}{R_0}x'^{-2} - 2\frac{R_0'}{R_0}\frac{x''}{(x')^3} + \frac{5}{4}\frac{(x'')^2}{(x')^4} - \frac{1}{2}\frac{x'''}{(x')^3}\right] \tag{109}$$

Differentiating this in order to fit the quantum Newton equation would be disorderly, so we will consider another variable to describe the trajectories first. We shall denote

our quantiles C as the following unique variable:

$$C = \int_{-\infty}^{x_0} \rho_0(x_0')dx_0 \tag{110}$$

Where $x \in (-\infty, \infty)$ and $C \in (0, 1)$. Now, differentiating this with respect to the initial position results in:

$$\frac{dC}{dx_0} = \rho_0(x_0) \rightarrow \rho_0(C) = 1 = R_0(C) \tag{111}$$

Being that R_0' and R_0'' are now both equal to zero, the quantum Newton equation simplifies to the following:

$$m\ddot{x} + V'(x) + \frac{\hbar^2}{2m}\left[\frac{1}{2}\frac{x''''}{(x')^4} - 4\frac{x'''x''}{(x')^5} + 5\frac{(x'')^3}{(x')^6}\right] = 0 \tag{112}$$

With our expression for the probability density in equation (37) and our new variable C, we can now determine the density at a time t as a function of C as follows:

$$\rho(x,t) = \frac{\rho_0(x_0)}{x'} \rightarrow \rho(C,t) = \frac{\rho_0(C)}{x'} = \frac{1}{x'} \tag{113}$$

Which can be used to once more simplify the quantum Newton equation in terms of density:

$$m\ddot{x} + V'(x) + \frac{\hbar^2}{2m}\left(\rho\rho'\rho'' + \frac{1}{2}\rho^2\rho'''\right) = 0 \tag{114}$$

Using this final result, the density is computed which allows for the acceleration $\ddot{x}$ of the particle to be computed. Then, the acceleration is used to formulate the velocity field and determine the trajectory for the particle at some time t, and the whole process is repeated numerically for the duration of the trajectory.

4 Method of Solving the Time-Dependent Schrödinger Numerically

In the section (2.2.7) we established a way to obtain a vector field from $|\psi(x,t)|^2$. However, ψ is not easily solvable. This section will cover the theory behind the technique we use to solve for ψ. In order to solve the one dimensional TDSE we will use the Crank-Nicolson scheme. The Crank-Nicolson scheme is a method that have been designed to solve the heat equation numerically. We will also need to implement absorbing boundary conditions (ABC) to the Crank-Nicolson scheme in order to get rid of unwanted reflections at the boundary of the simulation.

4.1 Methodology

4.1.1 Boundary conditions

Before we get to the Crank-Nicolson scheme will tackle the ABC which are in a way independent to the Crank-Nicolson scheme. After covering the Crank-Nicolson scheme we will cover how to implement the ABC in the Crank-Nicolson scheme.

As have been discussed previously in the introduction the time dependent Schrodinger equation (TDSE) can be express like so:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$$

where $\hat{H}$ is the Hamilton operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$.

First we need to establish the dispersion relation. By substituting the anzats $\psi = e^{i(kx-\omega t)}$ in the TDSE and by taking the partial derivatives we get:

$$i\hbar\frac{\partial}{\partial t}e^{i(kx-\omega t)} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{i(kx-\omega t)} + Ve^{i(kx-\omega t)}$$
$$\hbar\omega e^{i(kx-\omega t)} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}ike^{i(kx-\omega t)} + Ve^{i(kx-\omega t)}$$

Here, lets highlight the two following correspondences that will be useful later on.

$$k \longleftrightarrow -i\frac{\partial}{\partial x} \qquad \omega \longleftrightarrow i\frac{\partial}{\partial t} \tag{115}$$

$$\hbar\omega e^{i(kx-\omega t)} = \frac{\hbar^2}{2m}k^2e^{i(kx-\omega t)} + Ve^{i(kx-\omega t)}$$
$$\hbar^2k^2 = 2m(\hbar\omega - V) \tag{116}$$

This expression can be rewritten in terms of omega.

$$\omega(t) = \frac{\hbar k^2}{2m} + \frac{V}{\hbar} \tag{117}$$

There are many ABCs that could be use to get rid of the unwanted reflections. We will take the approach describe in [Wat17], which starts by assuming the potential to be constant, such that $V=$ {finite set of constant values}. That way, we can calculate the group velocity of a wave packet as it evolved accordingly to the TDSE. In order to obtain the group velocity we need to take the derivative of equation w, which form equation (117) give

$$C(k) = \frac{\partial\omega}{\partial k} = \frac{\hbar k}{m}. \tag{118}$$

This expression will be approximated to

$$\frac{\hbar k}{m} \equiv q \tag{119}$$

where q is positive and real. Using the correspondence (115) we obtain the following differential operator:

$$(i\frac{\partial}{\partial x} + \frac{mq}{\hbar})\psi = 0 \tag{120}$$

If the differential equation is satisfied at the boundary then the wave can be absorbed and no reflection will occur. However, a wave is often composed of many group velocities, thus this expression needs to be generalize. To consider more group velocities the expression will take this form:

$$\prod_{l=1}^{p}(i\frac{\partial}{\partial x}+\frac{mq_l}{\hbar})\psi=0 \tag{121}$$

If $q_k \neq q_l$ for $k \neq l$ then p different group velocity will be absorbed to the first order for the computed solution and if $q_k = q_l$ for $k \neq l$, then the q_k group velocity is absorbed to the pth order. In this paper only $p = 3$ will be used, therefore, we will need some derivation for that special case.

Let's start with this:

$$(k+\frac{mq_1}{\hbar})(k+\frac{mq_2}{\hbar})(k+\frac{mq_3}{\hbar})=0 \tag{122}$$

here the correspondence (115) have be use and the k have been assumed to be positive for simplicity. By expending this equation we get:

$$k^3+\frac{k^2m(q_1+q_2+q_3)}{\hbar}+\frac{km^2(q_1q_2+q_1q_3+q_2q_3)}{\hbar^2}+\frac{m^3q_1q_2q_3}{\hbar^3}=0 \tag{123}$$

Let

$$\begin{aligned} h_1 &= m(q_1+q_2+q_3) \\ h_2 &= m^2(q_1q_2+q_1q_3+q_2q_3) \\ h_3 &= m^3q_1q_2q_3 \end{aligned}$$

By subbing h_1, h_2, h_3 in the previous equation we get:

$$k^3+\frac{k^2h_1}{\hbar}+\frac{kh_2}{\hbar^2}+\frac{h_3}{\hbar^3}=0 \tag{124}$$

From the dispersion relation (116) we get $k^2 = \frac{2m(\hbar\omega-V)}{\hbar^2}$. This can be use to substitute k^2 in equation (125), which give the following equation:

$$k\frac{2m(\hbar\omega-V)}{\hbar^2}+\frac{2mh_1(\hbar\omega-V)}{\hbar^3}+\frac{kh_2}{\hbar^2}+\frac{h_3}{\hbar^3}=0 \tag{125}$$

By combining the first term with the third term and the second term with the fourth term we get:

$$k\frac{(2m(\hbar\omega-V)+h_2)}{\hbar^2}+\frac{2mh_1(\hbar\omega-V+h_3)}{\hbar^3}=0 \tag{126}$$

Finally, by bringing the second term to right and by multiplying both sides by $\hbar^3$and $(2m(\hbar\omega-V)+h_2))^{-1}$ we get:

$$\pm\hbar k=\frac{2mh_1(\hbar\omega-V)+h_3}{2m(\hbar\omega-V)+h_2} \tag{127}$$

We will let the ABC in that form for now. After the following subsection the ABC will be tweaked a bit more in order to be implemented in the Crank-Nicolson scheme.

4.1.2 Crank-Nicolson Scheme

The Crank-Nicolson is a combinations of the forward Euler (explicit) method and the backward Euler method (implicit) which are based on the trapezoidal rule. This approach benefits from the accuracy of the explicit method and the stability of the

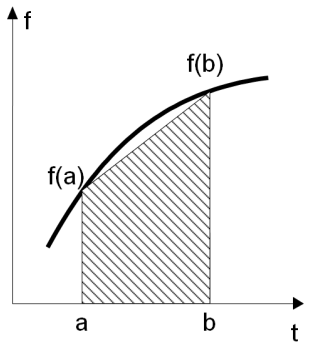

Figure 9: Trapezoidal Rule

implicit method.

In order to illustrate the forward Euler method we will use the time-dependent heat equation.

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} \tag{128}$$

where k is a constant. The technique consist of expressing u by its value as a set of grid point. For the spatial domain we choose $x = x_j = x_0 + j\Delta x$, with $j \in [0, J]$ and in a similar fashion the time domain will have a range $t = t_n = n\Delta t$, with $n \in [0, N]$. The first-order time derivative will be approximated in the following way

$$\frac{\partial u}{\partial t} = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t}. \tag{129}$$

The notation of this expression can be simplified to give

$$\frac{\partial u}{\partial t} = \frac{u_j^{n+1} - u_j^n}{\Delta t}. \tag{130}$$

The second derivative with respect to x can be approximated in the following way

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left[\frac{u(x_j + 1, t_n) - u(x_j, t_n)}{\Delta x}\right] \\ &= \frac{u(x_{j+2}, t_n) - 2u(x_{j+1}, t_n) + u(x_j, t_n)}{(\Delta x)^2}. \end{aligned} \tag{131}$$

Again the notation will be simplified, but the indices will also be shifted by minus one.

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \tag{132}$$

If we put equation (131) and equation (132) together we get the explicit or forward Euler method.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = k\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \tag{133}$$

Making reference to the grid point discussed earlier, this method can be visualized with the following figure 10:

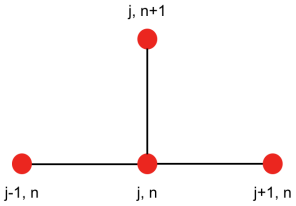

Figure 10: Grid point connectivity for explicit Euler

In order to obtain the implicit or backward Euler we will evaluate u at time step $n+1$ on the second derivative to the right hand side.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = k \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} \tag{134}$$

For the implicit Euler method the grid point diagram looks like:

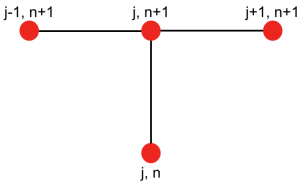

Figure 11: Grid point connectivity for implicit Euler

The Crank-Nicolson scheme consists of expressing the time derivative as the average of the space derivative of the explicit and implicit Euler method. This allows to combine the accuracy of the explicit method with small time step and the stability of the implicit method.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{k}{2} \left[\frac{(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (u_{j+1}^n - 2u_j^n + u_{j-1}^n)}{(\Delta x)^2} \right] \tag{135}$$

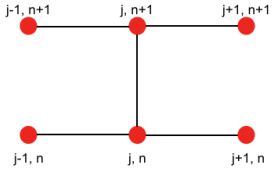

Figure 12: Grid point connectivity for Crank-Nicolson

4.1.3 Solving the Time dependent Schrödinger Equation with the Crank-Nicolson Method

Now that we acquired a good understanding of the Crank-Nicolson scheme with the heat equation we will see how it applies to the TDSE. One of the key feature of the Crank-Nicolson method for our application is that it is unitary meaning that it will conserve probability. Again let's consider the time dependent Schrödinger equation.

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$$

When the Hamiltonian operator is not time dependent then the solution to the TDSE is given by:

$$\psi(x,t) = \hat{U}\psi(x,0) = e^{\frac{-i\hat{H}t}{\hbar}}\psi(x,0) \tag{136}$$

After applying the same technique of discretization that was used with the heat equation the solution in (138) reads

$$\psi_j^{n+1} = e^{\frac{-i\hat{H}t}{\hbar}}\psi_j^n = \hat{U}\psi_j^n \tag{137}$$

Now we need to expend the matrix $\hat{U}$, but since $\hat{U}$ is unitary any approximation of $\hat{U}(\Delta t)$ also needs to be unitary to preserve the norm of the wave function. In order to do so we can use Cayley's form for the finite-difference representation of $e^{-i\hat{H}t}$.

$$\hat{U}\Delta t = e^{-i\hat{H}\Delta t} \simeq \frac{(1-\frac{\hat{H}\Delta t}{2})}{(1+\frac{\hat{H}\Delta t}{2})} \tag{138}$$

To get to that result we will first split $\hat{U}(\Delta t)$ as follows

$$\psi_j^{n+1} = e^{\frac{-i\hat{H}\Delta t}{2}}e^{\frac{-i\hat{H}\Delta t}{2}}\psi_j^n \tag{139}$$

and multiply the equation from the left with the conjugate transpose $\hat{U}(\frac{\Delta t}{2})$, which give

$$e^{\frac{i\hat{H}\Delta t}{2}}\psi_j^{n+1} = e^{\frac{-i\hat{H}\Delta t}{2}}\psi_j^n. \tag{140}$$

Now, by expending the exponential functions into a Taylor series keeping only the two firm terms of the series we get

$$\left(1+\frac{i\hat{H}\Delta t}{2}\right)\psi_j^{n+1} = \left(1-\frac{i\hat{H}\Delta t}{2}\right)\psi_j^n, \tag{141}$$

which is equivalent to Cayley's approximation. So far the relation with the Crank-Nicolson scheme might not have been so obvious, but a few remaining step is needed to get to the same form we got with the heat equation. First, we will distribute the two ψ and replace the Hamiltonian operator symbol by $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$.

$$\psi_j^{n+1} - \frac{\hbar^2}{2m}\frac{i\Delta t}{2}\left[\frac{\partial^2}{\partial x^2}\psi_j^{n+1} - V\psi_j^{n+1}\right] = \psi_j^n + \frac{\hbar^2}{2m}\frac{i\Delta t}{2}\left[\frac{\partial^2}{\partial x^2}\psi_j^n - V\psi_j^n\right] \tag{142}$$

Note that the terms $\frac{\hbar^2}{2m}$ cancelled out on each side. Now by rewriting $\frac{\partial^2}{\partial x^2}\psi_j^{n+1}$ and $\frac{\partial^2}{\partial x^2}\psi_j^n$ in the same way we did for the heat equation in (132) we get

$$\psi_j^{n+1} - \frac{i\Delta t}{2}\left[\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta x)^2} - V_j\psi_j^{n+1}\right] = \psi_j^n + \frac{i\Delta t}{2}\left[\frac{\psi_{j+1}^{n} - 2\psi_j^{n} + \psi_{j-1}^{n}}{(\Delta x)^2} - V_j\psi_j^{n}\right]. \tag{143}$$

In order to write (145) in matrix form will will use the following vector notation $\boldsymbol{\psi^n} = (\psi_0^n, ..., \psi_j^n, ..., \psi_J^n)$. The equation (145) can then be written in matrix form as follow:

$$\mathcal{U}_1\boldsymbol{\psi^{n+1}} = \mathcal{U}_2\boldsymbol{\psi^n} \tag{144}$$

where

$$\mathcal{U}_1 = \begin{pmatrix} \xi_0 & -\alpha & & & \\ -\alpha & \xi_1 & -\alpha & & \\ & \ddots & \ddots & \ddots & \\ & & -\alpha & -\xi_{J-1} & -\alpha \\ & & & -\alpha & -\xi_{J-1} \end{pmatrix}, \quad \mathcal{U}_2 = \begin{pmatrix} \gamma_0 & \alpha & & & \\ \alpha & \gamma_1 & \alpha & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha & \gamma_{J-1} & -\alpha \\ & & & -\alpha & \gamma_{J-1} \end{pmatrix}$$

with

$$\alpha = \frac{i\Delta t}{2\Delta x^2}, \xi_j = 1 + \frac{i\Delta t}{2}\left(\frac{2}{\Delta x^2} + V_j\right), \gamma_j = 1 - \frac{i\Delta t}{2}\left(\frac{2}{\Delta x^2} + V_j\right). \tag{145}$$

4.1.4 Implementation of the ABC in the Crank-Nicolson Scheme

In this section we will implement the ABCs in the Crank-Nicolson Scheme. The goal is to determine how to rewrite the boundary conditions in a way that they can become the first and last entries of the tridiagonal matrix $\mathcal{U}_1$ and $\mathcal{U}_2$. First they need to be discretized. By applying the correspondence (115) and assuming $\hbar = 1$ the equation (128) becomes

$$\pm i(\frac{h_2}{2m} - V)\frac{\partial\psi}{\partial x} \mp \frac{\partial^2\psi}{\partial t\partial x} - ih_1\frac{\partial\psi}{\partial t} - (\frac{h_3}{2m} - h_1V)\psi = 0. \tag{146}$$

We will use the finite-difference discretizations as describe in [FJ99] to approximate the derivative in (148).

$$\begin{aligned} \psi &\approx \frac{1}{4}(\psi_{j\pm1}^{n+1} + \psi_j^{n+1} + \psi_{j\pm1}^n + \psi_j^n), \\ \frac{\partial\psi}{\partial x} &\approx \pm\frac{1}{2\Delta x}(\psi_{j\pm1}^{n+1} - \psi_j^{n+1} + \psi_{j\pm1}^n - \psi_j^n), \\ \frac{\partial\psi}{\partial t} &\approx \frac{1}{2\Delta t}(\psi_{j\pm1}^{n+1} + \psi_j^{n+1} - \psi_{j\pm1}^n - \psi_j^n), \\ \frac{\partial^2\psi}{\partial t\partial x} &\approx \pm\frac{1}{\Delta t\Delta x}(\psi_{j\pm1}^{n+1} - \psi_j^{n+1} - \psi_{j\pm1}^n + \psi_j^n \end{aligned} \tag{147}$$

Those discritization yields the two following equations:

$$\beta_1^{p=3}\psi_0^{n+1} + \beta_2^{p=3}\psi_1^{n+1} = \beta_3^{p=3}\psi_0^n + \beta_4^{p=3}\psi_1^n, \tag{148}$$

$$\zeta_1^{p=3}\psi_{J-1}^{n+1} + \zeta_2^{p=3}\psi_{J-2}^{n+1} = \zeta_3^{p=3}\psi_{J-1}^n + \zeta_4^{p=3}\psi_{J-2}^n \tag{149}$$

where

$$\begin{aligned}
\beta_1^{p=3} &= \left(-\frac{ia_0}{2\Delta x} + \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} - \frac{b_0}{4}\right), \\
\beta_2^{p=3} &= \left(\frac{ia_0}{2\Delta x} - \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} + \frac{b_0}{4}\right), \\
\beta_3^{p=3} &= \left(\frac{ia_0}{2\Delta x} + \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} + \frac{b_0}{4}\right), \\
\beta_4^{p=3} &= \left(-\frac{ia_0}{2\Delta x} - \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} + \frac{b_0}{4}\right),
\end{aligned} \tag{150}$$

$$\begin{aligned}
\zeta_1^{p=3} &= \left(-\frac{ia_J}{2\Delta x} + \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} - \frac{b_J}{4}\right), \\
\zeta_2^{p=3} &= \left(\frac{ia_J}{2\Delta x} - \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} + \frac{b_J}{4}\right), \\
\zeta_3^{p=3} &= \left(\frac{ia_J}{2\Delta x} + \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} + \frac{b_J}{4}\right), \\
\zeta_4^{p=3} &= \left(-\frac{ia_J}{2\Delta x} - \frac{1}{\Delta t \Delta x} - \frac{ih_1}{2\Delta t} + \frac{b_J}{4}\right),
\end{aligned} \tag{151}$$

for which $a_j = \frac{h_2}{2m} - V_j$ and $b_j = \frac{h_3}{2m} - V_j$. We can now simply implement the ABC in the Crank-Nicolson scheme by adding those term to the matrix $\mathcal{U}_1$ and $\mathcal{U}_2$.

$$\mathcal{U}_1 = \begin{pmatrix} \beta_1 & \beta_2 & & & \\ -\alpha & \xi_1 & -\alpha & & \\ & \ddots & \ddots & \ddots & \\ & & -\alpha & -\xi_{J-1} & -\alpha \\ & & & \zeta_2 & \zeta_1 \end{pmatrix}, \quad \mathcal{U}_2 = \begin{pmatrix} \beta_3 & \beta_4 & & & \\ \alpha & \gamma_1 & \alpha & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha & \gamma_{J-1} & \alpha \\ & & & \zeta_4 & \zeta_3 \end{pmatrix}$$

4.2 Methods of Analysis

This section will cover the non-trivial pieces of code used in the simulation. The code presented simulate a simple Gaussian hitting a rectangular well. Variation of the potential well be presented in the results.

First we need to create the space in which the simulation will take space.

Listing 1: Simulation Parameters

```
    # Planck's constant is set to 1
mass = 0.5 # Mass of the particle

    # Time-related parameters
final_time = 5
time_steps = 5000
dt = final_time / time_steps

    # Space/mesh related parameters
```

```
xi = -20 # Left endpont
xf = +20 # Right endpoint
mesh_size = 3001
dx = (xf-xi) / (mesh_size-1)
```

Here note that mesh_ size refers to the domain $[0, J]$ discussed in the dicretization of the space domain and similarly time_steps the range from $[0, N]$.

We then need to create a potential well. In that case an upright potential well from 2 to 6. The well can vary in shape, value (- or +) and in quantity.

Listing 2: Setting up the potential

```
    # Our potential function
def V(x):
    return 8  if 2 <= x <= 6  else  0

    # Store the potential in a grid
potential = np.array([V(xi + i*dx)
for i in range(mesh_size)])
    # Define the X grid and the Psi array
Xgrid = np.linspace(xi, xf, mesh_size)
Psi = np.zeros((time_steps, mesh_size), complex)
```

As stated in equation (73) the the modulus squared of the wave function equal to the probability density of the particles; therefore, the chosen distribution, here Gaussian, needs to be squared rooted.

Listing 3: Parameters for the Initial Distribution

```
    # we need to specify the intial Psi values
k0 = 3 #wave number
sigma0 = 1 #the standard deviation of the initial Gaussian
mu0 = -9 #where the initial Gaussian is centered
Psi[0,:] = (1/(2*pi*sigma0**2)**(1/4))
*np.exp((1j)*k0*Xgrid - ((Xgrid-mu0)/(2*sigma0))**2)
```

In the following listing we set up the entries of the modified tridiagonal matrices $\mathcal{U}_1$ and $\mathcal{U}_2$ that implement the ABC in the Crank-Nicolson scheme. All the variables have been defined in (1.4.1) and (1.4.2)

Listing 4: Setting up the Absorbing Boundary Conditions

```
q = k0/mass
h1 = 3*mass*q
h2 = 3*(mass**2)*(q**2)
h3 = (mass**3)*(q**3)

ai = h2/(2*mass) - V(xi)
af = h2/(2*mass) - V(xf)
bi = h3/(2*mass) - h1*V(xi)
bf = h3/(2*mass) - h1*V(xf)
```

```
beta1 = -(1j)*ai/(2*dx) + 1/(dt*dx) - (1j)*h1/(2*dt) - bi/4
beta2 = (1j)*ai/(2*dx) - 1/(dt*dx) - (1j)*h1/(2*dt) - bi/4
beta3 = (1j)*ai/(2*dx) + 1/(dt*dx) - (1j)*h1/(2*dt) + bi/4
beta4 = -(1j)*ai/(2*dx) - 1/(dt*dx) - (1j)*h1/(2*dt) + bi/4

zeta1 = -(1j)*af/(2*dx) + 1/(dt*dx) - (1j)*h1/(2*dt) - bf/4
zeta2 = (1j)*af/(2*dx) - 1/(dt*dx) - (1j)*h1/(2*dt) - bf/4
zeta3 = (1j)*af/(2*dx) + 1/(dt*dx) - (1j)*h1/(2*dt) + bf/4
zeta4 = -(1j)*af/(2*dx) - 1/(dt*dx) - (1j)*h1/(2*dt) + bf/4
```

Here note that (1j) is the complex number i.

The ABC being defined, we can construct the modified matrices $\mathcal{U}_1$ and $\mathcal{U}_2$.

Listing 5: Making the matrix U1 and U2

```
    # setting up the tridiagonal matrices
ones = np.ones((mesh_size), complex)
alpha = (1j)*dt/(2*dx**2)
xis = np.array([2*mass + (1j)*dt/(dx**2)
+ (1j)*mass*dt*potential[i] for i in range(mesh_size)])
xis[0] = beta1
xis[mesh_size-1] = zeta1
up = -alpha*ones
up[1] = beta2
down = -alpha*ones
down[mesh_size-2] = zeta2
gamma = np.array([2*mass - (1j)*dt/(dx**2)
- (1j)*mass*dt*potential[i] for i in range(mesh_size)])
gamma[0] = beta3
gamma[mesh_size-1] = zeta3
ups = alpha*ones
ups[1] = beta4
downs = alpha*ones
downs[mesh_size-2] = zeta4
diags = np.array([-1, 0, 1])
vecs1 = np.array([down, xis, up])
vecs2 = np.array([downs, gamma, ups])

U1 = sp.spdiags(vecs1, diags, mesh_size, mesh_size)
U1 = U1.tocsc()
U2 = sp.spdiags(vecs2, diags, mesh_size, mesh_size)
```

Now that the matrices are set up we need a bit of code to compute ψ. Then we can compute the modulus of ψ to get the density, which can be used to plot the wave-packets.

Listing 6: Solving for Psi

```
LU = linalg.splu(U1)
    for i in range(time_steps - 1):
    b = U2.dot(Psi[i,:])
    Psi[i+1,:] = LU.solve(b)
```

```
    # Compute probability density
Density = np.abs(Psi * np.conj(Psi))
```

Listing 7: Utility method to compute derivatives

```
    # we need a little subroutine to compute derivatives
    # dim carries the dimension
    along which we will differentiate
def derivative(array, dim, dd):
    leng = array.shape[dim]
    der = np.zeros_like(array)
    for i in range(1, leng-1):
        indxl = [Ellipsis]*array.ndim
        indx = [Ellipsis]*array.ndim
        indxr = [Ellipsis]*array.ndim
        indxl[dim] = i-1
        indx[dim] = i
        indxr[dim] = i+1
        der[indx] = (array[indxr]-array[indxl])/(2*dd)
    indx0 = [Ellipsis]*array.ndim
    indx1 = [Ellipsis]*array.ndim
    indx0[dim] = 0
    indx1[dim] = 1
    der[indx0] = (array[indx1]-array[indx0])/dd
    indxm1 = [Ellipsis]*array.ndim
    indxm2 = [Ellipsis]*array.ndim
    indxm1[dim] = -1
    indxm2[dim] = -2
    der[indxm1] = (array[indxm1]-array[indxm2])/dd

    return der
```

In order to obtain the velocity field which will allows us to compute the trajectories we need to compute the action. This task is peform in the following listing.

Listing 8: Computing the action function

```
S = np.angle(Psi)
for i in range(time_steps):
S[i,:] = np.unwrap(S[i,:])

DisplayActionFunction = False
if DisplayActionFunction:
    figb, axb = plt.subplots()
    plt.axis([xi, xf, -100, 100])
    lineb, = axb.plot(Xgrid, S[0,:])

def animateb(i):
        lineb.set_ydata(S[i,:])  # update the data
```

```
        return line,

  # Init only required for blitting to give a clean slate.
    def init():
        lineb.set_ydata(np.ma.array(Xgrid, mask=True))
        return line,

ani = animation.FuncAnimation(figb, animateb,
np.arange(0, time_steps, 10), init_func=init,
interval=1, blit=True)
    plt.show()
```

Having the action we can extract the velocity field using equation (81).

Listing 9: Extracting the velocity field

```
    v = derivative(S, 1, mass*dx)
```

Finally, this is the listing that compute the trajectories.

Listing 10: Computing the trajectories

```
nt = 1000 #this is how many trajectories will be computed
x = np.zeros((nt, time_steps))
x[:,0] = np.linspace(mu0 - 3*sigma0, mu0 + 3*sigma0, nt)

for l in range(nt):
    # Compute the location of the particle
    for i in range(1,time_steps):
        # The grid index location
        loca = (x[l,i-1] - xi)/dx
        k = np.int(np.floor(loca))
        # Check if the particle reached the right end
        if k > mesh_size-2:
            x[l, i:time_steps] = xf

        # Check if the particle reached the left end
        elif k < 0:
            x[l, i:time_steps] = xi

        # Interpolate the position
        else:
            x[l,i] = x[l,i-1] +
            (v[i-1,k]*(loca-k)+v[i-1,k+1]*(1-loca+k))*dt

# Transpose X for ease of use
x = np.transpose(x)
```

5 Results

The results consists of two plots one is the a visualization of the wave packets as hits the potential barrier and the second one is a graphs showing the possible trajectories followed by the particle near the potential wall. The first case presented is the case described in the code, which is a single Gaussian hitting a rectangular wall. The right-

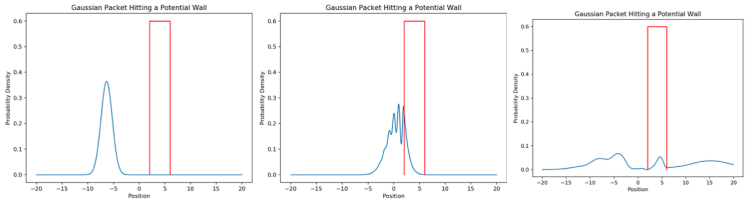

Figure 13: Single Gaussian Hitting a Rectangular Well

hand of the the third pictures shows that the simulation experienced no reflection at boundaries, which means that the implementation of the ABC have been a success. In this scenario we can see a big bulge travelling to the left, which indicate that most possibly the particle would bounce of the potential wall. Another interesting phenomenon is the small bump that appear in the potential wall, this bump stayed there after completion of the simulation. As can be seen in the other graph it is because the particle can get caught in the wall. As predicted by the pilot-wave theory

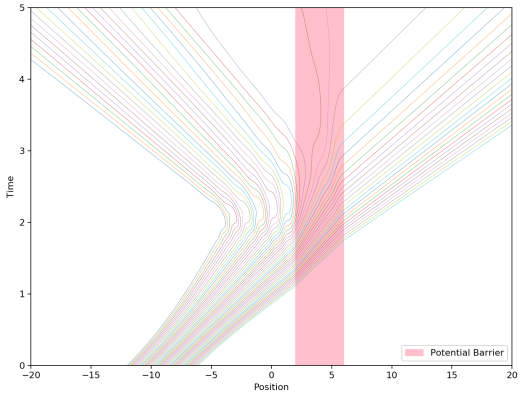

Figure 14: Trajectories of a Single Gaussian Hitting a Rectangular Wall

there is trajectories that do not even touch the bounds. Those are the reflections on the possible reflections of the particle on the wall. In order to understand this graph it is important to keep in mind that the on y-axis is time and on the x-axis position.

The second case presented is a double Gaussian hitting a rectangular wall. Notice that the two bumps appear smaller then the single one shown previously. It is because both have to sum up to one.

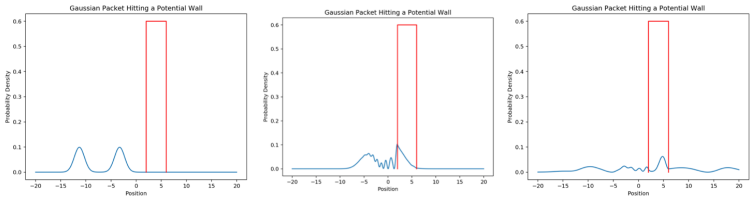

Figure 15: Double Gaussian Hitting a Rectangular Wall

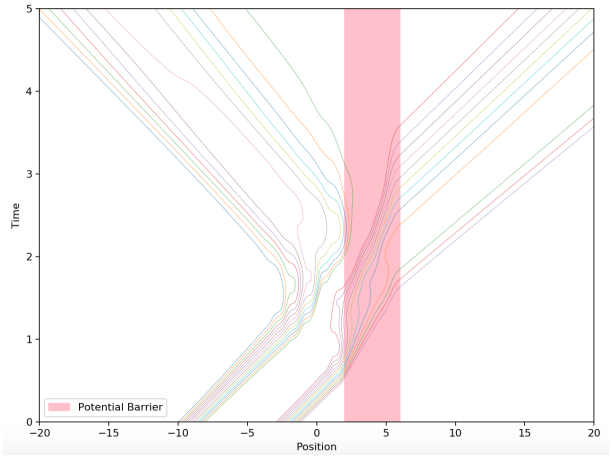

Figure 16: Trajectories of a Double Gaussian Hitting a Rectangular Wall

Finally the last case presented is a single Gaussian hitting a triangular wall. This was the smoothest graph, with very little erratic behavior. As can been seen in the two plot no particles get caught in the wall for this scenario.

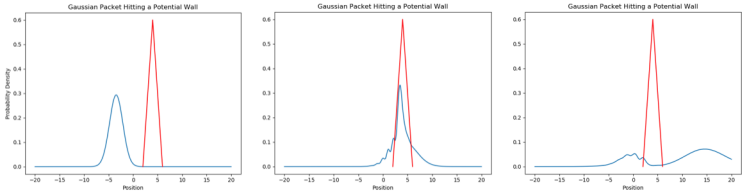

Figure 17: Single Gaussian Hitting a triangular Wall

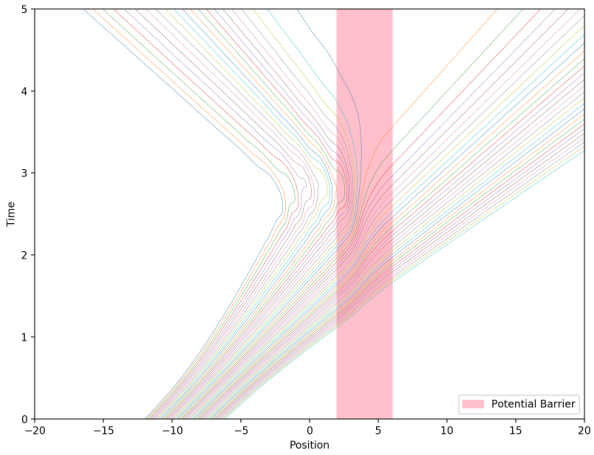

Figure 18: Trajectories of a Single Gaussian Hitting a triangular Wall

6 Conclusion

In this paper we discussed two potential way of plotting Bohmian trajectories in one dimension. The first consist of expressing the particles trajectories in terms of a differential equation that make no use of the wave function. The differential equation turned out to be very stiff which makes it very difficult to compute. On the other hand, with a bit more work this approach could potentially become very efficient and could be useful to generate data in order to train a neural net. The second approach consists of computing the one dimensional time dependent Schrodinger equation with the Crank-Nicolson scheme using absorbing boundary conditions in order to avoid reflections at the boundaries. This approach was success, the absorbing boundary conditions led to no reflections at the boundaries and it was possible to plot the wave packet hitting a potential well and to plot a relevant range of trajectories. The simulation works with different shapes of potential well and even variation of the Gaussian distribution.

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