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Constructing Numerical Methods For Solving The Guiding Equation In Bohmian Mechanics

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Abstract

The aim of this thesis was to simulate a part of a proposed experiment by Lev Vaidman by using Bohmian mechanics. To do this a numerical method for solving the Schrödinger equation and the guiding equation was created, with several ways of making the simulation more efficient.

To make the simulation work more efficiently the Schrödinger equation was applied to only a small region of the whole setup. This region followed the wavefunction of significant values and could change size during the simulation.

A beam splitter was constructed in the form of a thin potential barrier. The beam splitter was tested to verify that the reflected and transmitted angles agreed with expectations. A virtual detector was constructed and used for the calibration of the beam splitter to determine which potential resulted in dividing the wave packet into two wave packets of equal intensity.

A fixed angle mirror was used for testing the reflection of a wave packet for the reflected angle and concluded that it agreed with the expectations for it. Testing a time dependent mirror for different frequencies and amplitudes was performed, with the result that the numerical method could be used to determine the particles' trajectories.

These results were used to construct a larger setup that was a small part of Vaidman's proposed experiment. These setups were done in several version. All setups had one wave packet that went through one beam splitter and separated into two wave packets. These two wave packets reflected at two mirrors with different frequencies and then interfered with each other at either free space or at another beam splitter. The result of the simulation of these setups was that the particles' trajectories could be calculated with the guiding equation.

Keywords: Bohmian mechanics, Numerical methods.

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Sammanfattning

Syftet med denna avhandling var att simulera en del av det föreslagna experimentet av Lev Vaidman med hjälp av Bohmsk mekanik. För att göra detta skapades en numerisk metod för att lösa Schrödingerekvationen och den ledande ekvationen, ”the guiding equation”, med flera sätt att effektivisera simuleringen.

För att effektivisera simuleringen tillämpades Schrödingerekvationen på endast en liten region i hela uppställningen. Denna region följde vågfunktionen med betydande värden och kunde ändra storlek under simuleringen.

En stråldelare konstruerades i form av en tunn potentialbarriär. Stråldelaren testades för att verifiera att de reflekterade och överförda vinklarna överensstämde med förväntningarna. En virtuell detektor konstruerades och användes för kalibrering av stråldelaren för att bestämma vilken potential som resulterade i att vågpaketet delades in i två vågpaket med samma intensitet.

En spegel med fast vinkel användes för att testa reflektionen av ett vågpaket för den reflekterade vinkeln och kom fram till att den överensstämde med förväntningarna för den. Att testa en tidsberoendespegel för olika frekvenser och amplituder utfördes med resultatet att den numeriska metoden kunde användas för att bestämma partiklarnas banor.

Dessa resultat användes för att konstruera en större uppställning av ett experiment som var en liten del av Vaidmans föreslagna experiment. Dessa uppställningar gjordes i flera versioner. Alla uppställningar hade ett vågpaket som gick igenom en stråldelare och separerades i två vågpaket. Dessa två vågpaket reflekterades vid två speglar med olika frekvenser och interfererade sedan varandra antingen i en tom rymd eller vid en annan stråldelare. Resultatet av simuleringen av dessa inställningar var att partiklarnas banor kunde beräknas med ledande ekvation.

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1. Introduction

Lev Vaidman argues by means of a thought experiment [1,2], that it is not possible for a particle to travel in a way that Bohmian mechanics predicts. In his proposed experiment photons are sent through beam splitters and reflected by mirrors. When the photon beam is divided by a beam splitter the resulting light travels in different directions where they interact with the mirrors that oscillates with different frequencies and are then reflected towards more beam splitters where they interfere with each other. The resulting output is analysed by a detector that measures the power function of the wavefunction. This power function is analysed for its Fourier components, to determine which mirror frequencies that are contained in the wavefunction. He proposed an experiment where some of the oscillating frequencies of the mirrors do not appear in the power spectrum, while others do, in such a way that one can conclude that there exist path segments that are isolated from each other. Any particle's trajectory predicted by Bohmian mechanics can be described by a continuous function and the result of Vaidman's proposed experiment seems to contradict this

When quantum mechanics was discovered, its main interpretation was that the wavefunction could be used for determining the probability of measuring a certain outcome. The wavefunction is determined by solving the Schrödinger equation. The square of the magnitude of the wavefunction in position space is seen as the probability density of where the particle can be found. It was a common interpretation that there are only waves and by measuring the wavefunction, it collapses to a definite value, in some cases to result in a particle with a position. Another interpretation was that both the particle and wave exist, but the wave guides the particle. This is a pilot wave theory, also known as the de Broglie Bohm theory or as Bohmian mechanics. It incorporates the predictions of quantum mechanics and derives a formula similarly to Hamiltonian mechanics about the velocity of a particle. It could be considered a separate theory and not just as an interpretation of quantum mechanics because it can predict the position of a particle and its trajectory from a starting position. The uncertainty of the starting position corresponds to the probability of measurements, in quantum mechanics [3-9].

The equation which gives the velocity of a particle is known as the guiding equation which can be used to calculate the trajectory of a particle. This trajectory depends on the particle's starting position and the wavefunction for all times. Solving the Schrödinger equation for the analytic solution of the wavefunction is not possible in many problems so it is done by using numerical methods for both the solution of the partial differential equation of the wavefunction and for applying the guiding equation. Using this numerical solution of the wavefunction and by using the guiding equation it is possible to calculate a particle's trajectory given its initial position.

In this thesis, a numerical scheme adapted to analysing Bohm trajectories in the presence of oscillating mirrors is developed. This results in a method that can be regarded a first step towards analysing the Vaidman setup by means of Bohm trajectories.

The following section starts with a brief discussion of the Vaidman setup followed by a description of the de Broglie-Bohm theory. The numerical scheme to solve the combined Schrödinger and guiding equations is presented in section 3. The setups of the performed simulations are described in section 3. The results of these simulations are presented in section 4. The report ends with a discussion and the conclusions in sections 5 and 6, respectively.

2. Theory

2.1 Vaidman's proposed experiment

Vaidman's proposed experiment is depicted in Figure 1 [1,2]. It shows the setup with a particle source, the particles trajectories through the setup, beam splitters BS1-BS4, oscillating mirrors M1-M5, and a detector that measures the power from the wavefunction. The mirrors oscillate with different frequencies and these frequencies can be detected by Fourier transforming the power function measured by the detector. Vaidman proposed to slightly change the position of the mirror M2, so as to cause destructive interference at the beam splitter BS3, in the direction towards the mirror M5, and to prevent the particles to move towards that mirror, see Figure 2. Vaidman predicts in this setup that the oscillating frequencies of the mirrors M1 and M5, would not be present in the Fourier transform of the power function measured by the detector. On the other hand, the oscillation frequencies of the other mirrors M2, M3 and M4, would still be present in the Fourier transform of the power function. Since the oscillation frequencies of the mirrors M2 and M3 are present while those of mirrors M1 and M5 are absent, the particle needs to enter and exit the interferometer without hitting the mirrors M1 and M5, thereby creating and isolated path segment in the small interferometer loop defined by the mirrors M2 and M3, and the beam-splitters BS2 and BS3. Vaidman explains the result by using the two-vector formalism [10,11], in which a pre-selected forward going and a post-selected backward going wave function interfere constructively in the small interferometer loop. The constructive interference is marked by red lines in Figure 3. This results in creating isolated path segments, where the particles have a non-zero probability of being detected [1,2]. Vaidman's prediction has been verified in a photon experiment [12].

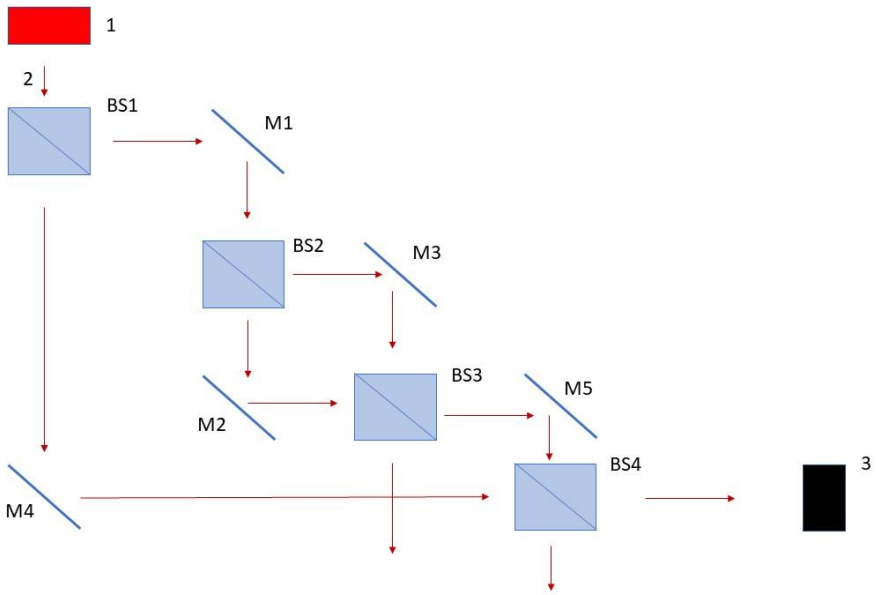

Figure 1. Depiction of Vaidman's proposed experiment. 1. A particle source, marked with a red rectangle. 2. Particle trajectories, marked with red arrows. 3. A detector marked with a black rectangle. BS1-BS4, Beam splitters, marked with blue rectangles. M1-M5, Oscillating mirrors, marked with blue lines.

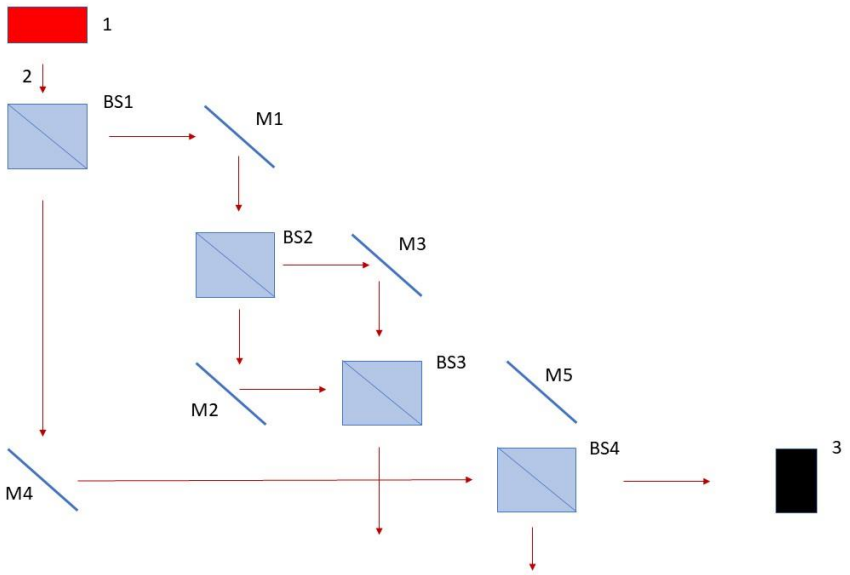

Figure 2. Depiction of Vaidman's experiment with M2 adjusted so as to create destructive interference along the path hitting the mirror M5.

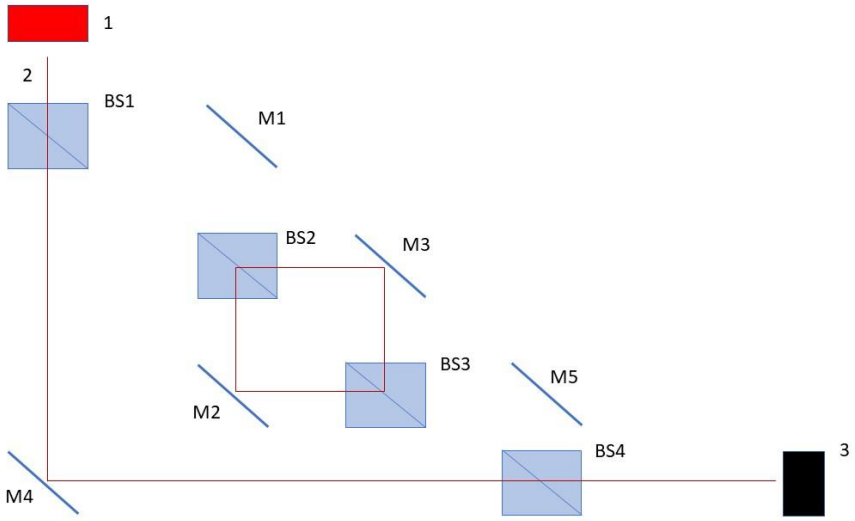

Figure 3. Trajectories associated with the setup in Figure 2. The absence of the frequencies of mirrors M1 and M5 implies an isolated path segment in the interferometer loop defined by the mirrors M2 and M3 and the beam-splitters BS2 and BS3.

2.2 De Broglie Bohm Theory

De Broglie Bohm theory is considered as an interpretation of quantum mechanics. It gives the same predictions as quantum mechanics, but it adds a different way of looking at quantum mechanics by using the wavefunction of quantum mechanics to predict a future position of a particle from a starting position. Quantum mechanics predicts the probabilities of detecting a particle at different positions and this still applies to de Broglie Bohm theory. The randomness in detecting a particle, in de Broglie Bohm theory, comes instead from the uncertainty of the starting position. The theory was originally suggested by de Broglie [3] (see also [4]), but it was considered a dead-end for quantum mechanics in its earlier years, thus de Broglie did not continue to work on it. The theory did not catch so much attention until Bohm [5,6] took up the idea in 1952, showing that it is able to capture all predictions of quantum mechanics. Therefore, the approach goes under the combined name de Broglie-Bohm theory,

but in more recent years it is also become known as Bohmian mechanics [7,8]. For a detailed monograph of the theory, see [9].

Bohmian mechanics is a pilot wave theory that uses a field consisting of the wavefunction, found by solving the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\bar{r},t) = \left[\frac{-\hbar^2}{2m}\Delta + V(\bar{r},t)\right]\psi(\bar{r},t). \quad (1)$$

The field affects the particle that the Schrödinger equation is calculated for. The theory is asymmetric, to use it one must first calculate the wavefunction from the Schrödinger equation and then the particle's trajectory from the wavefunction. In that way the wavefunction affects the particle's motion, but the motion of the particle do not affect the wavefunction [8,9].

The particle's trajectory can be calculated from the wavefunction that result from the Schrödinger equation. This is done with the guiding equation that is a result from Bohmian mechanics. The guiding equation can be used for the wavefunction that is solved either from a time independent Schrödinger equation or solved by the time dependent Schrödinger equation. Even if a particle is in free space, the particle is affected by a distant potential due to a quantum potential. This quantum potential is determined by the wavefunction and can affect the particle because the information of a remote potential is transmitted by the wavefunction and results in a quantum potential at the particle's position. The trajectories would be continuous and could not create isolated path segments as in Vaidmans explanation of the proposed experiment [8,9,13].

2.3 Derivation of the guiding equation

Hamiltonian mechanics use the Hamiltonian equations to determine motion classically and with those equations it is possible to determine the time derivative of the position. This equation has a corresponding equation in Bohmian mechanics where it is possible to derive an equation for a particle. This equation is defined differently since the wavefunction is a complex function and the fact that Schrödinger equation is a first order with respect of time. By taking that into account, the corresponded Hamiltonian equation for Bohmian mechanics gets defined somewhat differently. Deriving the equation is done with the probability flux or probability current. This is like a normal flux in a classical theory but corresponds to the probability density. It can be understood with help of an example with the probability of detecting a particle in a box. Integrating the probability density of the position with the volume of the box gives the total probability of locating the particle in the box. The changes of the total probability in time is equal to how much of this probability goes through the sides of the box by the probability flux or probability current [8,9].

The probability current is found by calculating how the probability density for a point changes in time and using the fact that the probability density is locally conserved. The time derivative of the square of the wavefunction is used as the time derivative of the probability density since the square of the magnitude of the wavefunction is the probability density. The change in the probability density is locally conserved and thus a continuity equation holds, applying the continuity equation for the probability density results in

$$\frac{d|\psi|^2}{dt} = \nabla\cdot\bar{J}, \quad (2)$$

where $\bar{J}$ is the probability current,

$$\bar{J} = \frac{\hbar}{2mi}(\psi^* \nabla\psi - \psi \nabla\psi^*). \quad (3)$$

After some cancelation and by using the imaginary and real components of the wavefunction, this is results to:

$$\bar{J} = \frac{\hbar}{m}\big(Re(\psi)\nabla Im(\psi) - Im(\psi)\nabla Re(\psi)\big). \quad (4)$$

The probability current can be considered as the streamlines of the probability density. If the time derivative of the position would be referred to as a flow of the probability density explained by streamlines instead this would result in that the probability current would be proportional to the derivative of the position. The probability current is thus a function of density multiplied by the time derivative

$$\bar{J}(\bar{r}, t) = |\psi(\bar{r}, t)|^2 \frac{d\bar{r}}{dt}. \quad (5)$$

If the current and the probability density is known, it is possible to get the time derivative of the position by dividing the current by the density. This formula of the probability current divided by the probability density can be rewritten to the more common form:

$$\frac{d\bar{r}}{dt} = \frac{\bar{J}(\bar{r}, t)}{|\psi(\bar{r}, t)|^2} = \frac{\hbar}{m} Im\left(\frac{\nabla\psi(\bar{r}, t)}{\psi(\bar{r}, t)}\right). \quad (6)$$

The way to connect this to the motion of the particle is to use a localised wavefunction of the position. This equation would then still hold, and the position of the non-zero parts wavefunction are very precise and thus only at that position would there be a non-zero probability of a particle to be located and so this is the position of the particle. The position of the particle called Q would replace r in this case, but this would also hold in the general case. So, rewriting it to the position of the particle, Q, is done by replacing r with Q:

$$\frac{d\bar{Q}}{dt} = \frac{\hbar}{m} Im\left(\frac{\nabla\psi(\bar{Q}, t)}{\psi(\bar{Q}, t)}\right) = \frac{\bar{J}(\bar{Q}, t)}{|\psi(\bar{Q}, t)|^2}. \quad (7)$$

This equation will have some issues if applying it to a place where the density is zero. This equation will only be used where there are a particle which demands a non-zero density.

This is the typical equation form of Bohmian mechanics and by using the definition of the probability current in equation (4), it is easily implemented in numerical methods. This equation is a first order in time, which could be compared with classical motion, where a second order time derivative is used to describe the motion. This difference will affect the result in the motion of the particle in Bohmian mechanics. The motion classically will be determined by both the position and the velocity in a given system but in Bohmian mechanics the motion of the particle is determined by only the position in a given system. From this equation it can also be derived that if particles are distributed according to the probability density from the wavefunction at any given time then they are always distributed according

to the probability density of the wavefunction. This result is derived from the continuity equation that uses that the total probability is locally conserved [8,9].

The equation (7) can be understood from another perspective, if the wavefunction is written in terms of the square root of the magnitude, R, and the phase, S, like this:

$$\psi = R * e^{iS}. \tag{8}$$

By using the wavefunction in this form the time dependent Schrödinger equation becomes two equations after separating the real and imaginary parts:

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}[R\Delta S + 2\nabla R \cdot \nabla S], \tag{9}$$

$$\frac{\partial S}{\partial t} = -\frac{1}{2m}\left[|\nabla S|^2 + 2mV + \hbar^2 \frac{\Delta R}{R}\right]. \tag{10}$$

The Schrödinger equation can be seen to have extra terms, were the last one in equation (10) is what can be referred to as a quantum potential. It is this potential that interfere with particles even if they are in free space [8,9].

The guiding equation can be rewritten when using the wavefunction, in equation (8), as:

$$\frac{d\bar{Q}}{dt} = \frac{\hbar}{m}\nabla S. \tag{11}$$

This equation shows that the velocity of a particle is proportional to change of the phase of the wavefunction [8,9].

2.4 Examples of use with the guiding equation

The guiding equation can be used in known solutions to Schrödinger equation for different potentials.

In the examples of an infinite wall or box, the result of using the guiding equation with the wavefunction for an eigenvalue of the energy gives a zero velocity of the particle everywhere. This means that the particle remains at a fixed position. Using several eigenvalue solutions to create a wave packet makes a non-zero velocity when using the guiding equation. This can also be observed in the Hydrogen atom, where the ground state eigenfunction also produces a zero velocity for the electron [8,9].

The fixed position solution of the trajectories is non-classically and is a result of the quantum potential. The quantum potential and the external potential can cancel each other to give the particle a zero velocity [8,9].

2.5 Creating a wave packet

Fixing the position of a particle to an exact position in space in quantum mechanics means that the range of the momentum of the wavefunction is infinitely large. By creating an uncertainty in the position by creating a wider range of possible detection positions will narrow the range of momentum. This can be done by creating a wave packet which travels like a wave with an almost fixed shape. The shape will be stretched when it is traveling. Inserting particles in the wave packet means that the particles must follow this wave packet. When the wave packet later interacts with its environment in

the form of a potential, the potential will affect the wave packet and thus the particles' trajectories by the guiding equation. The particles trajectories depend on their starting position at a specific time. The velocity at that time is dependent on the wavefunction and the position of the particle in the wavefunction and thus it is not possible to choose the velocity independently of those variables [8,9].

A wave packet can be described by as a gaussian wave packet like this:

$$\psi(\bar{r}, 0) = e^{-\frac{\bar{r}\cdot\bar{r}}{2a}+i\bar{k}\cdot\bar{r}}, \tag{12}$$

where $\bar{k}$ is the wavenumber and a is a value of the uncertainty of the position:

$$a = 2(\Delta x)^2, \tag{13}$$

where Δx is the uncertainty of the position. Since the wavefunction is gaussian the Heisenberg uncertainty principle is exact

$$\Delta x \Delta p = \frac{\hbar}{2}, \tag{14}$$

Where Δp is the uncertainty of the momentum [8,9].

Implementing a wave packet in a numerical simulation can be done by implementing it at a boundary. This is done by fixing the boundary to a function which is varied when time changes, referred as the boundary method. A wave packet can also be implemented by creating it over position space for a fixed starting time, referred as the fixed time method. The fixed time method is better than the boundary method because the simulation does not use any extra timesteps for the building of wave packet and the equation for the wave packet for a fixed time is easy to implement. If the construction of the wave packet is done by the boundary method, one would need to determine how much change is needed to be done to the boundary as the wave packet travels. The main negative part about the fixed time method is that it uses more grid points space to place it in the system at the starting time, but the size of the space is irrelevant if the numerical methods are made more efficient.

The phase of the complex wavefunction in each point needs to change slowly because of how the numerical method needs to differentiate the phase of the wavefunction in the guiding equation. The numerical methods will use a limited amount of grid points. Therefore, the size of the space between the grid points is significant. To get a good approximation of the velocity the phase needs to be small and that means that the wavenumber needs to be small. This in return makes the wave packet move slowly, which makes the numerical simulation to take a longer time to execute. This can be balanced by varying the size of the timestep to a bigger value to make the simulation take less amounts of timesteps in the numerical method. If the values of real and/or imaginary parts of the wavefunction change to much between grid points, then the simulation of the Schrödinger equation would be incorrect. This can be corrected by decreasing the value of the timestep, but the calculation of the particles' trajectories with the guiding equation will not be corrected this way. The result is that the particles may travel in a way that looks like they do not follow the wave packet.

When making a wave packet, the size of it needs to be defined in the position frame. If this is too small, then the uncertainty in the momentum becomes large. If the uncertainty of the momentum is large and the wavenumber is small, this would make the waves traveling all over and spreading the wave packet so its size will grow during the simulation. The size of uncertainty of the position must be

large enough to make the wave packet travel in one direction, but also large enough so the wave packet does not spread too much.

3. Method

The method in this thesis is to construct numerical methods for solving the Schrödinger equation with a general potential and a starting condition in form of a wave packet, the result is a wavefunction. By using the wavefunction, the particles' trajectories are determined with the guiding equation. In the Schrödinger equation and the guiding equation, there are constants such as the mass, m, and Planck's constant, ħ, both of which is put to 1. This is done by modifying the units of time and space making them dimensionless.

3.1 Solving the time dependent Schrödinger equation

The way of solving the time dependent Schrödinger equation is by using a cartesian coordinate grid system with grid points equally spaced and with a constant size of the timestep. By using the definition of a derivative

$$\frac{d\psi}{dt} \approx \frac{\Delta\psi}{\Delta t} = \frac{\psi(t+\Delta t)-\psi(t)}{\Delta t}, \tag{15}$$

a formula can be produced for how the wavefunction at one location changes when the time changes by an infinitely small amount

$$\psi(t+\Delta t) = \psi(t) + \frac{d\psi}{dt}\Delta t. \tag{16}$$

The partial time derivative is given by the time dependent Schrödinger equation which depends on the wavefunction and the Laplacian of the wavefunction. To solve how the wavefunction changes in a location it is needed to get the value of the wavefunction at that location and the Laplacian of the wavefunction at that location. Using the values of these it is possible to evolve the wavefunction at a small timestep at that location. Getting the value of the wavefunction can be done in an easy way by using the value for the wavefunction at that location and in the original time. This works well if the timestep is small, this is because the wavefunction do not vary much if the timestep is small. To get the Laplacian of the wavefunction is more complicated but can be done by using the definition of the derivative again for the position

$$\frac{\partial}{\partial x}\frac{\partial\psi}{\partial x} \approx \frac{\partial}{\partial x}\frac{\psi(x+\Delta x)-\psi(x)}{\Delta x} \approx \frac{\frac{\psi(x+\Delta x)-\psi(x)}{\Delta x} - \frac{\psi(x)-\psi(x-\Delta x)}{\Delta x}}{\Delta x}, \tag{17}$$

which reduces to:

$$\frac{\partial}{\partial x}\frac{\partial\psi}{\partial x} \approx \frac{\psi(x+\Delta x)-2\psi(x)+\psi(x-\Delta x)}{(\Delta x)^2}. \tag{18}$$

Then the second derivative is one part of the Laplacian of the wavefunction, where the other comes from the second derivative of the other axis. So, the Laplacian of the wavefunction uses the position of the wavefunction at the locations grid point and its neighbours. The neighbours are in the next position grid point in the grid system. The full Laplacian of the wavefunction in a 2-dimensional simulation

uses two perpendicular directions for the second derivative of the wavefunction. Thus, the value of the wavefunction at a grid point and its closes neighbours is used to calculate the wavefunctions value in the next timestep. The wavefunction is complex and could be numerically simulated in different ways. In this thesis it is done by separating the real and imaginary part of the wavefunction and using the time dependent Schrödinger equation for each part.

Coding this part is done by using matrix multiplication, since the experimental setup can be defined with a grid system and the experiment components can be defined with a potential. Thus, it is possible to solve the partial derivative equation by multiplying a matrix of the wavefunction with a matrix of the potential term by term to get the potential part of the Schrödinger equation. The Laplacian of the wavefunction is constructed by matrix multiplication with a helper matrix. The time derivative of the wavefunction is determined by the potential part of the Schrödinger equation and the Laplacian of the wavefunction for all grid points, by equation (1). Using the time derivative of the wavefunction and equation (16) to evolve the wavefunction at all grid points simultaneous.

Analytically, if the wavefunction has been normalised it should stay normalised. In a numerical simulation there could be a small deviation from this normalisation so the total sum of the squared magnitude of the wavefunction could go to infinity. This would make the numerical simulation stop due to error, but this deviation is assumed to be small, so this problem does not need to be considered. It is still needed to be considered that the wavefunction could deviate from the normalisation, if it is used for other purposes, like calculating mean position of wavefunction.

3.2 Solving the guiding equation

While solving the Schrödinger equation at the starting time, the wavefunction is defined in a certain way to create a wave packet. Then this wavefunction is used in the Schrödinger equation, this creates a wavefunction that has time and positions in the grid system as variables. With this wavefunction, it is possible to implement the guiding equation to solve the particle's trajectories. This can also be done by updating the wavefunction and the position of the particles at the same time. By updating the position parallel while simulating, the wavefunction do not need to be stored. If it was stored, the size of this data could become large if the grid system and the amount of timesteps is large. This is done by defining a particle's starting position at the starting time and using the definition of the guiding equation. In equation (7) the definition of the guiding equation is in terms of the probability current where it can be rewritten to the real and imaginary components of the wavefunction by equation (4).

Since the guiding equation needs to differentiate both the real and imaginary part of the wavefunction, it is possible to use the definition of the derivative again. The guiding equation also divides the probability current by the square of the magnitude of the wavefunction at the location. To avoid dividing by zero the numerical methods needs to be modified. It would be possible to divide by zero if a grid point's value of the wavefunction was used, like if that grid point is a mirror. Since the exact value of the wavefunction at a particle's position is not known when using numerical methods. The way of determining the value of the wavefunction is by using the mean value of the wavefunction of two grid points. Since this dividing in this method is used only at locations for the position of a particle and the particle should not be able to enter an area where the wavefunction is zero, this would avoid the problem.

This Schrödinger equation in equation (1) is used for a single particle with a spin of zero and a non-zero mass and thus when several particles is simulated this equation is not correct. For several particle systems the particle can affect each other which means that the Schrödinger equation must be modified to account for this.

This simulation will focus on a single particle system, but this does not mean that it is impossible to simulate several particles' trajectories at once. The particle in the simulation are there in an asymmetric way, in which the wavefunction affects the particle but the particle does not affect the wavefunction. Calculating a particle's trajectory is just to make a calculation using the wavefunction to get the velocity of a position in space and time and updating the position of the particle by adding the multiplication of velocity by a small value of the timestep to the original position. This is done

without changing the wavefunction and can be done to any position at a given time and thus can determine several particle starting positions in the same simulation.

A key point is to choose good starting positions of the particle, which is then used in this calculation. They should represent the probable trajectories a particle should follow, so picking starting positions should correspond to the probable positions the particle is in at the starting time. This information can be obtained from the wavefunction at the starting time. The square of the magnitude of the wavefunction is the probability density which corresponds to the probability of locating the particle in that position and an infinitesimal area around this point.

Thus, if the magnitude square of the wavefunction at the starting time is used to produce the starting positions of the particles to follow, they should give a good representation of trajectories. This can be done in several ways. Three methods are:

1. The first method is just to pick points randomly that is weighted by the probability from the wavefunction. Since it is unknow in any given wavefunction where the particle is this could be a good way of doing it. The negative side is that the positions is not easily replicated and may result in giving positions that do not result in giving trajectories that is informatic.
2. The second method is by picking points in a region of the wavefunction at a certain probability value. Like at a boundary around the most probable positions with an even step. This could be used if the simulation uses a wavefunction in the form of a wave packet, but it cannot be certain that nothing irregular happens to a starting position within this boundary.
3. The third method is to work in the region of most probable positions and pick out points with an even step. This can be done like in method 2 but the value of the probability used to define the boundary needs to be varied, this makes some of the starting position located in the interior of the boundary.

Using these starting positions with the guiding equation is done by using equation (4) and (7). When taking the derivative of an equation numerical, this uses:

$$\frac{dA}{dx} \approx \frac{A(x+\Delta x) - A(x)}{\Delta x}. \tag{19}$$

This works approximatively, when using the equation (19) for calculating the trajectories of the particles, this would use the grid points closes to particles' location. For one direction it would use two grid points, and these would be chosen by rounding off the position of the particle to the closes grid points. This would result in that all particles in a region would get the same velocity, which is not correct.

Modifying how the guiding equation is implemented is possible. Instead of using the value of a grid point by rounding off the particle's location, one can use the more exact position of the particle. It is possible to do a linear approximation of two grid points making the velocity more continues instead of jumping when changing grid point. This can be done in one dimension by using three grid points in a row or in a column in the grid system. Consider a 1-dimensional system, in this dimension it is possible to use the placement of the particle as a weight in the derivative

$$\frac{dA}{dx} \approx \beta \frac{A(x+\Delta x) - A(x)}{\Delta x} + (1-\beta) \frac{A(x) - A(x-\Delta x)}{\Delta x}. \tag{20}$$

So, this would use three grid points and the β would be determined by the position of the particle. If the particle is exactly between x and $x + \Delta x$ then β is 1, if the particle is exactly between x and $x -$

Δx then β is 0 and if the particle is exactly at x then β is 0.5. By using a linear fit the result should be smoother and more correct.

One could also use the other axis for improving the result of the velocity of the particle. This is done by using four grid points. This is possible for two or higher dimensional grid system and it uses the original way for the derivative with two grid points. It uses two of such derivatives, but they are placed in the perpendicular direction

$$\frac{dA}{dx} \approx \gamma \frac{A(x+\Delta x, y) - A(x,y)}{\Delta x} + (1-\gamma)\frac{A(x+\Delta x, y+\Delta y) - A(x, y+\Delta y)}{\Delta x}. \quad (21)$$

This is done for both axes, so it uses two squares of four grid points, but the grid points do not need to be the same in both squares but at least one grid point must overlap.

Now the γ is 1 if the particle is exactly at y, γ is 0 if the particle is exactly at $y + \Delta y$ and γ is 0.5 if the particle is exactly in between y and $y + \Delta y$. This linear fit uses positions in two dimensions for better trajectories.

Combining these two methods results in a 2-dimensional linear fit using six grid points. This is done by implementing equation (20) into equation (21). In that way the calculation uses either two rows with three grid points in each column or vice versa

$$\frac{dA}{dx} \approx \gamma C(x,y) + (1-\gamma)C(x, y+\Delta y), \quad (22)$$

where

$$C(x,y) = \beta B(x,y) + (1-\beta)B(x-\Delta x, y), \quad (23)$$

and

$$B(x,y) = \frac{A(x+\Delta x, y) - A(x,y)}{\Delta x}. \quad (24)$$

This will be a significant part in making the simulation perform better. If the wavefunction varies in each grid point, then there will be a jump when a particle change grid points in the basic method. Thus, by making a linear fit, the trajectories become smoother and looks more realistic.

There are other ways to make the trajectories smoother, like decreasing the length between each grid point. That will demand more grid points and make the simulation take longer. By making the guiding equation a linear fit in two dimensions will result in that the velocities of the neighbours of a point is in general different.

3.3 Boundary conditions

Since the Schrödinger equation are not in general bounded by a box but could be in free space, the boundary is to be treated separately. There should not be such restrictions that the wavefunction has to reflect at the boundaries in the simulation. If the box of grid points is small, then the wavefunction will interact with the boundaries of the grid system and this needs to be properly handled.

The numerical method works by having the wavefunction at a grid point change depending on the values of the wavefunction at the grid point itself and the grid point's neighbours' values of the wavefunction. This creates a problem at a boundary because a boundary grid point does not have some of its neighbours included in the simulation.

The way to solve this problem is to define the boundary as a mirror to avoid using its neighbours, this would cause any wavefunction to be reflected and go back towards any experimental setup that have been constructed. This is not what is desired, and this is corrected by using an imaginary potential of some width next to the boundary. Solving the Schrödinger equation in the imaginary potential will result in giving the wavefunction an extra term that makes the magnitude of the wavefunction to an exponential function. By picking a negative imaginary number will make the magnitude decreases for any wavefunction in the imaginary potential. By making the absolute value of the imaginary potential small will decrease any reflection of the imaginary potential. Then the width of the imaginary potential is decided so that the main part of the wavefunction do not reach the boundary.

3.4 Modelling the particles trajectories at the boundary

When simulating the particles' trajectories by using the guiding equation, the particles can reach a point where the simulation of the wavefunction is not updated because of the size of the grid. There is also a need to be aware of the imaginary boundary potential where a potential has been created just to interfere and lower the magnitude of the wavefunction. One way of doing it is to stop updating all the particles positions if one reaches a grid point where it is impossible for the simulation to calculate the velocity of a particle or to stop updating the position for only that particle. This could be at a point where the calculation itself would not be able to find the values it needs to implement the guiding equation. At this stage the particle has entered the complex boundary condition which could have interfered with the particle's trajectory. Thus, it would be better to terminate the updating of the particles position before they enter the imaginary potential region.

If the imaginary boundary potential does not affect the simulation of the wavefunction in the region of where the real potential acts, then this could be done be just terminate the particle when it would enter the last of the real potential grid points. In this point it actually has used the wavefunction in the complex potential region to calculate its trajectory, so it needs to be cancel at least 1.5 grid points before the imaginary potential because of the way the guiding equation was modelled in the 2-dimensional simulation.

3.5 Modelling a detector for measuring the wavefunction

In the article written by Vaidman, he measures the power of the laser. This is done in a detector which detects photons by converting the energy of the photons to an electric signal which current is proportional to the energy of the photons. The signal produced in the detector is proportional to the energy of a photon (which is nearly constant for each photon) and the number of photons that interact with the detector.

The exact proportionality is not important just the ratio for different times. The important terms in the detection is how many photons the detector measures. The number of photons the detector measures is proportional to total amount of photons that has entered it. This can be calculated with the probability current. The probability current is similar to the flux of particles and is therefore proportional to the number of photons entering the detector. By using the probability current of the wavefunction at the opening of the detector it is possible to numerically simulate the detectors power function.

By numerically calculating the sum of the probability current at a line will result in creating a virtual detector. It only uses the values of the wavefunction and does not affect the way the wavefunction behaves in the simulation. By recording the sums of the probability current for all timesteps will produce a power function measured by the virtual detector.

If a wave packet enters completely though a virtual detector then the area under the power function should be equal to 1, if the wavefunction has been normalised. If the area of a detectors power function is summed numerically, it would get a result of 1 divide by the sized of the timestep, because the summation is performed for each timestep.

3.6 Making a more efficient simulator

When simulating the wavefunction numerically it uses matrix multiplication to get the time derivative for the wavefunction at each grid point for each timestep. This is not completely necessary because the region of interest is where the wavefunction has significant values. In the simulation, this region is where the wave packets are.

By making the simulation to only simulate the wavefunction with the Schrödinger equation near the wave packets it becomes more efficient and will save a lot of time if the wave packets are much smaller than the whole system.

This is done by solving the matrix multiplication for a smaller matrix called box instead of the matrix corresponding for the whole grid system. The wave packet moves, and change location and the box has to move with it.

This can be done in several ways:

1. By following particles.
2. By testing the probability of detecting a particle at neighbour positions.
3. Calculating the mean position of the wavefunction.

The first method is to follow a particle or several particles in a wave packet and to use their mean position for the placement of the centre of the box. A problem with this method is to determine which particles to track to find the centred position of the wave packet. It is difficult to know which starting position of the particles is the best and how this might change during time. This method could be used when there is two wave packets and they are traveling separately and at a distance from each other, it is possible to have two small boxes that follows each of the wave packets. The main problem with this is when the wave packets interact, the particles used for tracking the two boxes can start following the other wave packet and thus it is needed to know how the particles are going to behave. This method of two boxes could even work when a wave packet goes through a beam splitter and produces two wave packets if it is known which particles is going to follow which wave packet.

The second method is that the tracking of the wavefunction is done by centring the box at a position where an even smaller region inside the box gets the highest probability that the particle will be detected in it. This is done by placing the box centred at the wave packets central position at the starting time. Then the solving of the Schrödinger equation is performed for the wavefunction inside the box and the solution for the particles' velocity is determined by the guiding equation. After every timestep or after some number of timesteps the box changes position by calculating the total probability of the wavefunction for a particle to by inside the region inside the box. This is done by summation of the square of the wavefunction for all grid points inside this region. Then this region change position by moving it one position up and the same calculation is performed for this position. This same procedure for the region is done for the down, left and right movement as well. This gives five different values of the probability and the one that gives the highest probability is the new centred position of the box.

The main problem with this method of tracking the wavefunction is that when the wave packet travels it leaves very tiny traces of the wave packet behind. These traces of the wave packet could intervein in the next calculations of the centre position. This is because it creates a small probability behind it but since the wave cannot travel in front of the box this will not happen in front of the wave packet in the same way, creating an asymmetry that affects this method. This will happen even if the box uses a boundary with an imaginary potential but will be smaller because of it.

The third method is to do this tracking by calculating the position of the centre of the box by the mean position of the wavefunction for all grid points. The square of the wavefunction is the probability density, it can be multiplied by the position vector and integrated for all positions. This would result in the mean position if the wavefunction is normalised. Numerically this is done by summation of the product of probability density and position of each axis and dividing by the total sum of the probability density for all grid points. This can be done for each timestep or after some amount of timesteps.

The mean position is easily implemented but it is not certain that it will result in the best position of the centre of the box. The mean position method is somewhat ineffective when the grid system is large, but it can be made to be more effective by only calculating the mean position using the wavefunction that is inside of the box. This would make it a lot faster when the box is small compared to the whole grid system.

The simulation can be modified with this box method in two ways to make it even more efficient, these are:

1. Have one small box that becomes two small boxes if the wave packet separates to two wave packets, like if a wave packet passes through a beam splitter which creates two wave packets.
2. Adjust the size of the box during the simulation

The first way of optimising is to use a box that solves the Schrödinger equation in just that box. If it is known that the wavefunction will be divided into two wave packets that travel away from each other the box could be separated and create two even smaller boxes, that follows each wave packet and solve the Schrödinger equation for each box. The tracking is done for two boxes in the ways as before with some modification when needed. When using two smaller boxes there might be an overlap of the boxes. This overlap is needed to be considered so that the Schrödinger equation is used in a correct way. For this to work a method for determine when to split the larger box into two smaller boxes needs to be used. This can be done in the box tracking with help of the particles' positions. If it is known that two particles separate and follow each wave packet, their distance can be used to determine when to use a large box or two small ones.

If particle 1 follow wave packet 1 and particle 2 follow wave packet 2, the position of the two small boxes centred around each of the particle's positions. If the particles are near each other one box can be used for both wave packets but in a larger size, the position of this box is centred at the mean position of the two particles. Doing it in this way an arbitrary large grid system can be used where the two wave packets will require each a small box compared to the one box method, which size will have to be very large when the wave packets separate. Since the time it takes to perform the matrix multiplication in the simulation depends on the size of the matrix this makes it more efficient.

The second way of optimising is to vary the size of the box in the one box method. The size of the box is increased or decreased when needed to make the calculation of the Schrödinger equation for the wave packet more efficient, thus the simulation will ignore regions which is not significant. The wavefunction will determine when to change the size of the box. The square of the magnitude of the wavefunction is used to get the probability that a particle is in a region in the box. This region will be a smaller size then the box. If the probability is less than desired, then the size of the box used for the simulation is increased and if it is larger than desired the size of the box used for simulation is decreased. The values can be set to a fixed amount of the probability or to a ratio of the total probability in the box used for the simulation. The ratios for the increase and decrease can be set to different constants. There will also be a constant for the size of the region which is a ratio of the size of the box used for simulation.

This check for the size change is done after a certain amount of timesteps and not for every timestep used in calculating the wavefunction because it is somewhat time consuming. When the size of the box change, some new matrices needs to be defined, like the matrix used in the simulation to calculate the Laplacian of the wavefunction. A new matrix with the imaginary boundary potential which is used in the box used for the simulation is also needed to be defined. The wave packet used in the simulation travel slowly and no big deviations will happen if this check of the box size happens after some number of timesteps instead of every timestep.

Decreasing the size of the box used for the simulation must be done slowly so that no important wavefunction behaviour is discarded but increasing of the size of the box can be done faster. If change is done in too small steps, the box will change often and must perform the procedure for the change in size more often, which is time consuming. If it is done in too big steps, the box could become larger than necessary, which makes the simulation of the Schrödinger equation less effective. Using this

method of changing the size of the box uses some extra time but if it is done correctly it can make the simulation more time efficient. The size of the wave packet will thus determine the size of the box. This method could be combined with the first method where it can create two boxes if the two wave packets separate and these boxes would have a size that can be modified during the simulation.

The setups in the next subchapters will use only this second method with one box that varies its size. They start with one wave packet were the size of the box is chosen to include the major parts of the wavefunction but limited to minimise the processing time. The position of the centre of the box will be determine by the mean position of the wavefunction evaluated by the wavefunction in the box.

3.7 Modelling a setup

To be able to simulate Vaidman's proposed experiment, setups with beam splitters and oscillating mirrors needs to be created. These will be simulated to verify that they give expected results.

Modelling a setup is done by having a Cartesian grid in a rectangular shape and putting objects in it which the wavefunction interacts with. This is done by defining a potential in the region of the objects. When there are no objects the potential is put to zero and for an object, like a piece of potential barrier, the potential is put to a non-zero real value. For a mirror, an infinitive value should be used so the wavefunction that travels towards it would result in getting a zero magnitude in it, this would result in a perfect mirror.

This cannot be done in a computer for several reasons. Computers cannot handle infinities and even if it could, this would result in that the wavefunction could grow to infinity in the mirror instead of being zero because of how the numerical methods in the simulation works. The solution to this problem in creating a mirror is instead done by declaring that the wavefunction must have a zero magnitude inside of the mirror, this is done after each timestep. This redefines both the real and imaginary part of the wavefunction to zero in the region of the mirror. Creating a mirror could also be done in another way and this is by creating a very thick potential barrier with a high but limited potential. If the mirror is created in this way would demand that the constants of the potential and the thickness of the potential are needed to be defined. Another problem is that in some setups the mirror could be constructed to be thin, in the second method the mirror needs to be thick to work properly. By creating the mirror by the first method of declaring the wavefunction to be zero in a region, can make the mirror very thin and it can also be used to construct a thin mirror with holes in it, like what is needed in a double split experiment.

Creating a beam splitter as a piece of potential barrier or creating a mirror can thus be done by modifying the potential or the wavefunction in some grid points. A completely horizontal or vertical mirror or beam splitter is created by using just parts of one row or one column. It is more complicated to create a mirror or beam splitter at an angle. Since in the simulation cartesian grid points are being used it is not possible to create straight lines if they are at an angle. The solution to this problem is to use a linear equation, that represent the surface of the mirror or beam splitter and round them off to closes whole numbers. This creates jumps in the grid points, so it looks like a staircase where the potential or wavefunction is defined differently than in the rest of the grid points. This could cause some imperfection in the simulation, but it is assumed that the deviation of the simulation is small when the grid points are small compared to size of the wave packet.

By these methods it is possible to construct mirrors and beam splitters and use them in a setup. A constant for the value of the potential in the beam splitter is needed, it can be set to a fixed value. The potential should have the same value in the whole beam splitter, and it should be a real value. It could be either negative or positive where the sign of it could have some interesting properties.

If it is a negative potential, this can be understood from the classical counterpart where particles entering it will result in decreasing their potential energy. If the particle's total energy is fixed it would result in that its kinetic energy would increase and thus the speed of the particle would increase. The counterpart in quantum mechanics will result in that the wavefunction travels faster in a negative potential.

If the potential is positive the opposite is true for both the classical and quantum mechanical theories. The unknown is how the particle, whom is traveling with the wavefunction in Bohmian mechanics, will behave. Since the particle will travel with any wave packet and the wave packet follows the rules of quantum mechanics this will also be true for the particle that are following the wave packet by the guiding equation.

There are some differences though. In the positive case some frequencies would result in getting a negative kinetic energy term in the potential region. A wave packet which is constructed of several frequencies would when traveling in a positive potential get the result that the contribution of these frequencies would decrease, and this may affect the wave packet. Having a negative potential could have the effect of creating a standing wave in the potential barrier, which could result in modifying the wave packet in another way. Near the intersection of a beam splitter and the free space surrounding it, there would be a quantum potential interfering with the particles. By constructing different kinds of potentials with different values of both signs is of interest to determine how this will affect the result of the particles' trajectories.

3.7.1 Creating a piece of thin potential barrier

To model a beam splitter is done with a thin piece of potential barrier. Making it thin have several advantages. Like that it has symmetry in the sense that it is possible to create a second wave packet input that produces outputs in similar directions as the first wave packet and can thus be used to construct interference between these two wave packets. A second advantage is that the time lag between a reflected and transmitted wavefunction will be smaller. When the wavefunction travels in a potential its kinetic energy is changed and thus its speed is different than the reflected wave, this could create problems if they should interfere later. In a symmetric setup with other components than the potential this would result in one wave reaching a point faster than the other, this could be fixed in several ways but still is a problem to be accounted for. A third advantage is that if the potential barrier is thick enough it would be able to create two reflections when a wave packet travels through it, one at the first surface and one at the second surface, where the potential barrier ends. If the potential is thin enough all these problems are approximately small and not an issue.

The piece of potential barrier is constructed by using one grid point as the thickness. To create a horizontal or vertical piece of the thin potential barrier is done by changing the potential in only one row or only one column. To create a piece of thin potential barrier at an angle is done with the method of defining a line and by rounding off the values of the line to integers to define the grid points where to change the potential.

Doing a simulation of a thin potential barrier can result in the separation of the wave packet into two wave packets and thus it is possible to get the angles of their path to see the reflected and transmitted properties. To get the angles of the reflected and transmitted wave packets is done by calculating the mean position of each wave packet. This can be done in different ways, but one way is to get a helper matrix which is defined to be 1 at the grid points of one side of the line were the potential is non-zero and zero for the grid points on the other side. By multiplying this matrix to the probability matrix term by term removes the other part of the wave packet, the corresponding calculation is done to get the other wave packet. Calculating the mean position is done with the resulting products.

The fixed angle and the potential are varied to see how this affects the results of the wave packets path. Measurements of the intensity of the two wave packets is done by using two virtual detectors in front of the outputs to see how the intensities vary when the potential value is varied. By using this method of measuring the intensities can determine the potential that gives an equal intensity of the resulting wave packets, which could be used in further experiments.

In the original setup proposed by Vaidman there is no use for a time-dependent beam splitter, but it is possible to create one where the angle varies in time. This is done by using the previous method of creating a piece of thin potential barrier but do it before each timestep and then deleting it after each timestep. When each run starts a new line is calculated using a new angle that depends on the time, as for example having a constant angle and add a small valued time-dependent function to that angle.

3.7.2 Creating a mirror

Creating a vertical mirror is done by zeroing the wavefunction at a column and creating a horizontal mirror is done by zeroing the wavefunction at a row. Creating a mirror at an angle uses a similar method as for a thin potential barrier but instead of defining the potential at the line a mirror is created by defining the wavefunction to be zero at the grid points on that line. This works because of how the numerical methods change the value of the wavefunction. The change of the wavefunction at a grid point depends on its and its neighbours' value of the wavefunction. By deleting the wavefunction in a complete boundary of a region for each timestep would result in that the wavefunction of all the grid points in the interior is unaffected by the wavefunction outside the boundary, resulting in that the boundary works as a mirror. Since nothing can travel through the mirror there is no need to modify any grid points behind the mirror and therefore it can be made thin.

Using a stationary mirror is done by using a fixed value of the angle. When a wavefunction reflects at the mirror, the reflected angle should be equal to the incident angle of the wave packet. This is tested to see that it works properly.

It is possible to create a mirror that has a time-dependent angle. The mirror is created as a stationary mirror by calculating a line and defining the wavefunction to be zero in the mirrors grid points, the equation for the line is changed for each timestep according to the angle of the mirror's time dependence. The main difference in doing a time dependent mirror by modifying the wavefunction than doing any time dependence in the potential is that there is no need to reset any changes after each timestep. Since the value of how fast and how big the angle changes will affect the result, the amplitude and the frequency of the oscillation are needed to be found. There will be tests of how much the angle changes by varying the amplitude and how fast the mirror vibrates by varying the frequency. This result will be used in the experimental setup in the next subchapter as a part of Vaidmans proposed experiment.

3.8 Testing parts of the experiment proposed by Vaidman

The main part of this thesis is to use the tools that has been created to determine how the particles' trajectories behave in the experiment proposed by Vaidman. Since Vaidman's proposed experiment is large and therefore time consuming to simulate, only a small part of it will be considered. The region in the red box in Figure 4 is where the focus of the setup is located. This region, with some modifications, will be simulated.

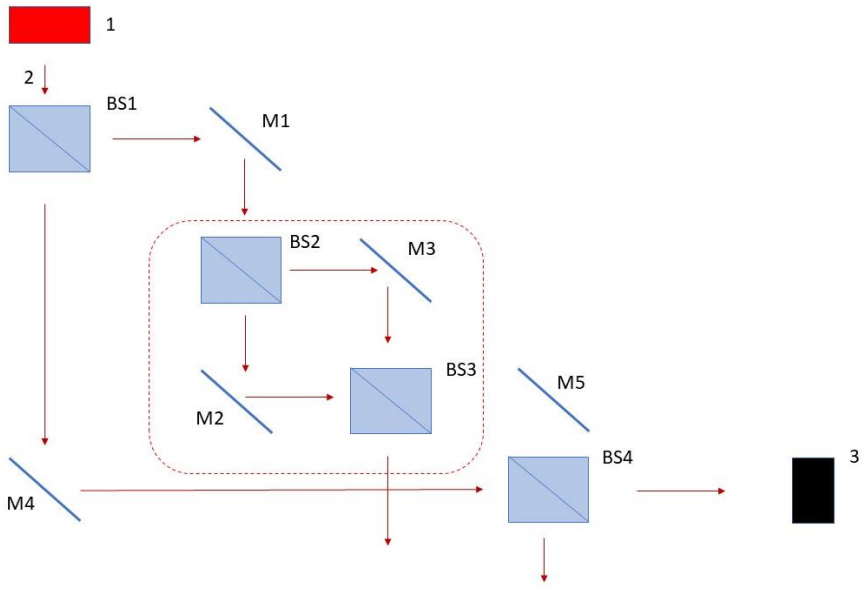

Figure 4. Depiction of Vaidman's proposed experiment with region of special interest mark in the red box.

The setup is to use one source of the wavefunction which is formed as a wave packet and send it through a beam splitter which should result in producing a transmitted and a reflected wave, with an equal intensity, to two perpendicular directions. The output waves travel towards two time-dependent mirrors to change the directions of the wave packets so they will approach each other again at a perpendicular direction. Then there are two versions of the setup, one where they interfere in free space and another variant is to use another beam splitter at the point of the interference of the wave packets. The result of this will create a wave packet that separates into two wave packets and then recombine to one or two wave packets. The particles will follow one of these wave packets after the first beam splitter and then interact with the second wave packet again. The guiding equation is used to solve the particles' trajectories and these trajectories is the result of the simulation.

4. Results

4.1 Test the virtual detector with a power plot

Testing the virtual detector is done by creating a wave packet that travels through the virtual detector and measuring the intensity. The particles' trajectories are displayed in Figure 5. The virtual detector measures the intensity when the wave packet travels through a line, the result of the measurement creates a power function, which is displayed in Figure 6.

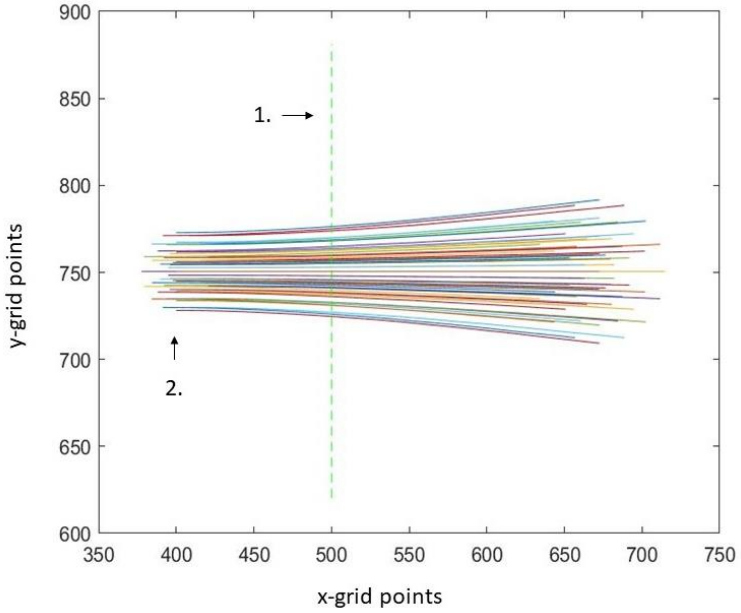

Figure 5. Particles' trajectories through a virtual detector. 1) Virtual detector. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

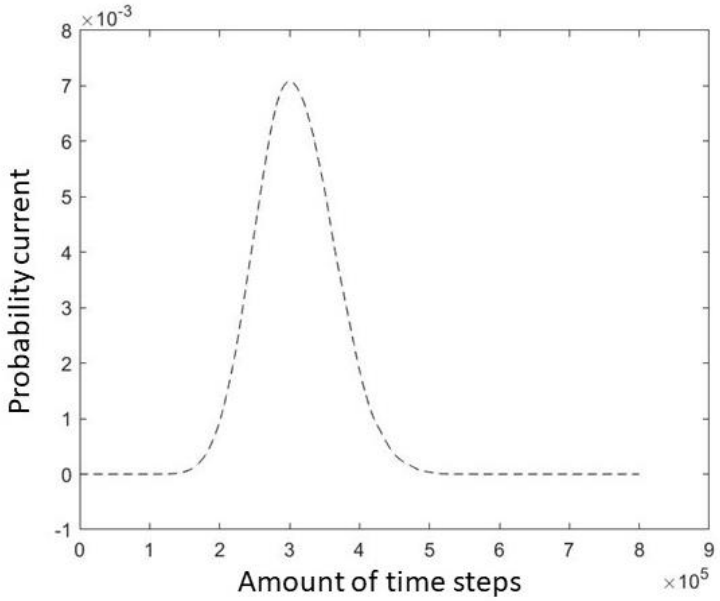

Figure 6. The intensity of wave function measured by the virtual detector with the probability current for all timesteps. The timestep size is 0.001.

Using one wave packet that travels through a virtual detector produces a power function, see Figure 6. The combine sum is equal to 993.23 as the wavefunction is normalised at the beginning and the timestep is 0.001, the expected sum is 1000.

4.2 Testing a thin potential barrier

4.2.1 Reflection and transmitted angles of a thin potential barrier

The test of the transmitted and reflected angles is done in the setup of Figure 7.

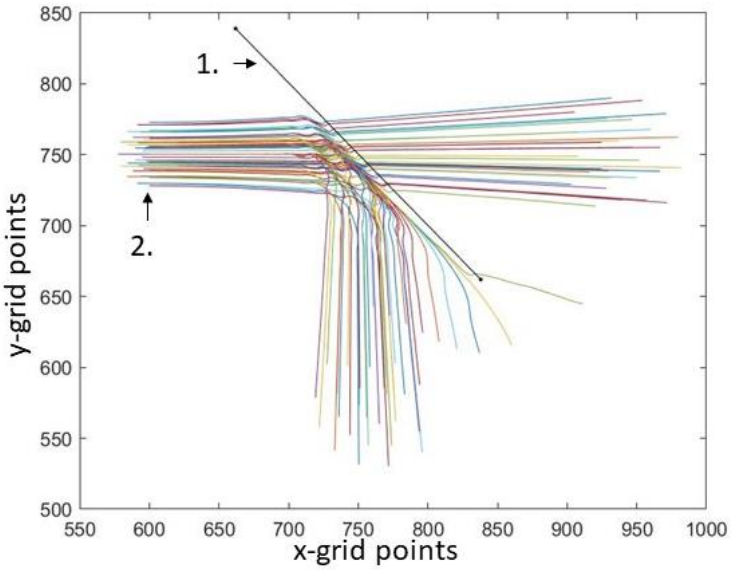

Figure 7. Example of the layout of testing the transmitted and reflected angles. 1) Thin piece of potential barrier with a varying potential and angle. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

This is done for several incident angles of the wave packet and for several values of the potential. The result is tabulated in Table 1.

Table 1. The result of the testing of the transmitted and reflected angles. This is done by varying the incident angle and the potential value.

Incident angle [degrees]	Potential value	Transmitted angle [degrees]	Reflected angle [degrees]
30	0.2	29.86	31.09
30	-0.2	29.41	30.76
30	0.3	29.64	30.79
30	-0.3	29.30	30.12
45	0.2	44.63	46.70
45	-0.2	43.76	45.75
45	0.3	44.29	46.18
45	-0.3	43.46	45.33
60	0.2	59.00	62.73
60	-0.2	57.48	61.02
60	0.3	58.54	61.96
60	-0.3	57.21	60.57

4.2.2 Power plot intensity

The test of the intensity of the transmitted and reflected wavefunction is done with a thin potential barrier with a fixed angle of 45 degrees and with two virtual detectors. This is simulated for several potentials. One example of the particles' trajectories is displayed in Figure 8 and the power plot of detectors are in the Figure 9-13. The result of these is tabulated in Table 2.

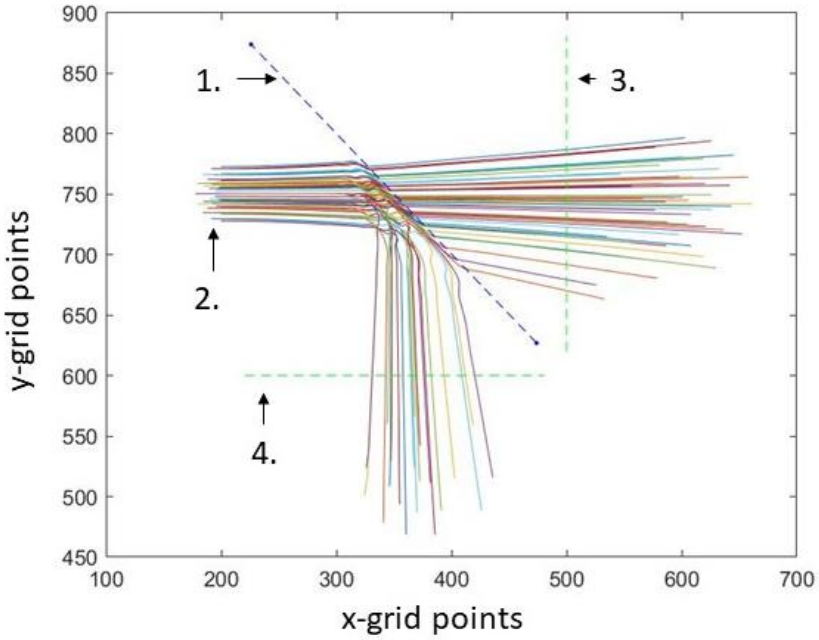

Figure 8. An example of the layout of testing intensity of the transmitted and reflected wave function. 1) Thin piece of potential barrier with a varying potential. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 3) Detector 2. 4) Detector 1.

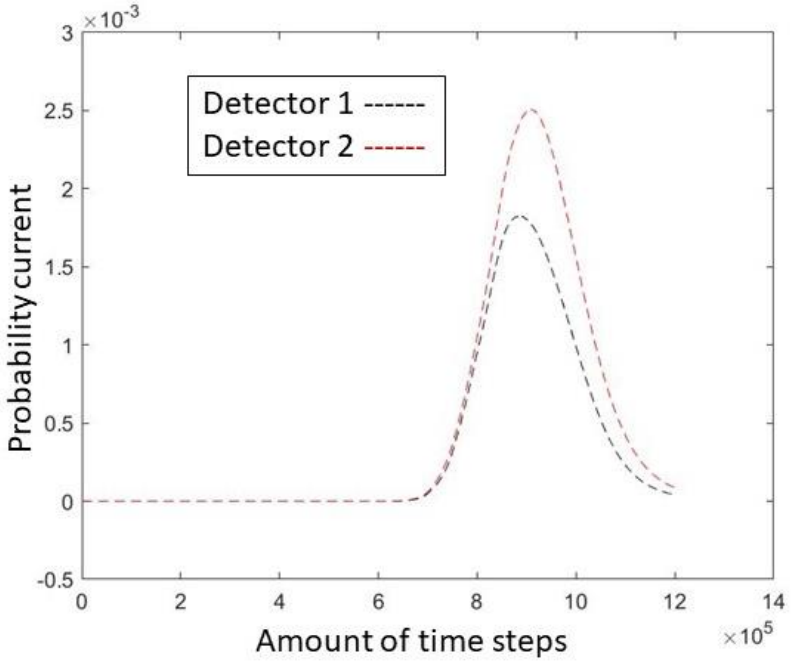

Figure 9. The intensity of wave function measured by the virtual detectors with the probability current for all timesteps. The timestep size is 0.001 and the potential 0.2.

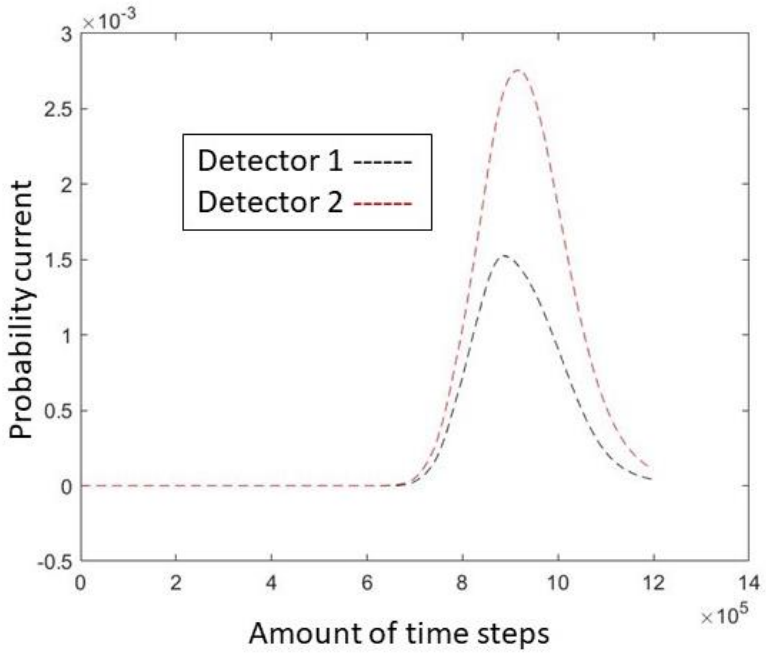

Figure 10. The intensity of wave function measured by the virtual detectors with the probability current for all timesteps. The timestep size is 0.001 and the potential -0.2.

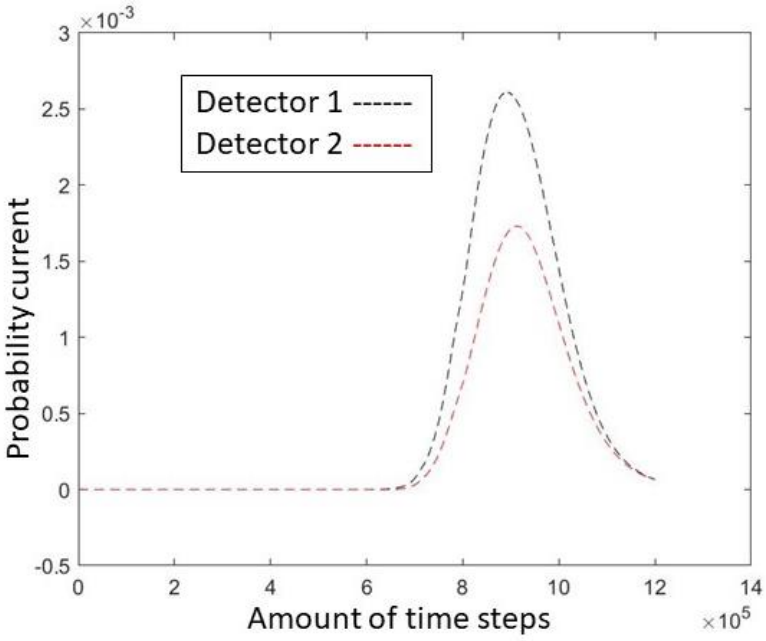

Figure 11. The intensity of wave function measured by the virtual detectors with the probability current for all timesteps. The timestep size is 0.001 and the potential 0.3.

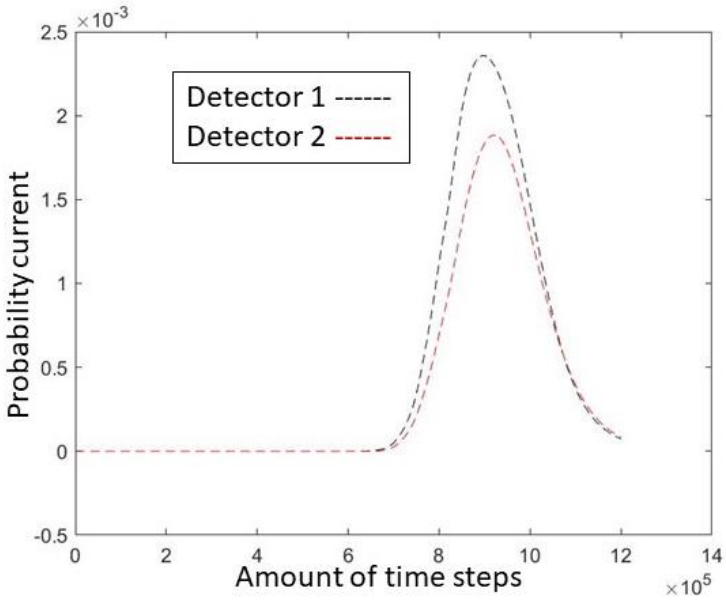

Figure 12. The intensity of wave function measured by the virtual detectors with the probability current for all timesteps. The timestep size is 0.001 and the potential -0.3.

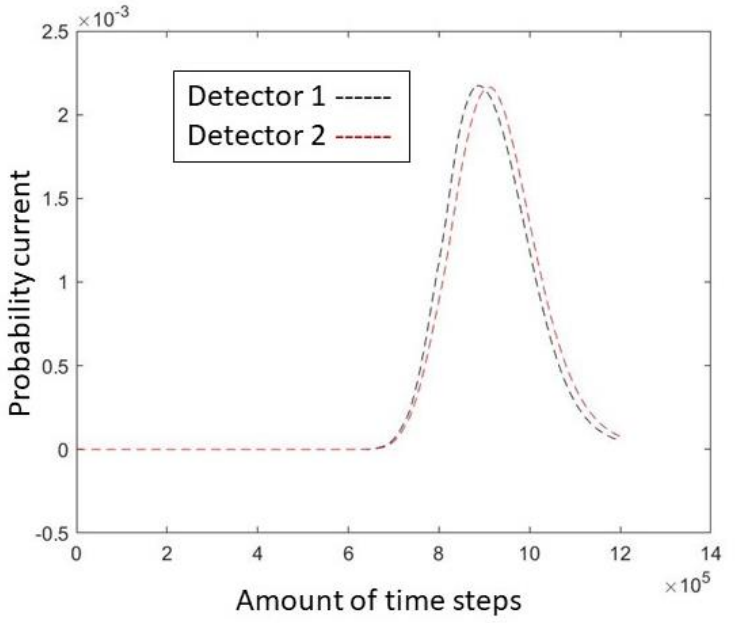

Figure 13. The intensity of wave function measured by the virtual detectors with the probability current for all timesteps. The timestep size is 0.001 and the potential -0.25.

Table 2. The result of the ratios in percentage for the sums of the intensity when the potential varies.

Potential value	Percentage ratio measured by detector 2	Percentage ratio measured by detector 1
0.2	55.75	44.25
-0.2	60.16	39.84
0.3	35.36	64.64
-0.3	41.86	58.14
-0.25	49.94	50.06

4.3 Testing the mirror

4.3.1 Test of the mirror with different fixed angles

The test of the reflection of a wave packet against a fixed mirror is done by varying the incident angle. The results of the particles' trajectories are displayed in the Figure 14-16. The result of the reflected angles is tabulated in Table 3.

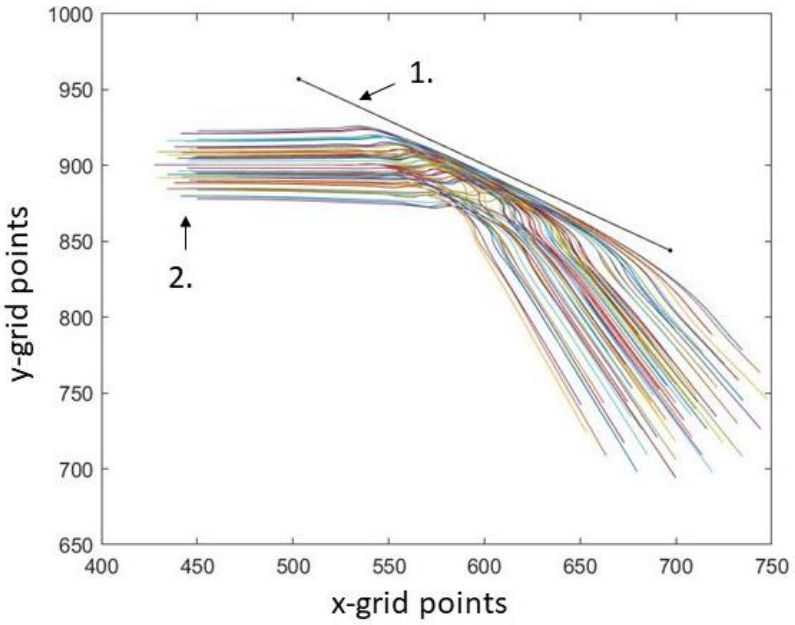

Figure 14. The result of reflecting a wave packet against a mirror with an incident angle of 60 degrees. 1) A Mirror. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

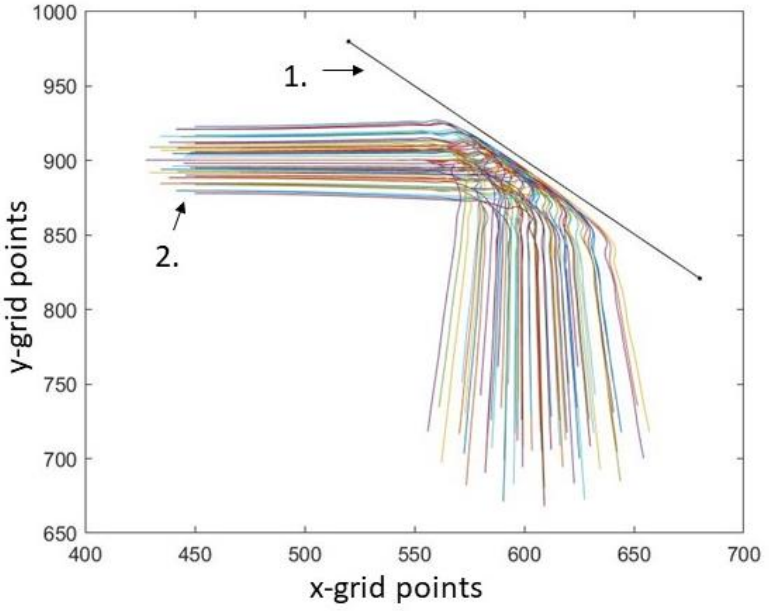

Figure 15. The result of reflecting a wave packet against a mirror with an incident angle of 45 degrees. 1) A Mirror. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot

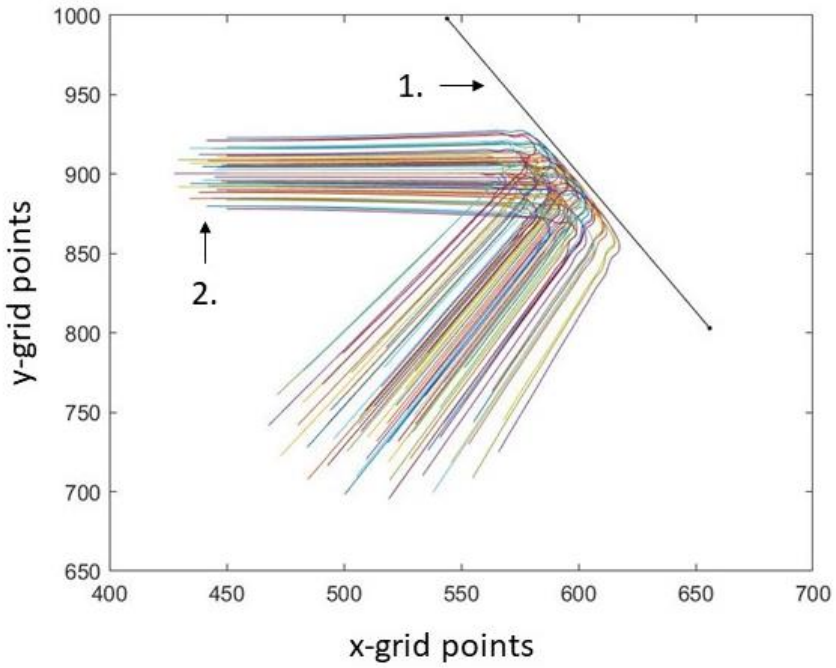

Figure 16. The result of reflecting a wave packet against a mirror with an incident angle of 30 degrees. 1) A Mirror. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot

It is observed that the wave packet reflects and spreads. The spreading would occur even if there was no mirror, this is due to the uncertainty of the momentum.

Table 3. The result of the reflected angles of reflection with a mirror for different incident angles.

Incident angle [degrees]	Reflected angle [degrees]
30	29.91
45	44.97
60	60.44

4.3.2 Testing a time-dependent mirror

The test of the mirror with a time dependent angle is done by having a mirror centred at a 45-degree incident angle of the wave packet approaching it. This angle is modified by an added sinusoidal function with a constant amplitude and frequency. The amplitude and frequency are varied, and the result of the particles' trajectories is displayed in Figure 17-20.

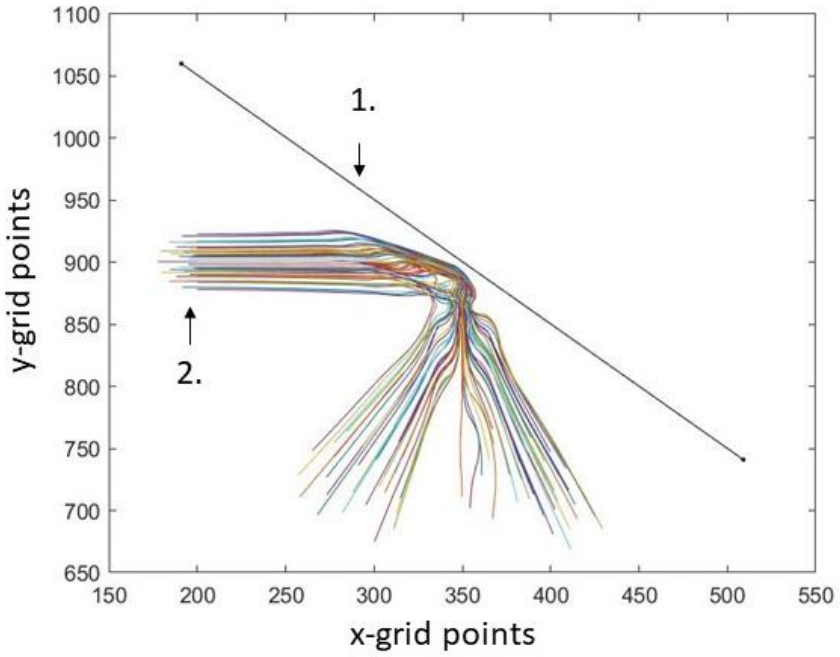

Figure 17. The result of reflecting a wave packet against a mirror with a time dependent angle. 1) A time dependent mirror with frequency of 100 and amplitude of 18 degrees. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

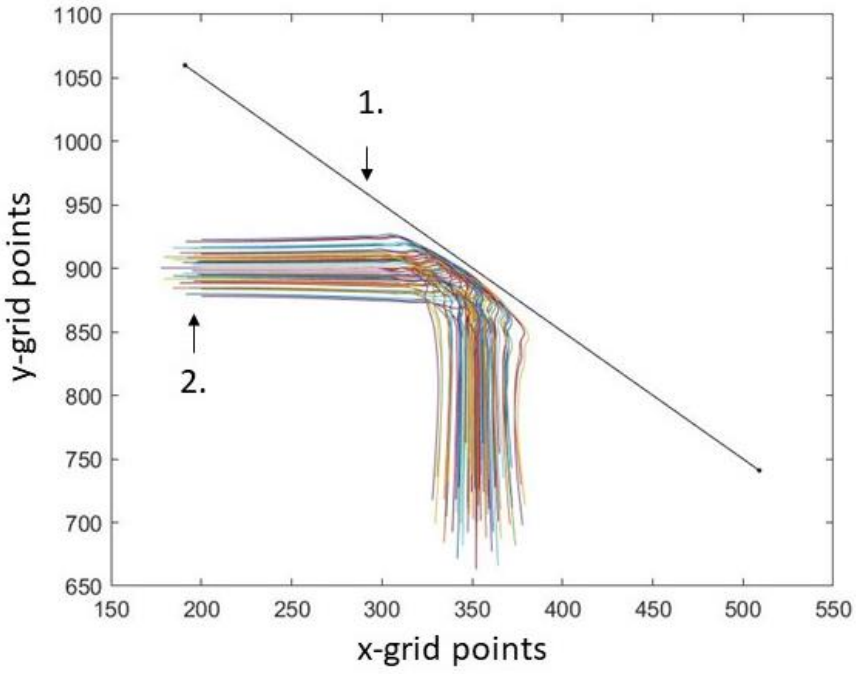

Figure 18. The result of reflecting a wave packet against a mirror with a time dependent angle. 1) A time dependent mirror with frequency of 100 and amplitude of 4.5 degrees. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

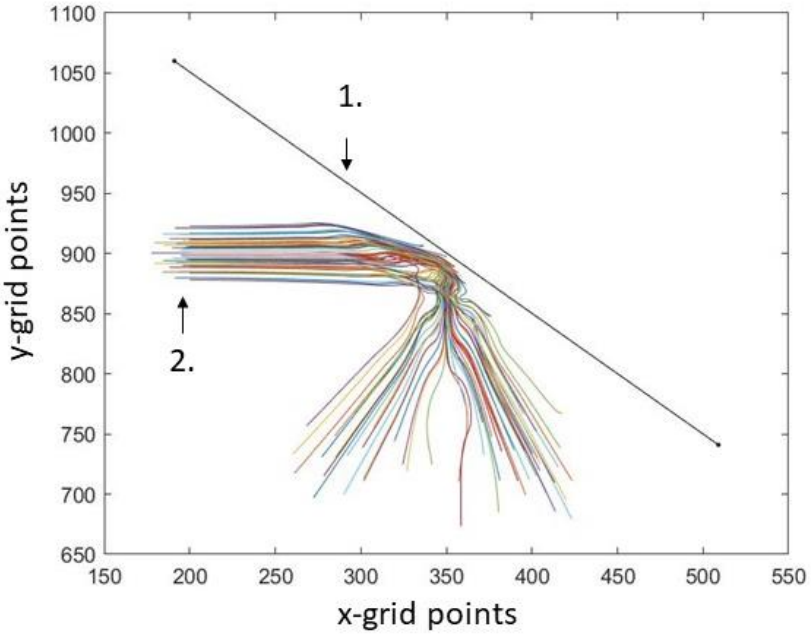

Figure 19. The result of reflecting a wave packet against a mirror with a time dependent angle. 1) A time dependent mirror with frequency of 1 and amplitude of 18 degrees. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

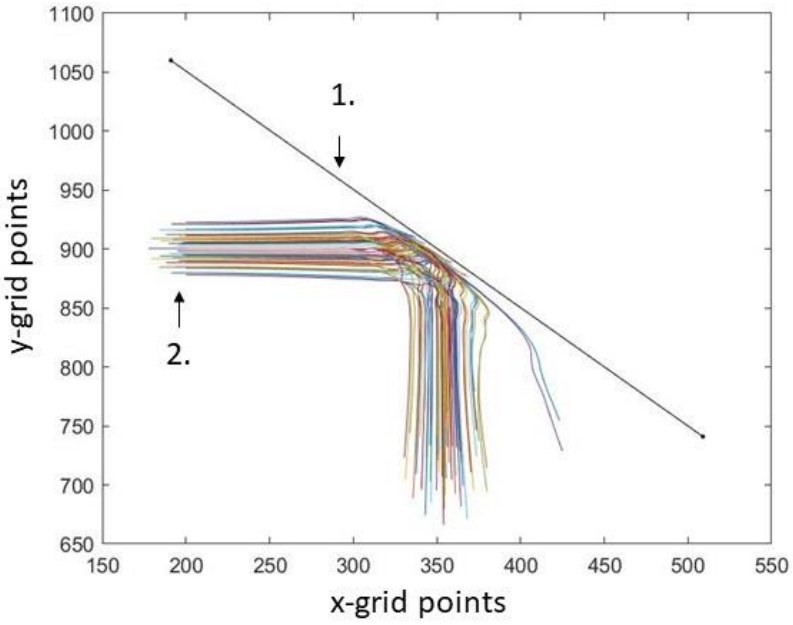

Figure 20. The result of reflecting a wave packet against a mirror with a time dependent angle. 1) A time dependent mirror with frequency of 1 and amplitude of 4.5 degrees. 2) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot.

It is observed that when the amplitude is large the wave packet separates and become two wave packets. When the frequency is large the resulting behaviour of the mirror becomes similarly to two mirrors overlapping with the angles at the extremes of the amplitude.

4.4 Test of a large setup

4.4.1 Using mirrors and beam splitters

This is test of a setup which is a part of the experimental setup proposed by Vaidman. The setup is constructed in two versions. It uses beam splitters with a potential of -0.25 and mirrors that uses the lower frequency range and amplitude from the previous setup with a time-dependent mirror. The result of simulating the particles' trajectories through one beam splitter and two mirrors is displayed in Figure 21-24.

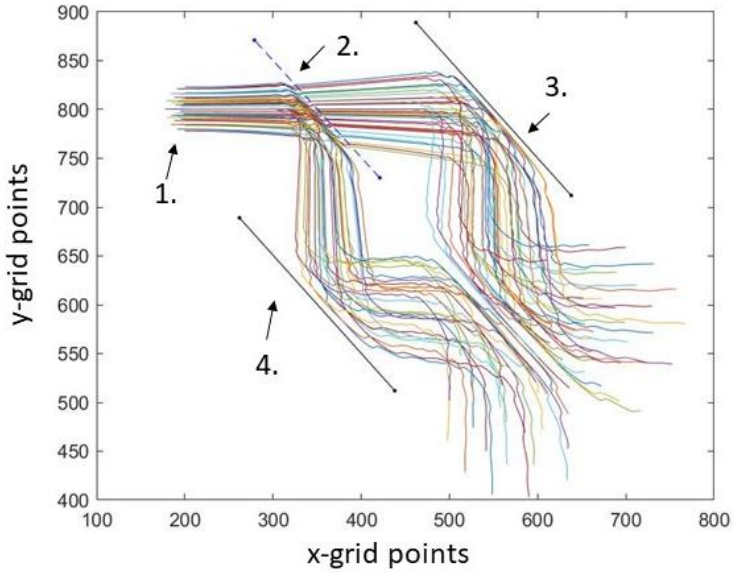

Figure 21. The result of a wave packet going through a setup with one beam splitter and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A stationary mirror 4) A stationary mirror.

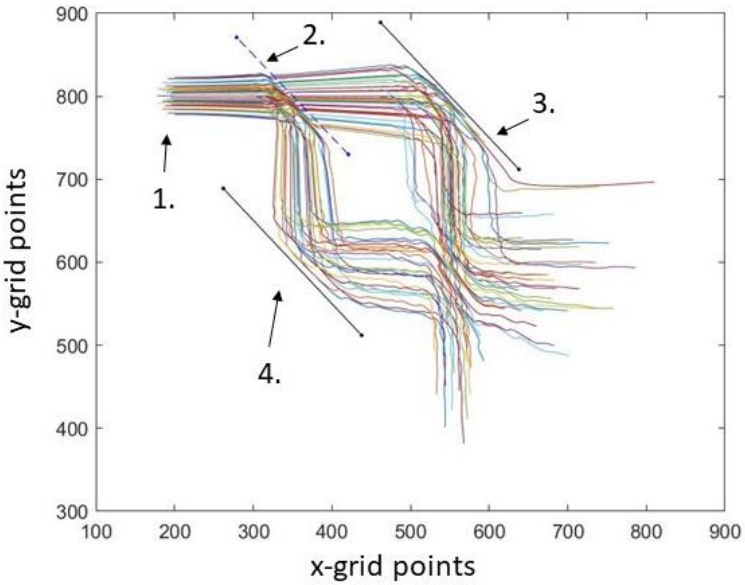

Figure 22. The result of a wave packet going through a setup with one beam splitter and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 4) A stationary mirror.

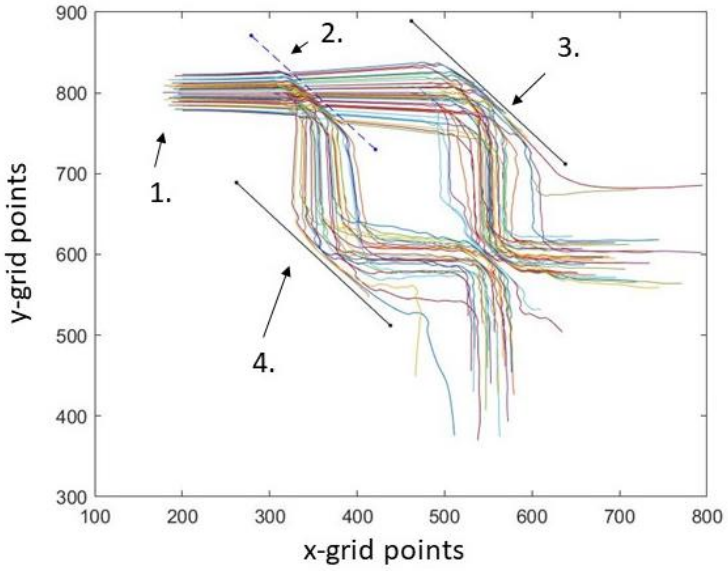

Figure 23. The result of a wave packet going through a setup with one beam splitter and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 4) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1.

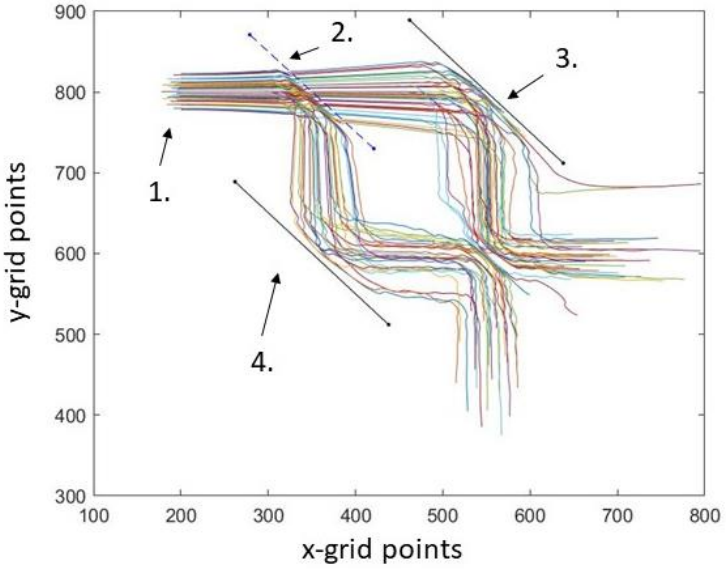

Figure 24. The result of a wave packet going through a setup with one beam splitter and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 4) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1.5.

The result of simulating the particles' trajectories through two beam splitters and two mirrors is displayed in Figure 25-28.

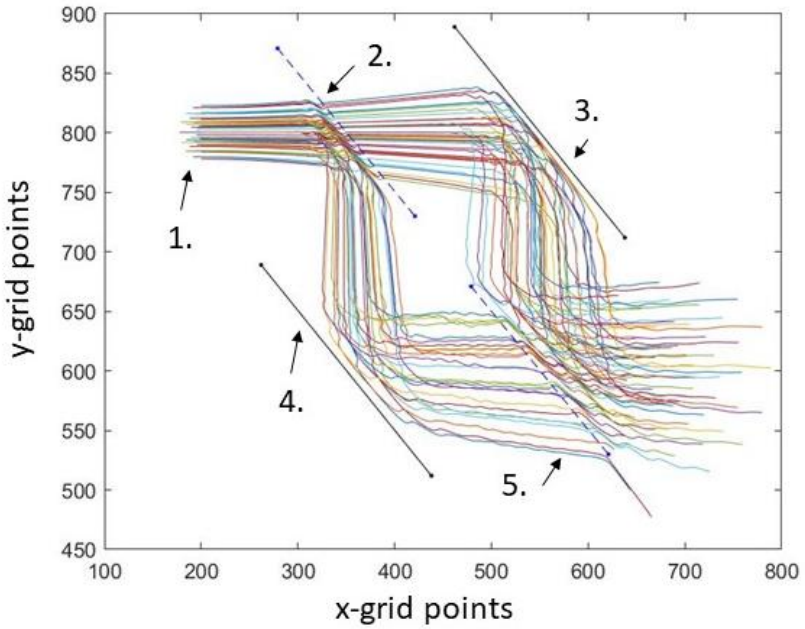

Figure 25. The result of a wave packet going through a setup with two beam splitters and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A stationary mirror 4) A stationary mirror. 5) A beam splitter with a potential of -0.25.

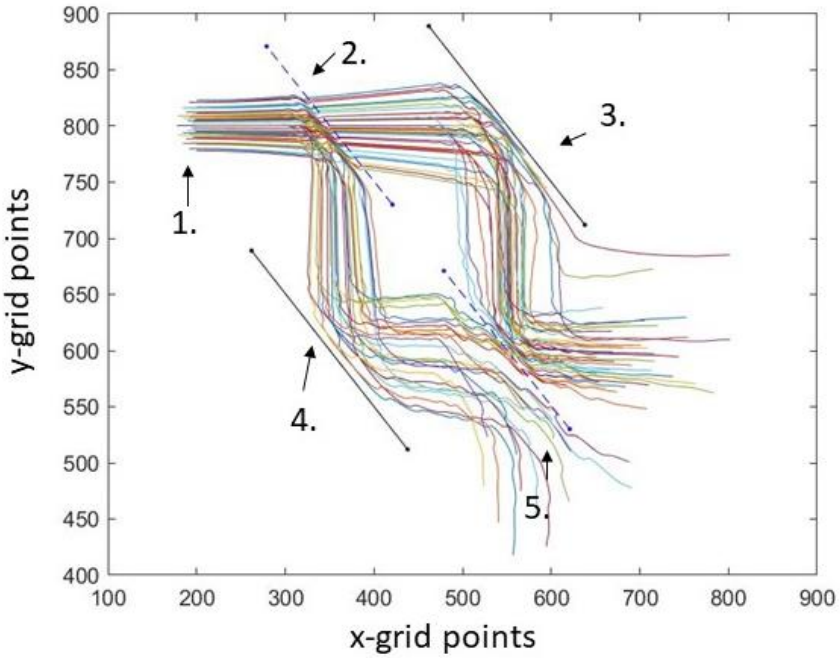

Figure 26. The result of a wave packet going through a setup with two beam splitters and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 4) A stationary mirror. 5) A beam splitter with a potential of -0.25.

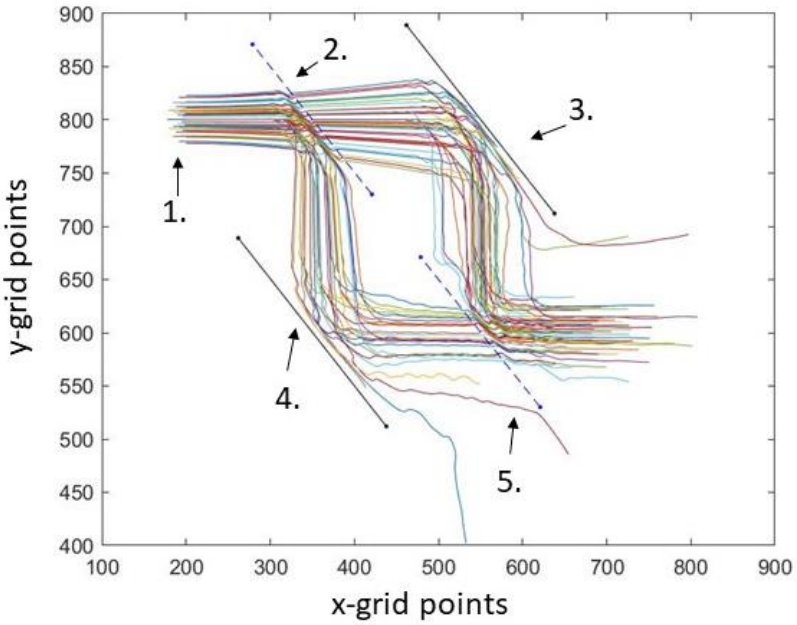

Figure 27. The result of a wave packet going through a setup with two beam splitters and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 4) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 5) A beam splitter with a potential of -0.25.

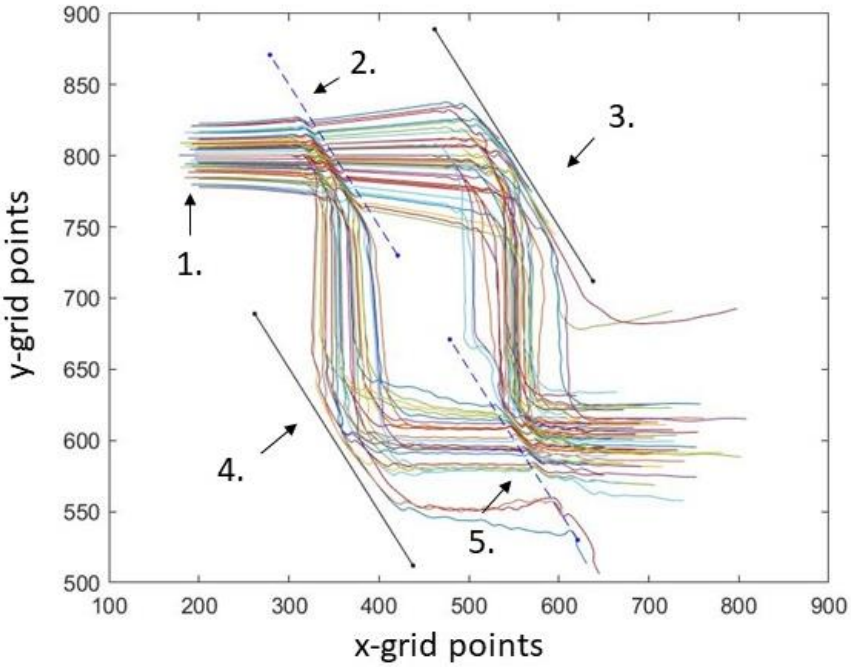

Figure 28. The result of a wave packet going through a setup with two beam splitters and two mirrors. 1) Starting position of the particles in the wave packet with their trajectories. The trajectories are plotted for all timesteps in the grid system with the x-direction grid points and y-direction grid points marked in the plot. 2) A beam splitter with a potential of -0.25 3) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1. 4) A time dependent mirror of amplitude of 4.5 degrees and a frequency of 1.5 5) A beam splitter with a potential of -0.25.

5. Discussion

The virtual detector gives a correct result when the wavefunction and the particles moves through it, see Figure 5. The result is a power function, displayed in Figure 6. The sum of the probability at each timestep is 993.23 and if the whole wave packet had gone through the virtual detector the sum should have been 1000, since the size of the timestep is 0.001. The normalisation could have been decreased but it is also possible that some of the wave packet has not gone through the virtual detector and the sum is therefore lower than 1000.

The angles of the reflected and transmitted waves when using a thin potential barrier as a beam splitter, is exemplified in Figure 7, which resulted in, see Table 1, that they are approximated equal to the incident angle. In the simulation these angles are not exactly equal to the incident angle. This could be because that the location of the point which is used for calculating the angles for the reflected and transmitted waves is difficult to know precisely but when this wave packet have travelled far this point is less important and these angle should approach the expected value. There is also some difference for the potential values. This is expected since the transmitted wave does travel a short while in the barrier which affects its trajectory. The transmitted and reflected waves are not independent from each other and thus the value of the potential in the barrier will affect both the transmitted and reflected angles.

Analysing a thin potential barrier with virtual detector resulted in Figure 8-13. The result of the intensity is tabulated in Table 2. Table 2 shows that the intensity of the transmitted wave is decreased when the magnitude of the potential is increased, independent of the sign of the potential. A value of the potential at -0.25 resulted in almost equal intensity of the transmitted and reflected waves. This value is the negative value of the potential which gives an equal intensity of the transmitted and reflected waves. It would be beneficial to find the positive value as well and use it in the larger setups.

The particles' trajectories of the reflection of a wave packet at a fixed mirror is displayed in Figure 14-16. The result of the angle of the reflected wave packet is tabulated in Table 3, the result is that the reflected angle is approximated equal to the incident angle. The difference is explained in that the point which is used for calculating the reflected angle is not known exactly.

The result of the particles' trajectories in the simulation of a time dependent mirror is displayed in Figure 17-20, the numerical method is observed to work in these setups. A large amplitude will make the wave packet separate and become two wave packets. A higher frequency will make the resulting behaviour of the mirror similarly to two mirrors overlapping with angles at the extreme amplitude. The trajectories are smooth, and the simulation seems to produce plausible trajectories.

The result of the particles' trajectories in the larger setups is displayed in Figure 21-28. The result of these shows that these setups is possible to simulate with this numerical method, but some of the particles seems to behave unexpectedly. This could be a result of using a negative value in the beam splitters. Since this is a start for the experiment proposed by Vaidman, it is recommended to continue with the complete proposed experimental setup. Since the complete setup is larger and the simulation would need more space in the form of grid points, it could be good to improve numerical methods further to limit the process time of simulating the setup. It is recommended to make the spacing between the mirrors and beam splitters larger in ratio to the size of the wave packet, this would give a better result of the experimental setup. It is recommended to follow up which potential value to use in the beam splitter and to vary its thickness. The simulations performed used a negative value in the potential, which made some of the wavefunction trapped in it. A positive value of the potential in the beam splitter could be used instead in the setup to observe any difference of the result in the simulation.

In this work, a wave packet was used as the wavefunction. This could give a different result than if a periodic wavefunction was used. In Vaidman's proposed experiment, a periodic wavefunction is used, so it would have been optimal to simulate the entire experiment with a periodic wavefunction starting at the particle source. The guiding equation, with the particles starting at the source, should be implemented after the wavefunction has reached a steady state. This could modify the result of the frequencies measured by the detector or the particles' trajectory compared with a wave packet.

What could happen is that the part of the wavefunction that propagates to M2 and M3 by reflecting at M1 is partly reflected at BS2 or BS3 and returns to BS1 through M1. The returning part of the wavefunction could then affect how the wavefunction behaves at BS1 in a steady state. This could result in that the part of the wavefunction that moves towards M4 consist of the frequencies of M2, M3 and M4 but not M1 and M5. This would explain the result attained by Vaidman.

6. Conclusions

This work resulted in a numerical method that simulates the Schrödinger equation and the guiding equation from Bohmian mechanics. The simulations were optimised with the help of a better method to determine the velocity of the particles with the guiding equation and with improved numerical methods of how to solve the Schrödinger equation. The numerical methods for simulating the Schrödinger equation was improved by only solving the Schrödinger equation in a small part of the whole system, this part of the system was the region of interest, where the wavefunction had significant values.

A beam splitter was created as a thin piece of a potential barrier. The beam splitter was tested in the reflected and transmitted angles as the incident angle of a wave packet changed. This resulted in that the angles of reflected and transmitted waves worked as ordinary optics would say a beam splitter would work, see Table 1 which is exemplified by Figure 7.

A virtual detector was constructed and tested, Figure 5-6, it was concluded that it works properly. The virtual detector was used to test the intensity of the reflected and transmitted waves when using the beam splitter, Figure 8-13 and Table 2. This was done to find the potential for a thin piece of potential barrier at 45 degrees that made the intensity of the reflected and transmitted waves to have an equal intensity. The result was that the potential had a value of -0.25 to give an output of two wave packets with almost equal intensity in the probability current over time.

A prefect mirror was tested to observe how the trajectories behaved for different fixed angles of incident for the wave packet, see Figure 14-16 and Table 3. The reflected angle was almost equal to the incident angle of a wave packet. The mirror was also tested for a time-dependent angle for different amplitudes and frequencies for the mirror at an average angle of 45 degrees, with the result that the numerical method works for a mirror if the value of the timestep is small, see Figure 17-20. The amplitude and frequency had to be small to be used in the experiment proposed by Vaidman.

Using the result of the mirror and beam splitter, two larger setups was constructed that was a small part of Vaidman proposed experiment. One with one beam splitter and two mirrors and one with the same setup but with an additionally beam splitter after the mirrors. The result is that it is possible to numerical simulate the setup. There needs to be more work towards optimising the numerical methods to make the simulation more effective and to make the setup larger and the spreading of the wave packet smaller to simulate the whole experiment proposed by Vaidman, Figure 21-28.

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