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Resumen

En este trabajo, investigamos el fenómeno de la inversión temporal de la función de onda de una partícula dentro del marco de la mecánica cuántica. La inversión temporal, o reversión temporal, es una simetría fundamental en la física cuántica, y comprender sus implicaciones sobre la función de onda proporciona una comprensión más profunda del comportamiento de los sistemas cuánticos.

Para explorar este fenómeno, utilizamos la interpretación de Bohm de la mecánica cuántica, que ofrece una perspectiva distinta al incorporar trayectorias de partículas deterministas guiadas por la función de onda. La interpretación de Bohm, también conocida como la teoría de de Broglie-Bohm, nos permite visualizar los efectos de la inversión temporal tanto en la función de onda como en la dinámica asociada de las partículas.

Además, un programa será desarrollado para simular el movimiento de un paquete gaussiano al mismo tiempo que un grupo de partículas distribuidas de manera gaussiana para observar la equivalencia con la interpretación de Bohm. En esta misma simulación, se llevará a cabo una inversión temporal.

Comenzamos revisando la formulación estándar de la inversión temporal en la mecánica cuántica y luego extendemos esto al marco de Bohm. Mediante el análisis de ejemplos específicos y la realización de simulaciones numéricas, demostramos cómo la función de onda y las trayectorias de las partículas evolucionan bajo la inversión temporal. Nuestros resultados muestran que las trayectorias Bohmianas proporcionan una representación intuitiva y clara del proceso de inversión temporal, destacando la naturaleza determinista del movimiento de las partículas incluso en el tiempo invertido.

Palabras clave: función de onda; dispersión; trayectorias; inversión temporal; diferencias finitas.

Abstract

In this work, the phenomenon of temporal inversion of the wave-function of a particle within the framework of quantum mechanics will be investigated. Temporal inversion, or time-reversal, is a fundamental symmetry in quantum physics, and understanding its implications on the wave-function provides a deeper understanding of the behavior of quantum systems.

To explore this phenomenon, the Bohmian interpretation of quantum mechanics will be used, which offers a distinct perspective by incorporating deterministic particle trajectories guided by the wave-function. Bohm's interpretation, also known as the de Broglie-Bohm theory, allows us to visualize the effects of time-reversal on both the wave-function and the associated particle dynamics.

Additionally, a program will be developed to simulate the movement of a Gaussian wave packet simultaneously with a group of particles distributed in a Gaussian manner to observe the equivalence with Bohm's interpretation. In this same simulation, a temporal inversion will occur.

We begin by reviewing the standard formulation of time-reversal in quantum mechanics and then extend this to the Bohmian framework. Through the analysis of specific examples and numerical simulations, how the wave-function and particle trajectories evolve under time-reversal will be demonstrated. The results show that Bohmian trajectories provide an intuitive and clear representation of the time-reversal process, highlighting the deterministic nature of particle motion even in reversed time.

Keywords: wave-function; dispersion; trajectories; time reversal; finite differences.

CHAPTER 1

Introduction

Quantum physics, a fundamental theory in physics, describes nature at the smallest scales of energy levels of atoms and subatomic particles. This work aims to delve into the intricate phenomenon of temporal inversion of the wave-function of a particle, providing a comprehensive study within the framework of quantum mechanics and Bohm's interpretation.

The structure of this work is organized to build a solid theoretical foundation. Initially, a brief introduction to quantum physics will be presented, covering essential principles and the solution to a free particle. This foundational knowledge is crucial for understanding the subsequent discussions.

Following this, Bohm's interpretation of quantum mechanics will be introduced, a distinct perspective that incorporates deterministic particle trajectories guided by the wave-function, exploring the quantum mechanics of a free particle within this framework and highlighting how Bohm's interpretation offers unique insights into particle dynamics.

Lastly,this work aims to delve into the concept of time reversal in quantum physics. Time reversal, or temporal inversion, is a fundamental symmetry in quantum mechanics. Understanding its implications on the wave-function and particle behavior is essential for the comprehensive study aimed to achieve.

Through these theoretical explorations, the groundwork for our primary objective will be laid: investigating the temporal inversion of the wave-function using Bohm's interpretation. By developing a simulation program, it will be possible to visualize the movement of a Gaussian wave packet and a group of particles distributed in a Gaussian manner. This will allow us to compare the standard quantum interpretation with Bohm's interpretation and examine the effects of temporal inversion in a detailed and rigorous manner.

This introduction sets the stage for a thorough exploration of quantum mechanics, Bohm's interpretation, and the intriguing phenomenon of time reversal, providing a clear pathway to understanding the core objectives of this work.

1.1. Basics about quantum mechanics

The first thing that we need to introduce is some basic concepts about Quantum mechanics, which is the Quantum physics applied to the movement of particles. In quantum mechanics, a particle is described by a wave-function [1] (we will call it $\psi(\vec{r},t)$). Such wave-function cannot be anything we propose as it must fulfill some conditions. One of the most important ones is that it must be a solution of a partial derivatives differential equation which is the Schrodinger's equation, that for the case of a free particle is:

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) \tag{1.1}$$

this expression can also be written using Dirac's notation as:

$$i\hbar\frac{d\,|\psi(t)\rangle}{dt} = \hat{H}\,|\psi(t)\rangle \tag{1.2}$$

Where $\hat{H}$ is called the Hamiltonian and it is related to the energy of the particle (for a free particle $\hat{H} = \frac{\hat{p}^2}{2m}$). Once we have obtained a solution that satisfies this equation we will have obtained our wave-function for free particles, where the product of its complex conjugate and the function itself is related to a density probability for the particle:

$$\psi^*(\vec{r},t)\psi(\vec{r},t) = |\psi(\vec{r},t)|^2 = \rho(\vec{r},t) \tag{1.3}$$

which can be interpreted as the probability density for the position of the particle. This is Born's interpretation of the wave function [2].

In the standard interpretation of Quantum Mechanics, the wave function encapsulates all information about the particle. This wave function enables us to calculate probabilities, but it does not provide definite information about the particle beyond its wave function. The particle does not possess a definite position; instead, it is described only by its wave function. Using the wave function, we can calculate the probabilities of finding the particle at various positions. However, the particle's position does not exist until it is measured [3]. Upon measurement, the particle exhibits a specific position value. This specific position is acquired through the measurement process, which also alters the wave function [4]. This alteration is known as the collapse of the wave function.

We have no control over this collapse, as the outcome is unknown before measurement. While we can calculate probabilities, we cannot predict specific results. The measurement problem is a significant issue in describing a particle as a wave. After collapse, the wave function must be normalized again, indicating that the measurement process cannot be described using the Schrödinger equation with a Hermitian Hamiltonian. Consequently, the measurement process lies outside the wave description of particles.

The problem is "solved" by distinguishing between two worlds: the quantum world, which includes subatomic particles, atoms, and molecules, and the classical world, which includes macroscopic objects and the instruments we use to measure physical properties. However, this solution is not entirely satisfactory, as there is no clearly defined boundary between these worlds.

One of the main proponents of the Copenhagen interpretation was John von Neumann, who proposed a theorem demonstrating that it is impossible to develop a mathematical framework for Quantum Theory that provides the same results as the Copenhagen interpretation while including hidden variables [5]. This theorem was later proven false by John Bell [6], who used the simplest method for his demonstration: a counter-example.

1.1.1. Solution for a free particle The general solution to equation (1.1) is a lineal superposition of harmonic waves [7] but we will analyze a particular solution to the Schrodinger's equation for a free particle in a three dimensional space which is known as a Gaussian wave packet. In our study we will propose that at the initial instant of time ($t = 0$) is defined by it's position ($\vec{r}$) and momentum ($\vec{p} = \hbar\vec{k}$) as:

$$\psi(\vec{r}, 0) = Ce^{-r^2/a^2} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \tag{1.4}$$

but in our approach, without loss of generality, we will only analyze the case of a particle with initial velocity on the y axis in order to simplify the expressions and because the results can be extended easily to the most general case:

$$\psi(\vec{r}, 0) = Ce^{-r^2/a^2} e^{-\frac{i}{\hbar}p_y y} = Ce^{-r^2/a^2} e^{ik_{y_0} y} \tag{1.5}$$

where C is a normalization constant and a is related to the initial dispersion of the packet. With this expression we can now calculate the expectation value of $\vec{r}$ at $t = 0$:

$$\langle\vec{r}\rangle = \langle\psi(\vec{r}, 0)|\,\vec{r}\,|\psi(\vec{r}, 0)\rangle = \int_V \psi^*(\vec{r}, 0)\vec{r}\psi(\vec{r}, 0)dV = \int_V \psi^*(\vec{r}, 0)r\psi(\vec{r}, 0)r^2\hat{u}_r sen\theta dr d\theta d\phi = 0 \tag{1.6}$$

where we have taken into account that integrating in all directions a vector which has the radial direction cancels out, and this result makes sense since it is a Gaussian centered at the origin.

To switch between the position and momentum representation, we will use the Fourier transform [8], which is defined as:

$$\tilde{\psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)e^{-ik_x x}dx \tag{1.7}$$

which in the case of three dimensions would be the composition of three consecutive transformations, each on in each direction:

$$\tilde{\psi}(\vec{k}) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\vec{r})e^{-i\vec{k}\cdot\vec{r}}dxdydz \tag{1.8}$$

In this integral, since the variables we integrate over are independent, and we have two different types of terms, we can solve it by taking into account that:

$$\int_{-\infty}^{\infty} e^{-x^2/a^2}e^{-ik_x x}dx = \int_{-\infty}^{\infty} e^{-(\frac{x^2}{a^2}+ik_x x)}dx = e^{-a^2\frac{k_x^2}{4}} \int_{-\infty}^{\infty} e^{-(\frac{x}{a}+ia\frac{k_x}{2})^2}dx \tag{1.9}$$

$$\int_{-\infty}^{\infty} e^{-y^2/a^2}e^{ik_{y_0}y}e^{-ik_y y}dy = \int_{-\infty}^{\infty} e^{-(\frac{y^2}{a^2}+i(k_y-k_{y_0})y)}dy = e^{-a^2\frac{(k_y-k_{y_0})^2}{4}} \int_{-\infty}^{\infty} e^{-(\frac{y}{a}+ia\frac{k_y-k_{y_0}}{2})^2}dy \tag{1.10}$$

where we have converted the exponent into a perfect square and taken out of the integral what does not depend on y. The integral can be quickly solved by making the variable change $s = \frac{y}{a} + ia\frac{(\cdots)}{2}$, $dy = ads$, and then $s^2 = b$, $ds = \frac{1}{2}b^{-1/2}db$, obtaining $a\sqrt{\pi}$:

$$\begin{aligned} \text{For } (1.9): \; & e^{-a^2\frac{k_x^2}{4}}a\sqrt{\pi} \\ \text{For } (1.10): \; & e^{-a^2\frac{(k_y-k_{y_0})^2}{4}}a\sqrt{\pi} \end{aligned} \tag{1.11}$$

since the integral in z is equal to the one in x, we therefore have:

$$\tilde{\psi}(\vec{k}) = \left(\frac{a}{\sqrt{2}}\right)^3 Ce^{-a^2\frac{k^2+k_{y_0}^2-2k_y k_{y_0}}{4}} = \left(\frac{a}{\sqrt{2}}\right)^3 Ce^{-a^2\left(\frac{\vec{k}-k_{y_0}\hat{u}_y}{2}\right)^2} \tag{1.12}$$

and, as we well know:

$$\tilde{\psi}(\vec{p}) = \frac{1}{\sqrt{\hbar}}\tilde{\psi}(\vec{k} = \frac{\vec{p}}{\hbar}) = \left(\frac{a}{\sqrt{2}}\right)^3 \frac{C}{\sqrt{\hbar}} e^{\frac{a^2}{4\hbar^2}\left(\frac{\vec{p}}{\hbar} - \vec{\hbar k_{y_0}}\right)^2} = Be^{\frac{a^2}{4\hbar^2}\left(\frac{\vec{p}}{\hbar} - \hbar\vec{k}_{y_0}\right)^2} \tag{1.13}$$

$$\rho_p(\vec{p}) = |\overline{\psi}(\vec{p})|^2 = \overline{\psi}(\vec{p})\overline{\psi}(\vec{p})^* = B^2 e^{\frac{a^2}{2\hbar^2}\left(\frac{\vec{p}}{\hbar} - \hbar\vec{k}_{y_0}\right)^2} \tag{1.14}$$

With this, we can now calculate the expectation value of $\vec{p}$ at $t = 0$:

$$\langle\vec{p}\rangle = \int_{V_{\vec{p}}} \vec{p}\rho_p(\vec{p})d^3\vec{p} = \int_{V_{\vec{p}}} p\rho_p(\vec{p})\hat{u_y}d^3\vec{p} = \hbar k_{y_0}\hat{u_y} = \hbar\vec{k}_{y_0} \tag{1.15}$$

The time variation of these expectation values according to Ehrenfest's theorem [9]:

$$\frac{d\langle\vec{r}\rangle}{dt} = \frac{\langle\vec{p}\rangle}{m} = \frac{\hbar\vec{k}_{y_0}}{m} = \frac{\vec{p_{y_0}}}{m} \tag{1.16}$$

$$\frac{d\langle\vec{p}\rangle}{dt} = -\left\langle\frac{dV(\vec{r})}{d\vec{r}}\right\rangle = 0 \tag{1.17}$$

To calculate the time evolution, it is enough to know $\psi(\vec{r}, 0)$ which is the function we are working on, and calculate $\tilde{\psi}(\vec{k}, 0)$. From this we will solve (1.2) in the momentum representation as the Hamiltonian is easier to work with. The result can be proven to be $\tilde{\psi}(k,t) = \tilde{\psi}(k,0)e^{-\frac{p^2}{2m}\frac{t}{\hbar}} = \tilde{\psi}(k,0)e^{-wt}$:

$$\psi(\vec{r},t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tilde{\psi}(\vec{k},0)e^{i(\vec{k}\cdot\vec{r}-wt)}d^3\vec{k} = \frac{a^3}{4\sqrt{\pi}}C\iiint_{\infty}^{\infty} e^{-a^2\left(\frac{\vec{k}-\vec{k}_{y_0}}{2}\right)^2} e^{i(\vec{k}\cdot\vec{r}-wt)}d^3\vec{k} \tag{1.18}$$

just as before, we have two types of integrals:

$$\int_{-\infty}^{\infty} e^{-a^2\frac{k_x^2}{4}}e^{i(k_x x - wt)}u_{\hat{k_x}}dk = \int_{-\infty}^{\infty} e^{-[\frac{-a^2}{4}k_x^2 - i(k_x x - \frac{\hbar k^2}{2m}t)]}u_{\hat{k_x}}dk \tag{1.19}$$

$$\int_{-\infty}^{\infty} e^{-a^2\frac{(k_y-k_{y_0})^2}{4}}e^{i(k_y y - wt)}u_{\hat{k_y}}dk = \int_{-\infty}^{\infty} e^{-[\frac{-a^2}{4}(k_y-k_{y_0})^2 - i(k_y y - \frac{\hbar k^2}{2m}t)]}u_{\hat{k_y}}dk \tag{1.20}$$

where it has been used that w is a function of $\vec{k}$ (according to the dispersion relation). Their solutions are similar to the previous ones (by obtaining a perfect square in the exponent and following analogous steps as done before), allowing us to easily verify that we arrive at:

$$\begin{aligned}
&\text{For (1.19)}: \ \frac{2\sqrt{\pi}}{a}\left(1 + i\frac{2\hbar t}{ma^2}\right)^{-1/2}\exp\left\{-\frac{x^2}{a^2 + i\frac{2\hbar t}{m}}\right\}u_{\hat{k_x}} \\
&\text{For (1.20)}: \ \frac{2\sqrt{\pi}}{a}\left(1 + i\frac{2\hbar t}{ma^2}\right)^{-1/2}e^{ik_{y_0}y - i\frac{\hbar k_{y_0}^2 t}{2m}}\exp\left\{-\frac{\left(y - \frac{\hbar k_{y_0}}{m}t\right)^2}{a^2 + i\frac{2\hbar t}{m}}\right\}u_{\hat{k_y}}
\end{aligned} \tag{1.21}$$

getting therefore:

$$\psi(\vec{r},t) = 2\pi C\left(1 + i\frac{2\hbar t}{ma^2}\right)^{-3/2}e^{ik_{y_0}y - i\frac{\hbar k_{y_0}^2 t}{2m}}\exp\left\{-\frac{r^2 + (\frac{\hbar k_{y_0}}{m}t)^2 - 2y\frac{\hbar k_{y_0}}{m}t}{a^2 + i\frac{2\hbar t}{m}}\right\}\hat{u_k} \tag{1.22}$$

with which we can calculate the probability density:

$$\rho(\vec{r},t) = |\psi(\vec{r},t)|^2 = \psi(\vec{r},t)\psi(\vec{r},t)^* = \\ = 4\pi C \left(1 + \left(\frac{2\hbar t}{ma^2}\right)^2\right)^{-3/2} \exp\left\{-\frac{2a^2(r^2 + (\frac{\hbar k_{y_0}}{m}t)^2 - 2y\frac{\hbar k_{y_0}}{m}t)}{a^4 + (\frac{2\hbar t}{m})^2}\right\} \tag{1.23}$$

From this formula, we can obtain the value of the dispersion by comparing $\rho(\vec{r},t)$ with a generic Gaussian:

$$\rho(s) = \frac{1}{\Delta s\sqrt{2\pi}} e^{-(s-\langle s\rangle)^2/2\Delta s^2} \tag{1.24}$$

which as we can observe is:

$$\Delta x = \Delta y = \Delta z = \sqrt{\frac{a^2}{2} + \left(\frac{2\hbar t}{ma}\right)^2} \tag{1.25}$$

1.1.2. Spin In quantum mechanics, the concept of spin is fundamental to fully describing the intrinsic angular momentum of some particles. Spin is a quantum property that does not have a classical counterpart; it represents an intrinsic form of angular momentum carried by some elementary particles, composite particles (hadrons), and some atomic nuclei. Each type of particle has a characteristic spin quantum number, which can take on values that are either integer or half-integer multipled by $\hbar$ [1].

Spin is crucial for understanding the behavior and properties of particles at a quantum level. It plays a key role in the Pauli exclusion principle, which governs the structure of atoms and the formation of the periodic table. Additionally, spin influences magnetic properties of materials, the interaction of particles with external magnetic fields (Zeeman effect), and is essential in the formulation of quantum statistics (Bose-Einstein and Fermi-Dirac statistics).

Following this, to fully describe a particle we would need a new representation that includes spin as well as the previous characteristics. For example, in one dimention and in the coordinates representatioon we will now need $\phi(x,t,s)$ as opposed to what would have from the previous section $\psi(x,t)$. However, in the case of a free particle, the Hamiltonian, which describes the total energy of the system, is independent of spin being able to express our new wave-function as the composition of two wave-functions [1] ($|\phi(t,s)\rangle = |\psi(t)\rangle\,|\chi(s)\rangle$):

$$\hat{H}\,|\phi(t,s)\rangle = \hat{H}\,|\psi(t)\rangle\,|\chi(s)\rangle = (\hat{H}\,|\psi(t)\rangle)\,|\chi(s)\rangle \tag{1.26}$$

meaning we can express (1.2) as:

$$i\hbar\frac{d\,|\phi\rangle}{dt} = \hat{H}\,|\phi\rangle \quad \Rightarrow \quad \left(i\hbar\frac{d\,|\psi\rangle}{dt}\right)|\chi\rangle = (\hat{H}\,|\psi\rangle)\,|\chi\rangle \quad \Rightarrow \quad i\hbar\frac{d\,|\psi\rangle}{dt} = \hat{H}\,|\psi\rangle \tag{1.27}$$

where we used that only $|\psi\rangle$ depends on time and for the last equation we multiplied both sides by $\langle\chi|$ and we took into account that $\langle\chi|\chi\rangle = 1$.

We can see from this that for a free particle, we can simplify our analysis by ignoring spin, focusing solely on the spatial and temporal evolution governed by the Schrödinger equation. This approach allows us to study the wavefunction of the particle without the added complexity of spin-dependent interactions. Thus, while spin is a fundamental aspect of a complete quantum description, in the specific case of a free particle, it is sufficient to describe the evolution using a spin-independent Hamiltonian.

By focusing on the Hamiltonian independent of spin, we can effectively describe the dynamics of the particle without loss of generality, making the mathematical treatment more straightforward while still keeping the essential physics of free particle motion.

1.2. Bohm's Interpretation

The problem highlighted in the previous section regarding the Copenhagen interpretation is not truly resolved, as there is no well-defined boundary between the quantum and classical worlds. David Bohm's book, "The Undivided Universe," [10] addresses this issue, emphasizing that such a boundary does not exist in Bohmian mechanics, which is effectively illustrated by Schrodinger's cat paradox.

Additionally, the wave description leaves us a little confused. What about the particle-like behavior of particles? Isn't an electron considered a particle? How can we observe distinct tracks of particles in a cloud chamber if they don't follow well-defined trajectories?

Bohm's interpretation of quantum mechanics, also known as the de Broglie-Bohm theory or the pilot-wave theory, offers a distinct perspective on quantum phenomena. Unlike the standard Copenhagen interpretation, which emphasizes the probabilistic nature of quantum mechanics, Bohm's interpretation introduces determinism into the quantum realm. This interpretation posits that particles follow well-defined trajectories, guided by a wave-function that evolves according to the Schrodinger equation. The interpretation proposed by David Bohm includes hidden variables such as position, momentum, and energy, allowing particles to be described as actual particles.

If we propose a wave function not as the sum of a real and an imaginary function but as its modulus and argument as follows:

$$\psi(\vec{r},t) = A(\vec{r},t)e^{\frac{i}{\hbar}S(\vec{r},t)} \tag{1.28}$$

with $A(\vec{r},t)$ and $S(\vec{r},t)$ being real functions that depend on the position and time, and we depart from the same equation as before, (1.1), we will get two equations that will be equivalent to the original equation but for these two functions. With that we will also have got rid of the imaginary unit i from the original equation, making it easier for us to obtain and analyse results.

Let´s obtain those two expressions for a one dimension wave-function, (1.1) in this case will be:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} \tag{1.29}$$

so:

$$\begin{aligned}
\frac{\partial\psi}{\partial t} &= \frac{\partial A}{\partial t}e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\frac{\partial S}{\partial t}e^{\frac{i}{\hbar}S} \\
\frac{\partial\psi}{\partial x} &= \frac{\partial A}{\partial x}e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\frac{\partial S}{\partial x}e^{\frac{i}{\hbar}S} \\
\frac{\partial^2\psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right) &= \frac{\partial^2 A}{\partial x^2}e^{\frac{i}{\hbar}S} + 2\frac{i}{\hbar}\frac{\partial A}{\partial x}\frac{\partial S}{\partial x}e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\frac{\partial^2 S}{\partial x^2}e^{\frac{i}{\hbar}S} - \frac{1}{\hbar^2}A\left(\frac{\partial S}{\partial x}\right)^2 e^{\frac{i}{\hbar}S}
\end{aligned} \tag{1.30}$$

We can see that there is a common factor $e^{\frac{i}{\hbar}S}$ which we can take out and we can now replace the results in (1.1):

$$\begin{aligned}
&i\hbar\left\{\frac{\partial A}{\partial t} + \frac{i}{\hbar}A\frac{\partial S}{\partial t}\right\}e^{\frac{i}{\hbar}S} = \\
&= -\frac{\hbar^2}{2m}\left\{\frac{\partial^2 A}{\partial x^2} + 2\frac{i}{\hbar}\frac{\partial A}{\partial x}\frac{\partial S}{\partial x} + \frac{i}{\hbar}A\frac{\partial^2 S}{\partial x^2} - \frac{1}{\hbar^2}A\left(\frac{\partial S}{\partial x}\right)^2\right\}e^{\frac{i}{\hbar}S}
\end{aligned} \tag{1.31}$$

Now we can cross out the exponentials and taking into account that the imaginary part of the left hand side must be equal to the imaginary part of the right hand side and that the same stands for the real part (and $i \cdot i = -1$), we can separate this expression into two equations:

$$i\hbar\frac{\partial A}{\partial t} = -\frac{i\hbar}{m}\frac{\partial A}{\partial x}\frac{\partial S}{\partial x} - \frac{i\hbar}{2m}A\frac{\partial^2 S}{\partial x^2} \tag{1.32}$$

$$-A\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 A}{\partial x^2} + \frac{1}{2m}A\left(\frac{\partial S}{\partial x}\right)^2 \tag{1.33}$$

In the first equation, we have $i\hbar$ as a common factor, being able to take both of them out and therefore making this equation independent of $\hbar$ and without imaginary units. When we find an equation that does not depend on $\hbar$, we can typically provide a classical interpretation of such an equation. This equation can be easily transformed into the following form:

$$\frac{\partial A^2}{\partial t} + \frac{\partial}{\partial x}\left(A^2\frac{1}{m}\frac{\partial S}{\partial x}\right) = 0 \tag{1.34}$$

As we can observe, this has the same structure as a continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\cdot(\rho v) = 0 \tag{1.35}$$

where the probability density is A^2; and this checks out because as $\psi = Ae^{\frac{i}{\hbar}S}$, the probability density is $\rho = |\psi|^2 = A^2$. If we interpret this probability as the probability density of a set of classical particles, this probability density satisfies the previous continuity equation with the following velocity field:

$$v = \frac{1}{m}\frac{\partial S}{\partial x} \tag{1.36}$$

Now, regarding the second equation, dividing it by A we get:

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + \frac{\partial S}{\partial t} - \frac{\hbar^2}{2m}\frac{1}{A}\frac{\partial^2 A}{\partial x^2} = 0 \tag{1.37}$$

where there is only one term depending on $\hbar$, which means that the quantum properties and behaviour are condensed in that term. Removing this term we can relate the consequent equation to the Hamilton-Jacobi's equation [11], which can be easily proven equivalent to Newton's equation [11] by just differentiating with respect to the position:

$$\frac{\partial}{\partial t}\frac{\partial S}{\partial x} + \frac{1}{m}\frac{\partial S}{\partial x}\frac{\partial^2 S}{\partial x^2} = 0 \tag{1.38}$$

and remembering from (1.36) that $\partial S/\partial x = mv$:

$$\frac{\partial}{\partial t}mv + v\frac{\partial}{\partial x}mv = \frac{d}{dt}mv = 0 \tag{1.39}$$

which is Newton's equation for a free particle.

Bohm's idea is to retain the last term that we removed before (the last part of (1.37)) and consider that particles have well-defined positions and velocities. However, the particles do not follow a classical trajectory, as we must include a new potential that affects their movement. This new potential, commonly referred to as the quantum potential, is:

$$V_q = -\frac{\hbar^2}{2m}\frac{1}{A}\frac{\partial^2 A}{\partial x^2} \tag{1.40}$$

with this potential depending obviously on position and time.

There are some considerations to take into account about this potential. First, the quantum potential depends on the shape of the amplitude A, not on its absolute value. If we multiply A by a constant, this constant does not affect the quantum potential value. Therefore, we do not need to normalize the wave function to calculate the particle trajectories. The second consideration is that the quantum potential affects the particle only in regions where A is non-zero. The last consideration is that the movement of the particle is influenced by the wave function through the amplitude A, but not the other way around: the wave function is not affected by the particle [10]. This is unlike what we typically observe in other physical processes.

1.2.1. Bohmian mechanics for a free particle In this part we will analyse the same case as before, the free particle. For this, we will reuse the results obtained from the solution for a free particle, which means that we will consider that the wave-function of the particle at the initial moment is of the form of (1.5), and therefore the wave-function with the time dependence is of the form of (1.22).

As we have that same expression we also have the same values for $\langle x\rangle(t)$, $\langle y\rangle(t)$, $\Delta x(t)$ and $\Delta y(t)$ (as well as the values for z which are of the same way as the ones for x). We can see from these values that the center for x and z doesn't move and is fixed in zero (as expected since our initial distribution is centered at 0 and there is only initial speed in the y direction).

On the other hand, the center of the distribution for the y axis moves with a velocity $\langle v_y\rangle = \hbar k_{y_0}/m = \langle p_y\rangle/m$. The meaning of the dispersion not being null and increasing over time even for the x and z values means that, obviously, at the initial time there is a dispersion in the values of the position for each axis as it is a Gaussian distribution, and that dispersion increases over time since the particle doesn't have a well defined velocity at the starting point [10].

Now let´s apply Bohm's interpretation to get the motion of the particle. If we write our wave-function as we did in (1.28), as we have seen the particles move following the equations:

$$\frac{dx}{dt} = \frac{1}{m}\frac{\partial S}{\partial x}\,, \quad \frac{dy}{dt} = \frac{1}{m}\frac{\partial S}{\partial y}\,, \quad \frac{dz}{dt} = \frac{1}{m}\frac{\partial S}{\partial z} \tag{1.41}$$

so we need to know how the phase of the wave-function varies with respect to the position. The term:

$$\left(1 + i\frac{2\hbar t}{ma^2}\right)^{-3/2} \tag{1.42}$$

has a phase but doesn't depend on the position, so that we only need to analyse the rest:

$$\begin{aligned} &e^{ik_{y_0}y - i\frac{\hbar k_{y_0}^2 t}{2m}} \exp\left\{-\frac{r^2 + (\frac{\hbar k_{y_0}}{m}t)^2 - 2y\frac{\hbar k_{y_0}}{m}t}{a^2 + i\frac{2\hbar t}{m}}\right\} = \\ &e^{ik_{y_0}y} e^{-i\frac{\hbar k_{y_0}^2 t}{2m}} \exp\left\{-\frac{r^2 + (\frac{\hbar k_{y_0}}{m}t)^2 - 2y\frac{\hbar k_{y_0}}{m}t}{a^2 + i\frac{2\hbar t}{m}}\right\} \end{aligned} \tag{1.43}$$

as we can also see, the second exponential doesn't depend on the position either so we get:

$$e^{ik_{y_0}y} \exp\left\{-\frac{r^2 + (\frac{\hbar k_{y_0}}{m}t)^2 - 2y\frac{\hbar k_{y_0}}{m}t}{a^2 + i\frac{2\hbar t}{m}}\right\} \tag{1.44}$$

Let's seperate the imaginary and real part of the second exponential:

$$\begin{aligned}\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^2+i\frac{2\hbar t}{m}} =& \frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^2+i\frac{2\hbar t}{m}}\cdot\frac{a^2-i\frac{2\hbar t}{m}}{a^2-i\frac{2\hbar t}{m}} = \\ a^2\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}} &- \left(i\frac{2\hbar t}{m}\right)\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}}\end{aligned} \tag{1.45}$$

so we get from (1.44):

$$\exp\left\{-a^2\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}}\right\}\exp\left\{\frac{i}{\hbar}\hbar k_{y_0}y+\frac{i}{\hbar}\left(\frac{2\hbar^2t}{m}\right)\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}}\right\} \tag{1.46}$$

and therefore:

$$\begin{aligned}\frac{1}{m}\frac{\partial S}{\partial x} =& \frac{1}{m}\frac{\partial}{\partial x}\left\{\hbar k_{y_0}y+\left(\frac{2\hbar^2t}{m}\right)\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}}\right\} = \\ =& \frac{2\hbar^2t}{m^2}\cdot\frac{2x}{a^4+\frac{4\hbar^2t^2}{m^2}} = \frac{\frac{4\hbar^2t}{m^2a^4}x}{1+\frac{4\hbar^2t^2}{m^2a^4}}\end{aligned} \tag{1.47}$$

$$\begin{aligned}\frac{1}{m}\frac{\partial S}{\partial y} =& \frac{1}{m}\frac{\partial}{\partial y}\left\{\hbar k_{y_0}y+\left(\frac{2\hbar^2t}{m}\right)\frac{r^2+(\frac{\hbar k_{y_0}}{m}t)^2-2y\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}}\right\} = \\ =& \frac{1}{m}\left\{\hbar k_{y_0}+\left(\frac{2\hbar^2t}{m}\right)\frac{2y-2\frac{\hbar k_{y_0}}{m}t}{a^4+\frac{4\hbar^2t^2}{m^2}}\right\} = \frac{\frac{\hbar k_{y_0}}{m}+\frac{4\hbar^2t}{m^2a^4}y}{1+\frac{4\hbar^2t^2}{m^2a^4}}\end{aligned} \tag{1.48}$$

as in previous sections, we will obviate the operations for the z component as the results are of the same way as those for x. The constant:

$$\frac{ma^2}{2\hbar}=\tau \tag{1.49}$$

has time dimensions, and if we define the mean value of the velocity as:

$$v_{y_0}=\frac{\hbar k_{y_0}}{m} \tag{1.50}$$

the equations transform into:

$$\frac{dx}{dt}=\frac{x\frac{t}{\tau^2}}{1+\frac{t^2}{\tau^2}} \tag{1.51}$$

$$\frac{dy}{dt}=\frac{v_{y_0}+y\frac{t}{\tau^2}}{1+\frac{t^2}{\tau^2}} \tag{1.52}$$

The solutions to these ordinary differential equations are:

$$x(t)=C\sqrt{t^2+\tau^2} \tag{1.53}$$

$$y(t)=v_{y_0}t+D\sqrt{t^2+\tau^2} \tag{1.54}$$

where C and D are constants of integration. To calculate them, we must now introduce the initial condition for the position of the particle:

$$x(0)=C\tau \;\longrightarrow\; C=\frac{x(0)}{\tau} \tag{1.55}$$

$$y(0) = D\tau \quad \longrightarrow \quad D = \frac{y(0)}{\tau} \tag{1.56}$$

and therefore:

$$x(t) = \frac{x(0)}{\tau}\sqrt{t^2+\tau^2} \tag{1.57}$$

$$y(t) = v_{y_0}t + \frac{y(0)}{\tau}\sqrt{t^2+\tau^2} \tag{1.58}$$

$$z(t) = \frac{z(0)}{\tau}\sqrt{t^2+\tau^2} \tag{1.59}$$

which are out motion equations for each particle (where we used as before that the z component follows the same equations as the x, component and so the calculations are the same leading us to the same expression but with the information about the z component)

The importance of these results lies in the fact that each particle follows a different trajectory that depends on its initial position ($x(0)$, $y(0)$ and $z(0)$). We can now see what would happen if we have a set of particles with the initial positions distributed following a Gaussian distribution centered at 0, as we had at the beginning, so:

$$\overline{x(0)} = x_0 = 0 \tag{1.60}$$

$$\overline{x^2(0)} = \Delta x^2(0) + x_0^2 = \frac{a^2}{4} \tag{1.61}$$

and the same way for the other components. Now, the mean value at the instant t:

$$\overline{x(t)} = \overline{\frac{x(0)}{\tau}\sqrt{t^2+\tau^2}} = 0 \tag{1.62}$$

$$\overline{y(t)} = \overline{v_{y_0}t + \frac{y(0)}{\tau}\sqrt{t^2+\tau^2}} = v_{y_0}t \tag{1.63}$$

which means that even though each particle follows a different trajectory, the mean value moves in the same way as the center of the wave packet (in the case of the x and z components the center isn't moving as there is no initial velocity in those directions and therefore the mean value for all the instants is 0) and as a classical particle. We can also calculate:

$$\overline{x^2(t)} = \overline{\left(\frac{x(0)}{\tau}\sqrt{t^2+\tau^2}\right)^2} = \frac{\overline{x^2(0)}}{\tau^2}(t^2+\tau^2) = \frac{a^2}{4}\frac{t^2+\tau^2}{\tau^2} \tag{1.64}$$

$$\begin{aligned}\overline{y^2(t)} =& \overline{\left(v_{y_0}t + \frac{y(0)}{\tau}\sqrt{t^2+\tau^2}\right)^2} = \\ = (v_{y_0}t)^2 + \frac{\overline{y^2(0)}}{\tau^2}(t^2+\tau^2) &+ 2v_{y_0}t\frac{\overline{y(0)}}{\tau}\sqrt{t^2+\tau^2} = \overline{y(t)}^2 + \frac{a^2}{4}\frac{t^2+\tau^2}{\tau^2}\end{aligned} \tag{1.65}$$

from where we can check that the initial dispersion is $a/2$ as it was for the initial wave packet, and after some time the dispersion increases like:

$$\frac{a}{2}\frac{t}{\tau} = \frac{a}{2}\frac{2\hbar t}{ma^2} = \frac{\hbar t}{ma} \tag{1.66}$$

again in the same way as for the wave packet.

We can attribute this increase due to the fact that there is an initial dispersion on the velocity which leads to a dispersion on the position. We will see why this is not correct according to Bohm's interpretation. The velocity of the particle is:

$$\begin{aligned} v_x(t) =& \frac{dx(t)}{dt} = \frac{d}{dt}\left(\frac{x(0)}{\tau}\sqrt{t^2+\tau^2}\right) = \frac{x(0)}{\tau}\frac{t}{\sqrt{t^2+\tau^2}} = \\ =& \frac{x(0)}{\tau}\frac{t\sqrt{t^2+\tau^2}}{t^2+\tau^2} = x(t)\frac{t}{t^2+\tau^2} \end{aligned} \tag{1.67}$$

$$\begin{aligned} v_y(t) =& \frac{dy(t)}{dt} = \frac{d}{dt}\left(v_{y_0}t + \frac{y(0)}{\tau}\sqrt{t^2+\tau^2}\right) = v_{y_0} + \frac{y(0)}{\tau}\frac{t}{\sqrt{t^2+\tau^2}} = \\ =& v_{y_0} + \frac{y(0)}{\tau}\frac{t\sqrt{t^2+\tau^2}}{t^2+\tau^2} = v_{y_0} + (y(t) - v_{y_0}t)\frac{t}{t^2+\tau^2} \end{aligned} \tag{1.68}$$

As we can see, at the beginning all particles have the same velocity without dispersion. But we can observe that after some time, a dispersion in the velocity appears. We can now check the following values:

$$\overline{v_x(t)} = \overline{x(t)\frac{t}{t^2+\tau^2}} = 0 \tag{1.69}$$

$$\overline{v_y(t)} = \overline{v_{y_0} + (y(t) - v_{y_0}t)\frac{t}{t^2+\tau^2}} = v_{y_0} \tag{1.70}$$

$$\overline{v_x^2(t)} = \overline{\left(x(t)\frac{t}{t^2+\tau^2}\right)^2} = \frac{a^2}{4}\frac{t^2+\tau^2}{\tau^2}\frac{t^2}{(t^2+\tau^2)^2} = \frac{a^2}{4}\frac{t^2}{\tau^2(t^2+\tau^2)} \tag{1.71}$$

$$\begin{aligned} \overline{v_y^2(t)} =& \overline{\left(v_{y_0} + \frac{y(0)}{\tau}\frac{t}{\sqrt{t^2+\tau^2}}\right)^2} = \\ v_{y_0}^2 + \overline{\frac{y^2(0)}{\tau}\frac{t^2}{t^2+\tau^2}} -& \overline{2v_{y_0}\frac{y(0)}{\tau}\frac{t}{\sqrt{t^2+\tau^2}}} = v_{y_0}^2 + \frac{a^2}{4}\frac{t^2}{\tau^2(t^2+\tau^2)} \end{aligned} \tag{1.72}$$

The dispersion for the velocity at the instant t

$$\Delta v_x(t) = \sqrt{\overline{v_x^2(t)} - \overline{v_x(t)}^2} = \frac{a}{2}\frac{t}{\tau\sqrt{(t^2+\tau^2)}} \tag{1.73}$$

which we can check that is equal for the three components, and it is null at the beginning but after some time it tends to:

$$\frac{a}{2\tau} = \frac{2a\hbar}{2ma^2} = \frac{\hbar}{ma} = \frac{\hbar}{2m\Delta x(0)} \tag{1.74}$$

again with the same value for the other two components.

This result was obtained on the previous section but with a very different interpretation. The initial velocity for the particles has no dispersion, but it appears after some time. That same dispersion is the same as the one from Heisenberg's uncertainty principle. We can see that by calculating what the dispersion of the momentum tends to after some time is:

$$\Delta p = m\Delta v \quad \Rightarrow \quad \Delta p_x \to \frac{\hbar}{2\Delta x(0)} \tag{1.75}$$

$$\Delta p_x \Delta x(0) \to \frac{\hbar}{2} \tag{1.76}$$

again equal for the other two components.

1.2.2. General equation of motion We have seen the equation of motion using Bohm's interpretation for a specific wave-function. Now we will see the general way to calculate it, meaning that this is applicable to any wave-function. We know how to work with a wave-function that has the structure of (1.28). Any wave-function can be expressed like that by taking into account that the phase can we calculated as:

$$\frac{1}{\hbar}S = \arctan\left(\frac{\mathrm{Im}\{\psi\}}{\mathrm{Re}\{\psi\}}\right) \tag{1.77}$$

so taking into account that:

$$\frac{d}{dx}\arctan(f(x)) = \frac{1}{1+f(x)^2}\frac{df(x)}{dx} \tag{1.78}$$

it is clear that:

$$\frac{1}{m}\frac{\partial S}{\partial x} = \frac{\hbar}{m}\frac{1}{1+\left(\frac{\mathrm{Im}\{\psi\}}{\mathrm{Re}\{\psi\}}\right)^2}\left(\frac{\frac{\partial \mathrm{Im}\{\psi\}}{\partial x}\mathrm{Re}\{\psi\} - \frac{\partial \mathrm{Re}\{\psi\}}{\partial x}\mathrm{Im}\{\psi\}}{(\mathrm{Re}\{\psi\})^2}\right) \tag{1.79}$$

so therefore:

$$v_x(t) = \frac{dx(t)}{dt} = \frac{1}{m}\frac{\partial S}{\partial x} = \frac{\hbar}{m}\frac{\frac{\partial \mathrm{Im}\{\psi\}}{\partial x}\mathrm{Re}\{\psi\} - \frac{\partial \mathrm{Re}\{\psi\}}{\partial x}\mathrm{Im}\{\psi\}}{(\mathrm{Re}\{\psi\})^2 + (\mathrm{Im}\{\psi\})^2} \tag{1.80}$$

and analogous expressions for the other directions.

1.3. Uncertainty principle

The uncertainty principle is one of the foundational concepts of quantum mechanics, highlighting the inherent limitations in simultaneously knowing certain pairs of measurable physical properties which are complementary to each other. In this section, we will explore the theoretical underpinnings of the uncertainty principle through the lens of both of the previous interpretations. By examining these perspectives, we aim to understand how each interpretation approaches the uncertainty inherent in quantum mechanics and the implications for our understanding of reality at the quantum level.

This principle, as commented before, affirms that we cannot simultaneously determinate certain pairs of physical measurements with arbitrarily high precision such as the position and the momentum of a particle [8]. In other words, the higher the certainty sought in determining a particle's position, the less is known about its linear momentum, and therefore about its velocity. This principle was formulated by the German theoretical physicist Werner Heisenberg in 1927. The measurements of the observable object will have a standard deviation, Δx, in position and Δp in momentum. They thus satisfy the uncertainty principle, mathematically expressed as [8]:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} \tag{1.81}$$

To get to this expression, we just need to know that $\Delta\Box = \sqrt{\langle\Box^2\rangle - \langle\Box\rangle^2}$, and that $\langle ...\rangle = \int \psi^* ... \psi$. From here we will take ψ as $Ae^{\frac{i}{\hbar}S}$ as we did before, and remember:

$$\begin{aligned} &\text{Copenhagen's interpretation: } p_x = -i\hbar\frac{\partial}{\partial x} \\ &\text{Bohm's interpretation: } p_x = \frac{v_x}{m} = \frac{\partial S}{\partial x} \end{aligned} \tag{1.82}$$

and the same for the other components. We will start solving for Bohm's interpretation. The general results are the same for all components so we will only work on the x component and denote p_x as p for simplification in this section. We then have:

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* p \psi dx = \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \frac{\partial S}{\partial x} A e^{\frac{i}{\hbar}S} dx = \int_{-\infty}^{\infty} \frac{\partial S}{\partial x} A^2 dx \tag{1.83}$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^* p^2 \psi dx = \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \left(\frac{\partial S}{\partial x}\right)^2 A e^{\frac{i}{\hbar}S} dx = \int_{-\infty}^{\infty} \left(\frac{\partial S}{\partial x}\right)^2 A^2 dx \tag{1.84}$$

Now let's calculate the same results on the other interpretation:

$$\begin{aligned}
\langle p \rangle &= \int_{-\infty}^{\infty} \psi^* p \psi dx = \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \left(-i\hbar \frac{\partial}{\partial x}\right) A e^{\frac{i}{\hbar}S} dx = \\
&= \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} (-i\hbar) \left[\frac{\partial A}{\partial x} e^{\frac{i}{\hbar}S} + \frac{i}{\hbar} A \frac{\partial S}{\partial x} e^{\frac{i}{\hbar}S}\right] dx = -i\hbar \int_{-\infty}^{\infty} A \frac{\partial A}{\partial x} dx + \int_{-\infty}^{\infty} \frac{\partial S}{\partial x} A^2 dx = \\
&= -i\hbar \int_{-\infty}^{\infty} \frac{1}{2} \frac{\partial A^2}{\partial x} dx + \int_{-\infty}^{\infty} \frac{\partial S}{\partial x} A^2 dx = \left.\frac{-i\hbar}{2} A^2\right|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial S}{\partial x} A^2 dx = \int_{-\infty}^{\infty} \frac{\partial S}{\partial x} A^2 dx
\end{aligned} \tag{1.85}$$

where we have used that A^2 evaluated in $\pm\infty$ is zero due to the fact that it is equal to the probability density and for it to be normalized it must be zero in both limits. We can see that this result is the same as the one from Bohm's interpretation. The other term:

$$\begin{aligned}
\langle p^2 \rangle &= \int_{-\infty}^{\infty} \psi^* p^2 \psi dx = \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \left(-i\hbar \frac{\partial}{\partial x}\right)^2 A e^{\frac{i}{\hbar}S} dx = \\
&= \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \left(-\hbar^2 \frac{\partial^2}{\partial x^2}\right) A e^{\frac{i}{\hbar}S} dx = \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \left(-\hbar^2 \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\right)\right) A e^{\frac{i}{\hbar}S} dx = \\
&= -\hbar^2 \int_{-\infty}^{\infty} A e^{-\frac{i}{\hbar}S} \left[\frac{\partial^2 A}{\partial x^2} e^{\frac{i}{\hbar}S} + 2\frac{i}{\hbar}\frac{\partial A}{\partial x}\frac{\partial S}{\partial x} e^{\frac{i}{\hbar}S} + \frac{i}{\hbar} A \frac{\partial^2 S}{\partial x^2} e^{\frac{i}{\hbar}S} - \frac{A}{\hbar^2}\left(\frac{\partial S}{\partial x}\right)^2 e^{\frac{i}{\hbar}S}\right] dx = \\
&= -\hbar^2 \int_{-\infty}^{\infty} A \frac{\partial^2 A}{\partial x^2} dx - 2i\hbar \int_{-\infty}^{\infty} A \frac{\partial A}{\partial x}\frac{\partial S}{\partial x} dx - i\hbar \int_{-\infty}^{\infty} A^2 \frac{\partial^2 S}{\partial x^2} dx + \int_{-\infty}^{\infty} A^2 \left(\frac{\partial S}{\partial x}\right)^2 dx = \\
&= -\hbar^2 \int_{-\infty}^{\infty} A \frac{\partial^2 A}{\partial x^2} dx - i\hbar \int_{-\infty}^{\infty} \frac{\partial}{\partial x}\left(A^2 \frac{\partial S}{\partial x}\right) dx + \int_{-\infty}^{\infty} A^2 \left(\frac{\partial S}{\partial x}\right)^2 dx = \\
&= -\hbar^2 \int_{-\infty}^{\infty} A \frac{\partial^2 A}{\partial x^2} dx - \left. i\hbar \frac{\partial S}{\partial x} A^2\right|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} A^2 \left(\frac{\partial S}{\partial x}\right)^2 dx = \\
&= -\hbar^2 \int_{-\infty}^{\infty} A \frac{\partial^2 A}{\partial x^2} dx + \int_{-\infty}^{\infty} \left(\frac{\partial S}{\partial x}\right)^2 A^2 dx
\end{aligned} \tag{1.86}$$

as we can see, we followed the same reasoning as before to explain that one term disappears. This value has one term that is the same as the one obtained with Bohm's interpretation. However, there is an additional term which gives us different dispersion values for each interpretation. This leads to the fact that the uncertainty principle is not faced the same by both perspectives, so which one is correct? Well that is a very good question, but it remains unsolved due to its complexity and difficulty to be proved. Nevertheless the results are not that different since after some time both terms are equal due to the fact that the different value tends to zero, what is interesting is that this differentiating term can be related to the quantum potential.

1.4. Temporal Inversion

Temporal inversion, also known as time reversal, is a fundamental symmetry in quantum physics. This concept involves reversing the direction of time in a physical system, effectively transforming the system's evolution as if time were running backward. Understanding temporal inversion provides crucial insights into the behavior and symmetries of quantum systems.

In classical physics, time reversal symmetry implies that the fundamental laws of motion remain invariant if the direction of time is reversed. However, in quantum mechanics, the situation is more nuanced. The wave function, which encapsulates all the information about a quantum system, transforms in a specific way under time reversal. This transformation often involves complex conjugation and a reversal of momenta.

In this section, we will explore the theoretical framework of temporal inversion in quantum mechanics. We begin by introducing the mathematical formalism of time reversal and its implications for the wave function. We then examine how temporal inversion is treated within Bohmian mechanics, highlighting the differences and similarities with the standard interpretation. Finally, we will discuss practical examples and applications of temporal inversion, providing a comprehensive understanding of its role in quantum physics.

By studying temporal inversion, we aim to deepen our comprehension of the symmetries governing quantum systems and to shed light on the fundamental nature of time in the quantum realm.

1.4.1. Time reversal operator One might assume that time reversal is closely analogous to space inversion, where the operation $t \to -t$ would replace $x \to -x$. However, this simple analogy proves to be misleading in almost every respect [9].

Firstly, the term itself misleading. The operation discussed in this section would be more accurately described as motion reversal. Despite this, we will continue to use the traditional but less precise term "time reversal" due to its widespread use. The effect of the time reversal operator $\hat{T}$ is to reverse both linear and angular momentum while leaving the position unchanged [9]. Therefore by this definition:

$$\begin{aligned} \hat{X} \to \hat{X} \quad &\Rightarrow \quad \hat{T}\hat{X}\hat{T}^{-1} = \hat{X} \\ \hat{P} \to -\hat{P} \quad &\Rightarrow \quad \hat{T}\hat{P}\hat{T}^{-1} = -\hat{P} \\ \hat{J} \to -\hat{J} \quad &\Rightarrow \quad \hat{T}\hat{J}\hat{T}^{-1} = -\hat{J} \end{aligned} \tag{1.87}$$

To satisfy these conditions, we just rely on the general and plausible assumptions that space is homogeneous and isotropic under time reversal.

With these relations let's now see what happens with the commutator position-momentum:

$$\begin{gathered} \left[\hat{X}, \hat{P}\right] = \hat{X}\hat{P} - \hat{P}\hat{X} = i\hbar \\ \downarrow \\ \hat{T}\left[\hat{X}, \hat{P}\right]\hat{T}^{-1} = \hat{T}\hat{X}\hat{T}^{-1}\hat{T}\hat{P}\hat{T}^{-1} - \hat{T}\hat{P}\hat{T}^{-1}\hat{T}\hat{X}\hat{T}^{-1} = \hat{T}i\hbar\hat{T}^{-1} \\ \downarrow \\ \hat{X}(-\hat{P}) - (-\hat{P})\hat{X} = \hat{P}\hat{X} - \hat{X}\hat{P} = -i\hbar = \hat{T}i\hbar\hat{T}^{-1} \end{gathered} \tag{1.88}$$

where we have taken into account $\hat{T^{-1}}\hat{T} = \hat{I}$. For this to be true it is logical that $\hat{T}i\hbar\hat{T}^{-1}$ must be $-i$. Operators that act like this on complex numbers are called *anti-linear* operators [9].

Time Reversal of Schrodinger's equation

One might assume that the effect of a time reversal operation over the evolution equation for a particle (1.2) is to change t for $-t$. However, as mentioned before, we must tread carefully when it comes to apply this operator and the considerations it carries. Since t is merely a parameter, it cannot be directly affected by an operator. Therefore, the connection between the action of $\hat{T}$ and the parameter t can only be indirect. The time reversal transformation of (1.2):

$$\left.\begin{aligned}\hat{T}i\hbar\frac{d\left|\psi(t)\right\rangle}{dt} &= -i\hbar\frac{d}{dt}\hat{T}\left|\psi(t)\right\rangle \\ \hat{T}\hat{H}\left|\psi(t)\right\rangle &= \hat{T}\hat{H}\hat{T^{-1}}\hat{T}\left|\psi(t)\right\rangle\end{aligned}\right\} \quad -i\hbar\frac{d}{dt}\hat{T}\left|\psi(t)\right\rangle = \hat{H}\hat{T}\left|\psi(t)\right\rangle \tag{1.89}$$

where we wrote now the time dependency to see how the operator works and we supposed that the time reversal operator is time independent and $\hat{H}$ was time reversal invariant ($\hat{T}\hat{H}\hat{T^{-1}} = \hat{H}$) [9]. If we replace t (which is a dummy variable) by $-t$:

$$\left|\psi(t)\right\rangle \rightarrow \left|\psi(-t)\right\rangle : \quad \frac{d}{dt}\left|\psi(-t)\right\rangle = -\frac{d}{dt}\left|\psi(t)\right\rangle \tag{1.90}$$

we will get that if we use this change in (1.89), then $\left|\psi_r\right\rangle = \hat{T}\left|\psi(-t)\right\rangle$ is also a solution for (1.2):

$$\left.\begin{aligned}-i\hbar\frac{d}{dt}\hat{T}\left|\psi(t)\right\rangle \rightarrow & i\hbar\frac{d}{dt}\hat{T}\left|\psi(-t)\right\rangle = i\hbar\frac{d\left|\psi_r\right\rangle}{dt} \\ \hat{H}\hat{T}\left|\psi(t)\right\rangle \rightarrow & \hat{H}\hat{T}\left|\psi(-t)\right\rangle = \hat{H}\left|\psi_r\right\rangle\end{aligned}\right\} \quad i\hbar\frac{d\left|\psi_r\right\rangle}{dt} = \hat{H}\left|\psi_r\right\rangle \tag{1.91}$$

While the invariance of $\hat{H}$ under a linear transformation leads to a conserved quantity (such as the parity eigenvalue in the case of space inversion), no equivalent conserved quantity exists for the anti-linear time reversal transformation [9]. Instead, the solutions of the Schrodinger equation appear in pairs: $\left|\psi(t)\right\rangle$ and $\hat{T}\left|\psi(-t)\right\rangle$.

As we can also see, when we applied the time reversal operator over our equation we only changed i for $-i$ (it's complex conjugate) and applied it to the wave-function too, reinforcing the idea that our operator over the equation doesn't "invert time" but rather inverts the motion of the particle as said before since it changes the sign of the equation and the wave-function that contains how our particle is moving.

We have learnt about the operator and how it acts on Schrodinger's equation but we don't yet know the explicit form of our operator. We know that the time reversal operator implies a complex conjugation so let's see what happens when we make the complex conjugate of (1.2):

$$-i\hbar\frac{d\left|\psi(t)^*\right\rangle}{dt} = \hat{H}^*\left|\psi(t)^*\right\rangle \tag{1.92}$$

As we can see, this equation and (1.89) (again we are taking that $\hat{H}$ is time invariant) are very similar assuming that $\hat{H}$, is an hermitian operator ($\hat{H} = \hat{H}^\dagger \Rightarrow \hat{H} = \hat{H}^*$), which for a free particle checks. This means that we can associate the time reversal operator with the complex conjugation operator in this representation: .

$$\hat{T}\psi(t) = \psi^*(t) \tag{1.93}$$

In the position representation, the effect of the position operator is simply to multiply by x, so we can see that (1.93) satisfies equations (1.87). The momentum operator, which has the form $-i\hbar\nabla$, has its sign reversed by complex conjugation, thereby satisfying again equations (1.87). It is also evident that (1.87) holds for the orbital angular momentum operator, $\hat{L} = \hat{x} \times (-i\hbar\nabla)$. Therefore, equation (1.93) is valid in the position representation for spinless particles.

Time reversal and spin

In one of the previous sections the importance of spin to define a particle was discussed, highlighting the relevance of that property to fully describe it while explaining that it does not affect the motion of the particles we are characterising and therefore we could get rid of it to detail their dynamics.

However, it is worth mentioning how spin is affected by time reversal since it will not be unaffected by it and this is the purpose of this section. Spin is an angular momentum [12] and following the definitions from (1.87):

$$\hat{T}\hat{S}\hat{T}^{-1} = -\hat{S} \tag{1.94}$$

Let's work on the representation where the s_z operator (the z component operator of the spin) is diagonal and we will be describing particles with spin 1/2. All the operators for the components of spin in this representation can be expressed as matrices related to Pauli's matrices:

$$\hat{s}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\hat{\sigma}_x \qquad hats_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\hat{\sigma}_y \qquad hats_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\hat{\sigma}_z \tag{1.95}$$

where the $\hat{\sigma}$ are the Pauli's matrices. From this representation we can clearly see that applying the time reversal operator on each component as we have defined it before:

$$\hat{T}\hat{s}_x\hat{T}^{-1} = \hat{s}_x \qquad \hat{T}\hat{s}_y\hat{T}^{-1} = -\hat{s}_y \qquad \hat{T}\hat{s}_z\hat{T}^{-1} = \hat{s}_z \tag{1.96}$$

which as we can observe is not completely correct since only the y component behaves following the (1.87) relations. This is because the previous definition of the time reversal operator is only valid while not describing spin. When we want to include it in our description of the time reversal operator we have to complete our definition of the operator.

We will now call the previous definition of the time reversal operator as $\hat{K}_0$ and the complete time reversal operator $\hat{T} = \hat{Y}\hat{K}_0$, where $\hat{Y}$ is a new operator. The conditions it must fulfill is that it mustn't affect the position, the momentum or the orbital angular momentum since they already follow the (1.87) conditions with the effect of $\hat{K}_0$ [12]. Therefore $\hat{Y}$ must only act on the spin operators, and not in any way since it must only invert the x and z components as $\hat{s}_y$ did follow the previous conditions too with the effect of $\hat{K}_0$. We then have:

$$\hat{Y}\hat{s}_x\hat{Y}^{-1} = -\hat{s}_x \qquad \hat{Y}\hat{s}_y\hat{Y}^{-1} = \hat{s}_y \qquad \hat{Y}\hat{s}_z\hat{Y}^{-1} = -\hat{s}_z \tag{1.97}$$

which we can interpret as a rotation of π radians around the y direction on the spin space [12].

We can conclude then that $\hat{Y} = e^{-i\pi s_y/\hbar}$, and therefore the time reversal operator consists of a complex conjugation and a rotation of the spin around the y axis being its form $\hat{T} = e^{-i\pi s_y/\hbar}\hat{K}_0$ with $\hat{K}_0$ the complex conjugation operator.

CHAPTER 2

Objectives

The primary objectives of this work are as follows:

1. **Investigate Temporal Inversion in Quantum Mechanics**:
   - Analyze the phenomenon of temporal inversion of the wavefunction of a particle within the framework of quantum mechanics.
   - Understand the implications of temporal inversion on the behavior and properties of quantum systems.
2. **Use Bohmian Interpretation**:
   - Apply the Bohmian interpretation of quantum mechanics to the study of temporal inversion.
   - Explore how Bohm's interpretation, with its deterministic particle trajectories, provides insights into the time-reversal process.
3. **Develop Simulation Program**:
   - Create a program to simulate the movement of a Gaussian wave packet.
   - Simulate a group of particles distributed in a Gaussian manner to observe the equivalence with Bohm's interpretation.
   - Incorporate a temporal inversion in the simulation to study its effects.
4. **Compare Interpretations**:
   - Compare the results obtained from the standard quantum interpretation and the Bohmian interpretation during the simulation.
   - Evaluate the equivalence and differences between these interpretations, particularly in the context of temporal inversion.
5. **Perform Numerical Analysis**:
   - Conduct numerical simulations to visualize the evolution of the wavefunction and particle trajectories under time-reversal.

- Analyze specific examples to demonstrate the practical implications of temporal inversion.
- Highlight how the integration of Bohm's interpretation with temporal inversion analysis can open new avenues for exploring quantum phenomena.

By achieving these objectives, this work aims to provide a comprehensive understanding of temporal inversion in quantum mechanics and demonstrate the value of the Bohmian interpretation in studying this fundamental symmetry.

CHAPTER 3

Development

In this development section, we aim to explore the evolution of a free particle using two fundamental interpretations of quantum mechanics: the Copenhagen interpretation and Bohm's interpretation. Our objective is to simulate the behavior of a free particle under both interpretations, analyze the results from previous sections, and compare the outcomes to gain a deeper understanding of quantum dynamics.

First, we need to solve the time-dependent Schrödinger equation to obtain the wave-function evolution over time for the Copenhagen interpretation (1.1). The Schrödinger equation is central to quantum mechanics, describing how the quantum state of a physical system changes over time. To solve this equation numerically in Matlab, we will discretize the spatial domain, define the initial wave-function $\psi(x, 0)$ (typically as a Gaussian wave-packet centered at some position with a certain momentum), and use numerical methods such as the Crank-Nicholson method, known for its stability and accuracy, to evolve the wave-function over time. By solving this equation, we will obtain the wave-function $\psi(x, t)$ at each time step, representing the probability amplitude of finding the particle at position x at time t.

Next, we will use the wave-function obtained from the Schrödinger equation to calculate the particle trajectories in Bohm's interpretation. In Bohm's interpretation, the particle's motion is guided by the wave-function through the quantum potential, and the trajectory of a particle is determined by the guidance equation (1.36). To compute these trajectories, we will numerically integrate the equation to find the particle's position at each time step. This will provide us with the deterministic paths that particles follow according to Bohm's interpretation. To observe the similarities of this interpretation and the previous one, we will generate several particles that will follow a Gaussian distribution to see if the Gaussian packet follows the same trend as the Gaussian wave-function

Visualization is key to understanding and comparing the results from both interpretations. For this purpose, we will generate plots of the wave-function over time to show how the probability distribution evolves and overlay the particle trajectories on the wave-function plots to illustrate how particles move according to Bohm's interpretation. These visualizations will help in comparing the probabilistic nature of the Copenhagen interpretation with the deterministic trajectories of Bohm's interpretation.

Additionally, we will introduce a temporal inversion to both evolutions to study the symmetry of quantum systems with respect to time. Temporal inversion, or time-reversal, involves reversing the motion in the simulation. To implement temporal inversion, we

will modify the time evolution algorithm to simulate that temporal inversion, solve the "inverted" Schrödinger equation to see how the wave-function evolves for the Copenhagen interpretation, and recalculate the particle trajectories using the time-reversed wave-function for Bohm's interpretation. By simulating temporal inversion, we can examine if the quantum dynamics remain consistent when time is reversed and analyze any deviations or asymmetries.

The development section will involve a detailed simulation process that includes solving the Schrödinger equation, computing particle trajectories, and visualizing the results. By comparing the Copenhagen and Bohm's interpretations, and introducing temporal inversion, we aim to gain deeper insights into the nature of quantum mechanics and the behavior of free particles. This comprehensive approach will allow us to explore the fundamental principles and differences between these interpretations, ultimately contributing to our understanding of quantum dynamics.

3.1. Numerical resolution of Schrodinger's equation

The equation we need to solve to model our free particle is (1.1). This equation resembles to a heat diffusion equation which is a parabolic partial differential equation. These kind of equations have the following shape:

$$u_t = \alpha \nabla^2 u \tag{3.1}$$

from which we can realize that $\alpha = i\hbar/2m$ and we need initial and boundary conditions.

To solve a problem like this numerically, the first step is to discretize the domain $\Omega(\vec{r}, t)$. This means converting the problem from one with an infinite dimension degrees of freedom at every point in $\Omega(\vec{r}, t)$ to one with a finite number of points in the domain which will simplify our problem and will let us to take some approximations as we will now see in one of the most used methods for this.

3.1.1. Finite differences The simplest way to discretize a partial differential equation's problem is to reduce the spatial domain to a finite number of equally spaced points located at the nodes of a uniform rectangular grid [13] (and take regular intervals of time to solve its value at each point if there are time partial derivatives). The partial derivatives of the solution function, u, are obtained using difference quotients, which gives this discretization method its name. We will use $u_{i,j}$ to denote the value of the unknown function at the node (x_i, y_j) (where i and j refer to the ith and jth point in the grid for each axis). Let h be the step size in x and g the step size in y, then:

$$x_{i+1} = x_i + h \qquad and \qquad y_{i+1} = y_i + g \tag{3.2}$$

The partial derivatives of u (for time and space) can be approximated at each node in different ways and to different orders depending on the method used. Finite differences numerical methods are of two types: explicit and implicit. In the former, the unknown variables are calculated successively in terms of known values or previously computed variables. In implicit methods, a system of equations must be solved at each step to determine the unknowns.

Crank-Nicholson method

This method of finite differences is obtained when we discretize (3.2) between two consecutive instants and we take the mean value, it is a mixture of the completely explicit and implicit methods. It presents a great improvement with respect those methods since it gives really good approximations (it is a method of second order on time and space, which means that the error on the approximation decreases quadratically when we decrease the step for both variables) and it is unconditionally stable, which means that the method to be stable independently of the step taken [13].

As our differential equation doesn't have crossed partials and we know that our solution and initial condition can be expressed as a multiplication of functions for each direction separately, we can solve the problem individually for each direction and then multiply them all (each term of the solution for a direction by its corresponding term of the solution for the other direction) for the total solution or just analyse each direction individually. For that we will explain the procedure only using the x direction as all directions are solved the same just by changing and using the corresponding initial condition for that direction. We will take as the step of time k.

The procedure is the following, first we approximate u_t at the instant t_{j-1} and t_j and for $\nabla^2 u$ we approximate with a fraction of progressive difference (using t_j terms for the spatial approximation) and a fraction of regressive difference (using t_{j-1} terms for the spatial approximation) [13]. The formula is (taking both fractions as $1/2$ so that we are using the mean value of the progressive and regressive difference):

$$\frac{u_{i,j} - u_{i,j-1}}{k} = \alpha \left\{ \frac{1}{2} \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{1}{2} \frac{u_{i+1,j-1} - 2u_{i,j-1} + u_{i-1,j-1}}{h^2} \right\} \tag{3.3}$$

This formula comes from the approximations:

$$\frac{\partial f}{\partial \beta} \approx \frac{f(p + \Delta\beta) - f(p)}{\Delta\beta} \tag{3.4}$$

$$\frac{\partial f}{\partial \beta} \approx \frac{f(\beta) - f(\beta - \Delta\beta)}{\Delta\beta} \tag{3.5}$$

where f is a function, p the point where we are approximating and β the parameter with respect we are deriving. Both approximations are constructed by similar ideas and they are only true when $\Delta\beta \to 0$.

For the temporal part since we only have a first order derivative we can choose any of those since it will only change the numeration on j, in this case we used:

$$\frac{\partial u(x_i, t_j)}{\partial t} \approx \frac{u(x_i, t_{j-1} + \Delta t) - u(x_i, t_{j-1})}{\Delta t} = \frac{u(x_i, t_j) - u(x_i, t_{j-1})}{k} \tag{3.6}$$

On the other hand, for the spatial part, as there appears second order derivatives and we will construct them from first order derivatives we will make a mix of both approximations. This is to make our second order derivative "centered on the point" and with a better result since we are mixing the values of before and after the point instead of only one of those two:

$$\frac{\partial^2 u(x_i, t_j)}{\partial x^2} \approx \frac{\frac{\partial u(x_i + \Delta x, t_j)}{\partial x} - \frac{\partial u(x_i, t_j)}{\partial x}}{\Delta x} \approx \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} \tag{3.7}$$

As we can see, we constructed the approximation for the second order derivative using first order derivatives with the structure of (3.4) but then for the values of each derivative we used the formula from (3.5)

If we clear away the j terms from (3.3) we get the Crank-Nicholson formula.

$$2(1+\omega)u_{i,j} - \omega(u_{i+1,j} + u_{i-1,j}) = 2(1-\omega)u_{i,j} - \omega(u_{i+1,j-1} + u_{i-1,j-1}) \tag{3.8}$$

where $\omega = \frac{k\alpha}{h^2}$. For each fixed value for j we can transform into a matrix times a vector equation whose independent terms are obtained through the solution at the instant t_{j-1}. This matrix can we written as:

$$\mathcal{A}u_j = \mathcal{B}u_{j-1} \tag{3.9}$$

where u is a solution column vector for the time of the sub-index and $\mathcal{A}$ and $\mathcal{B}$ are tridiagonal matrices that contain the parameters with which each vector must be multiplied by in order to get equation (3.8). This last equation can also be written as:

$$\mathcal{A}u_j = b \tag{3.10}$$

since we knew the values of the second term. This equation is a linear equation system written as a matrix ($\mathcal{A}x = b$). These kind of linear systems can be easily and quickly solved by different methods. For example, if it wasn't a very large system thanks to Matlab we could just do it in a line of code by using:

$$\mathcal{A}^{-1}\mathcal{A}u_j = \mathcal{A}^{-1}b \quad \Rightarrow \quad u_j = \mathcal{A}^{-1}b \tag{3.11}$$

with u_j the vector solution for the time t_j and $\mathcal{A}^{-1}$ the inverse of the $\mathcal{A}$ matrix. We can do this since Matlab is a language specially designed for mathematics and sciences applications but if we were using another language or if the systems were very large (the computing time would become excessive in this case) we would need another method such as the so known Gauss method for linear systems or others such as the "LU" factorization or the Cholesky method [13].

The initial condition in the points of the mesh will let us build the b vector in $t_{j-1} = t_0$ for the first iteration of the method that will let us find our first solution for $t_j = t_1$. This solution will become our t_{j-1} in the next iteration that will let us calculate the new $t_j = t_2$ term and so on. Our initial condition is the corresponding part for our direction of the initial Gaussian wave-packet (1.5) since we will be simulating the results obtained in the theoretical framework of the previous charapters

The boundary conditions are inside the b vector too, more precisely on the first and last position of the vector since they are referring to the first and last points in our mesh since those are our borders. They will be renewed each iteration to the value that the border must have and that way we are imposing that value on the limits. Our boundary conditions will be 0 for forth borders since there is no drain or source for our wave-function.

Equation (3.8) can also be solved by regrouping terms, imposing the initial and border conditions and resolving each equation and unknown value individually by looping through the solution vector up and down instead of as matrices but the process is more extensive to solve and to explain so it will only be mentioned in this work.

Now that we know how to solve the problem we have to take into account that our function is a complex function. This is very important when it comes to solve the equation for each iteration since not all programming languages can work with complex numbers. In those where it is not possible we will have to divide our function into two different function into $u = u_r + iu_i$ which correspond to the real and imaginary part of the function and we will solve each one separately in each iteration. This was not our case since we will use Matlab and it is prepared to work with complex numbers.

3.2. Absorbing Boundary Conditions

To accurately simulate the behavior of a free particle, it is crucial to implement conditions that allow for the exchange of information at the boundaries of the computational domain. Without such conditions, the wavefunction of the particle would begin to reflect off the domain boundaries, resulting in unphysical behaviors and distorting the simulation. These artificial reflections can introduce errors and make it difficult to analyze the true dynamics of the particle. To address this, we employ Absorbing Boundary Conditions (ABC), which effectively prevent such reflections and ensure the simulation remains consistent with the expected behavior of a free particle in an infinite domain.

Absorbing Boundary Conditions (ABC) are numerical techniques designed to minimize or eliminate unwanted reflections at the artificial boundaries of a computational domain [14]. These non-physical reflections occur when modeling wave propagation phenomena in a finite domain that does not represent an infinite space. Also known as non-reflecting or radiating boundary conditions, ABCs allow for the simulation of open or radiating conditions at the domain's boundaries.

The primary purpose of ABCs is to prevent waves incident at the domain boundaries from reflecting back into the system, as these reflections can distort simulation results. This is particularly important in wave propagation problems, such as acoustic, elastic, or electromagnetic waves, where accurate modeling of infinite space is required. ABCs achieve this by applying techniques such as one-way wave equations, damping regions, or Perfectly Matched Layers (PML) [15].

Implementing ABCs numerically requires careful discretization to ensure both numerical stability and accuracy. Techniques like finite difference schemes are commonly used to approximate partial derivatives in wave equations, but special care is needed near the boundaries to make the absorbing conditions effective.

An approach involves introducing a *damping region* near the domain's boundaries. In this region, waves are gradually attenuated as they approach the edges, reducing reflections [16]. Although effective, this method increases computational cost significantly [16], especially in three-dimensional simulations, as the domain must be expanded to accommodate the damping region.

For our simulation, we will employ damping regions to simulate free exchange at the boundaries, ensuring that the wavefunction evolves as expected for a free particle. In our case, this approach yields excellent results and is computationally feasible since we are not simulating an overly complex or large system. The implementation involves multiplying the wavefunction by a damping function that equals 1 inside the domain and smoothly decreases to 0 near the boundaries. This decrease is achieved using the function $1 - e^{-(x/2a)^2}$, which transitions to 0 at the edges with appropriately chosen parameters for the simulation. Notably, this damping function is 1 minus a Gaussian, matching the shape of the wavefunction we are simulating. This similarity ensures effective attenuation at the boundaries, and selecting a damping Gaussian width several times larger than the original wavefunction's width provides very accurate results.

Absorbing boundary conditions are essential for simulating finite domains that accurately mimic infinite spaces. Techniques such as one-way wave equations, damping regions, and PMLs effectively reduce non-physical reflections at the boundaries, ensuring precise results. However, careful implementation is required to avoid numerical instability and computational overhead, particularly in 3D models. ABCs are a fundamental tool for simulating wave propagation in fields like acoustics, electromagnetism, ...

3.3. Units

In order to solve our equation we need some initial conditions and information about the wave-function. Besides we can extract information and properties of the solution at each point where it is solved. All these initial values and information at each point are measures which have units so in order to analyse the results we need first to specify which units we are using.

Plus, depending on the units used the behaviour of our function can change (for example changing the units of the velocity will make our wave-function propagate faster or slower). Hence, we must define the system of units that we will be using. For our system of units, we will take as basic units length, mass and the reduced Plank's constant, $\hbar$.

We will take the Armstrong ($\mathring{A}$) as our basic unit to measure length. Therefore, when we use or take information about a measure with units of length, we will have to multiply the value times 10^{-10} to work with the international system's units. For example for our problem we will take that the initial amplitude of the wave-packet in our program is 1. This means that the initial dispersion is of $10^{-10}m = 1\mathring{A}$.

For our simulation we will for example use electrons as our particles. For this reason we will take the mass of the electron as our basic mass unit ($m_e = 9.1 \cdot 10^{-31}kg$). This way wherever we have a mass unit it will be 1 ($1\ m_e$) in our program.

The unit for Plank's constant is Plank's constant itself, meaning that $\hbar = 1$ ($1\ \hbar$) in our program. This means that whenever we have a value that involves this unit we have to remember that $1\ \hbar = 1.05 \cdot 10^{-34}kg\, m^2/s$. As mass, length and time appear in the units of $\hbar$ and we have the values for all of them but time for the program, we can get it from the ones we got:

$$[\hbar] = ML^2T^{-1} \quad \Rightarrow \quad T = ML^2[\hbar]^{-1} \quad \Rightarrow \quad a.u.t. = \frac{9.1 \cdot 10^{-31}kg \times (10^{-10}m)^2}{1.05 \cdot 10^{-34}kg\, m^2/s} \tag{3.12}$$

We get that the unit of time in our program is $a.u.t. = 8.6667 \cdot 10^{-17}s$.

For this program we also need the velocity of the wave-packet. In order to get this value, we know that the velocity is related to the energy. In our case since it is a free particle $p_0 = \sqrt{2mE}$. Now we will use that the energy is of $10\, eV$ so let's see what will be the units in our program. The units of energy are:

$$[E] = ML^2T^{-2} \quad \Rightarrow \quad a.u.e. = \frac{9.1 \cdot 10^{-31}kg \times (10^{-10}m)^2}{(8.6667 \cdot 10^{-17}s)^2} \tag{3.13}$$

So $a.u.e. = 1.2115 \cdot 10^{-18}J$. As we have the energy in eV we need to make a conversion:

$$Energy(eV) \times \frac{1.6 \cdot 10^{-19}J}{1\ eV} \times \frac{1\ a.u._e}{1.2115 \cdot 10^{-18}J} = Energy(eV) \times 0.13207 \left(\frac{a.u.e.}{eV}\right) \tag{3.14}$$

and therefore:

$$p_{y_0} = \sqrt{2mE} = \sqrt{2 \times 1 \times Energy \times 0.13207} = 0.3634\sqrt{2}\sqrt{Energy} = 5.14\frac{m_e\mathring{A}}{a.u.t.} \tag{3.15}$$

As $k_{y_0} = p_{y_0}/\hbar$ and in our system $\hbar = 1$ we can say that $k_{y_0} = 5.14\mathring{A}^{-1}$.

3.4. Simulation of particles following Bohm's interpretaton

In this section, we aim to simulate particles in the framework of Bohm's interpretation of quantum mechanics and demonstrate the equivalence in the dynamics of these particles with the predictions of the Copenhagen interpretation.

To illustrate this equivalence, we will focus on the evolution of a Gaussian wave-packet, a common and illustrative example in quantum mechanics. A Gaussian wave-packet represents a particle with a Gaussian distribution of positions and momenta. In the Copenhagen interpretation, the wave-packet evolves according to the Schrödinger equation, spreading over time due to the uncertainty principle.

By simulating a large number of particles with a Gaussian distribution and their trajectories, we aim to show that the collective behavior of these particles under Bohm's interpretation reproduces the statistical predictions of the Copenhagen interpretation. Specifically, the Gaussian wave and particle packet will be seen to evolve in a similar manner although each one follows a different interpretation, thus highlighting the equivalence of the two approaches in describing quantum dynamics.

The motion equations for the particles, obtained in a previous section, will be central to our simulation. These equations are derived from the guidance equation in Bohm's theory, which relates the velocity of a particle to the gradient of the phase of the wave-function. For a Gaussian wave-packet, this results in trajectories that mirror the spread and evolution of the wave-packet itself.

Through this simulation, we will gain deeper insights into the relationship between the deterministic trajectories in Bohm's interpretation and the probabilistic evolution of the wave-function in the Copenhagen interpretation. This exercise not only reinforces the conceptual understanding of both interpretations but also demonstrates the practical equivalence in predicting quantum phenomena.

First we will need to create the position for the particles we want to simulate. In order to do that we will introduce a theorem.

3.4.1. Central limit theorem

The Central Limit Theorem (CLT) is a fundamental principle in the field of probability and statistics. It provides a crucial bridge between the behavior of individual random variables and the properties of their collective sum or average, thereby explaining why the Gaussian distribution (also known as the normal distribution) is so prevalent in natural phenomena and various fields of study.

At its core, the Central Limit Theorem states that, given a sufficiently large sample size, the distribution of the sum (or average) of a large number of independent and identically distributed random variables, each with a finite mean and variance, will approximate a normal or Gaussian distribution, regardless of the original distribution of the variables [17]. This remarkable result holds true even if the underlying variables are not normally distributed themselves.

The CLT takes a crucial part in our simulation since it states that we are able to reproduce a Gaussian distribution even if we don't have a command to specifically create it [18]. For example in our program we will use equally distributed aleatory numbers between 0 and 1 (which almost all programming languages have an easy way to give those aleatory numbers) although another aleatory distribution gives the same result. In the specific case of Matlab, it already has an aleatory Gaussian distribution number generator,

but it is far more interesting and worth learning about this theorem and how to apply it as well as making it possible to adapt it to any programming language.

With this theorem we will be able to generate the position of any wanted number of particles following a Gaussian distribution. The procedure is the following:

- First we define the number of particles we want to simulate and we create an empty position vector with the same dimension number as the number of particles.
- Then we fill each component of the vector with an aleatory equally distributed number between 0 and 1 and we repeat this part a large number of times.
- When we had the first aleatory number we had a number between 0 and 1, and they were all equally probable. When added the first new aleatory number the possibilities were between 0 and 2 and the numbers around the middle (which is 1) were more probable. Therefore when we make m iterations the numbers in the middle will be more probable than those of the edges and they will have a similar distribution to a Gaussian centered in $m/2$, so to center it in 0 we will have to subtract $m/2$ to the vector.
- It can be proven that the standart deviation of the numbers we generated is $\sigma = \sqrt{m/12}$. Therefore, to make our width equal to 1 in our distribution we will have to multiply our vector by $1/\sigma$

Now that we have the position of the wanted number of particles (the more the better to get a best adjusted Gaussian distribution as seen), there is something important to comment before representing them. If we represent them at the same height in a graph it would be difficult to observe clearly their evolution and to appreciate their distribution (if we wanted to check if they were generating properly), and so it would be a good idea to represent them at different altitudes. Particles were given a random height between a range in the created program to avoid that.

3.4.2. Motion equation Now that we have determined the positions of the particles, we can evaluate how they move by referring to the equations outlined in the introduction section. There were two approaches to describe the particle dynamics: a specific result for our case (1.68) and the general method (1.80). For flexibility and broader application, we will utilize the latter. This allows us to use the program with different distributions, even though we are currently working with a Gaussian distribution.

To proceed, we need the results obtained from evolving the Schrödinger equation and the initial positions of the particles. Both of these have been addressed in previous sections. It is important to note that the solution of the Schrödinger equation was computed at specific, equally distributed points in space. However, the randomly generated particle positions are unlikely to match these points exactly. Therefore, we will employ an interpolation method to estimate the values at the particle positions based on the two nearest points from the Schrödinger solution.

This interpolation ensures that the evaluation of particle movement is accurate and consistent with the evolved wave-function. By doing so, we can effectively track the dynamics of our particle ensemble and verify the equivalence of Bohm's interpretation with the Copenhagen interpretation in describing the evolution of a Gaussian wave-packet. The procedure to obtain the interpolated value between two points is the following, if we are doing a linear interpolation, the general formula for a line:

$$f(x) = mx + n \quad \Rightarrow \quad f(x) - f(x_i) = m(x - x_i) \tag{3.16}$$

where x is the point where we are doing the interpolation, $f(x)$ the interpolated value, m the slope, n the value at $x = 0$, x_i the first point of the interpolation and $f(x_i)$ its value. To calculate the slope:

$$f(x_i) = mx_i + n \ , \quad f(x_{i+1}) = mx_{i+1} + n \quad \Rightarrow \quad m = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \tag{3.17}$$

where now the $i + 1$ sub-index refers to the second point of the interpolation. The interpolated value then is:

$$f(x_p) = f(x_i) + \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}(x_p - x_i) \quad \Rightarrow \quad \psi_p = \psi_i + \frac{\psi_{i+1} - \psi_i}{h}(x_p - x_i) \tag{3.18}$$

with h the spatial step from the previous section and x_p the position obtained with the CLT for the particle. We will choose x_i and x_{i+1} so that x_p is between them to get a good estimation of $f(x_p)$.

Once we have this we can apply (1.80) to calculate the velocity value of a particle at the wanted point. As we do not now the values of the partials we can do a similar procedure as we did when we wanted to approximate the value of the partials for the Crank-Nicholson method. We will proceed in the following way, the parts of the wave-function that are not affected by a partial will be the interpolated values we have calculated. The partials will be approximated as:

$$\left.\frac{\partial \psi}{\partial x}\right|_{x=x_p} \approx \frac{\psi_{i+1} - \psi_i}{x_{i+1} - x_i} = \frac{\psi_{i+1} - \psi_i}{h} = m \tag{3.19}$$

as we can see we are approximating the partial at x_p as the increment on the value of the wave-function divided by the step in space with the values of the two closest results of the wave-function to the point where we are calculating the partial (taking into account that the point is between those values as we did for the interpolation to get a good estimation). Our approximation of partial gives us the slope, which makes sense since for a line its partial is that value and we are using a linear interpolation.

If we substitute these values and the values of the mass and $\hbar$ in our program our velocity ends up being:

$$v_p = \frac{\mathrm{Im}\{m\}\mathrm{Re}\{\psi_p\} - \mathrm{Re}\{m\}\mathrm{Im}\{\psi_p\}}{(\mathrm{Re}\{\psi_p\})^2 + (\mathrm{Im}\{\psi_p\})^2} \tag{3.20}$$

it is important to note that for each particle the points that we use for the estimations are different and so the value of m is not the same between particles.

Before we move on we must not forget that the wave-function evolves through time and therefore the values we have are for a certain equally distributed times. Taking that into account, the value of the velocity obtained from the previously mentioned equation is calculated with the values of the wave-function at a specific time t_j and so, the velocity for the particle is for that designed time, as well as the wave-functions from before (for example ψ_i is actually $\psi_{i,j}$).

Now that we have the velocity of the particle at a specific moment t_j and point x_p we can see how the particle will evolve. For that we have to know that:

$$v = \frac{dx}{dt} \quad \Rightarrow \quad vdt = dx \tag{3.21}$$

If we want to know the new position x'_p that the particle will have past a time equal to the step of time used for the solutions of the wave-function (k), we will have to resolute:

$$\int_{x_p}^{x'_p} dx = \int_{t_j}^{t_{j+1}} vdt \quad \Rightarrow \quad x'_p - x_p = v(t_{j+1} - t_j) \tag{3.22}$$

getting therefore the new position for our particle as:

$$x'_p = x_p + vk \tag{3.23}$$

All the velocities and new positions are obtained in the same way for all the particles and for all the instants of time, so to watch our particles evolve we just have to solve these equations for each iteration of time.

3.5. Temporal Inversion

In two of the previous sections of this chapter, we outlined the process of solving and simulating both the solution to the Schrödinger equation, the wave-function —and specifically the probability density which is used within the framework of the Copenhagen interpretation— and the motion and dispersion of particles according to Bohm's interpretation. In this new section, we will introduce time-reversal in both descriptions. We chose not to include this in the respective earlier sections because the procedure is identical for both interpretations and relatively straightforward.

If we recapitulate by going back to the first chapter, a temporal inversion can be achieved by applying a complex conjugation and a rotation of the spin around the y axis of π radians on the wave function. As we are simulating spinless particles (particles with no spin), the methodology is reduced since the rotation on the spin space is not necessary to recreate a temporal inversion and we can just proceed by only making the complex conjugation to our wave-function.

In the first section of this chapter we developed the way of obtaining the wave-function and its evolution by approximations to Schrodinger's equation. Therefore we just have to choose the instant of time where the temporal inversion will take place and replace the wave-function with its complex conjugate and let it evolve over time. This will give us the behaviour of our wave-function under a temporal inversion. The way to obtain the complex conjugate is to multiply the imaginary part of the solution by -1 since this operation is a reflection over the real axis for a complex number. In our case, in a Matlab program we can achieve the same by using the command "conj( )", and the complex number inside.

As for the Bohmian particles, we have obtained the equations that simulate their motion. In those equations we saw that the motion of the particle is affected by its own wave-function, more exactly the velocity is affected by it (which can be explained by thinking that there is a potential intrinsic to the particle and that affects its own movement). So following the same reasonings, by just choosing the instant of time when the time reversal will take place, we just have to change the wave function with its complex conjugate as before and let it evolve. In order to analyse both interpretations and their similarities and differences on the results, we will solve and represent the wave-function and the particles at the same time, using the same wave-function for the representation and to calculate the velocity of the particles.

3.6. Results and analysis

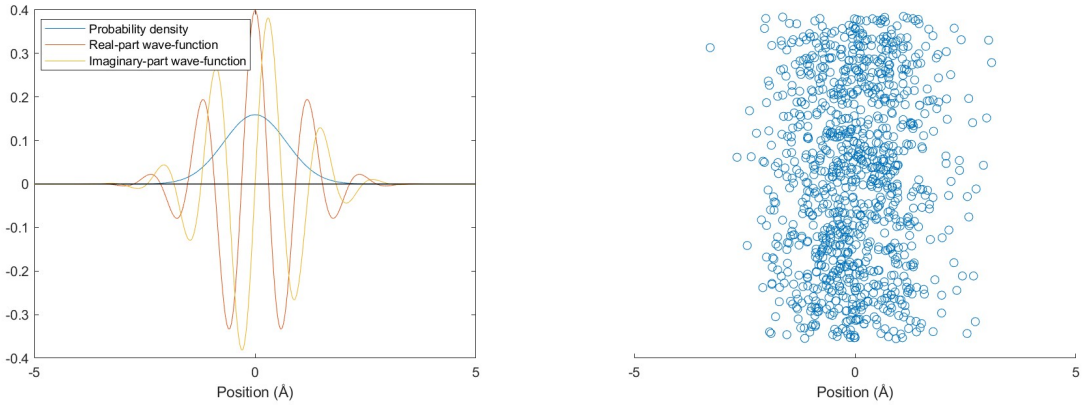
In this section, we present the results obtained from simulations comparing the Copenhagen and Bohm interpretations. We have solved the time-dependent Schrödinger equation using Matlab, starting with a Gaussian wave-packet. The solution yields a time-evolving wave-function, which in turn provides the probability density distribution. This distribution represents the probability of finding a particle in a particular position and momentum at a given time, which is central to the Copenhagen interpretation.

Additionally, within the same program, we implemented a simulation based on Bohm's interpretation. We randomly distributed particles according to the initial Gaussian distribution and evolved them over time using the equations derived from Bohm's theory. For this, we required a wave function, and we used the same time-evolving wave-function previously obtained from the Schrödinger equation. Both interpretations, Copenhagen and Bohm, were represented simultaneously in order to observe the similarities and differences in the particle trajectories and probability distributions.

Finally, we carried out another set of simulations where time-reversal was applied to both interpretations. This allowed us to analyze how each interpretation behaves under time-reversed conditions, offering insights for both interpretations.

All the simulations were made for a mesh with a length of $80\mathring{A}$ that contains $4 \cdot 10^5$ points inside (corresponding to a step of $2 \cdot 10^{-4}\mathring{A}$) and during an interval of time of $6\,a.u.t.$ with 600 instants of time inside (a step of $0.01\,a.u.t.$) for 1000 particles.

3.6.1. Evolution on both interpretations In the firsts results, we present in **Figure** 3.1 the time evolution of the wave-function and probability density obtained solving the time-dependent Schrödinger equation, related to the Copenhagen interpretation.

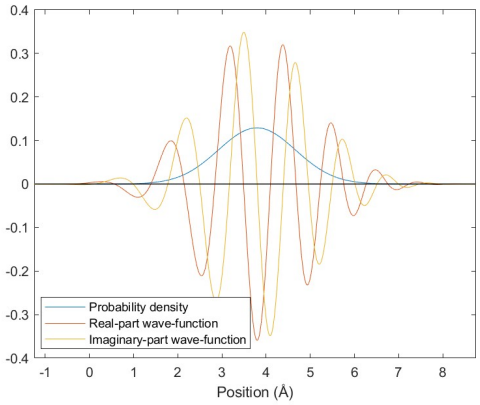


(a) Probability density, real and imaginary part of the gaussian wave-function at the begining.

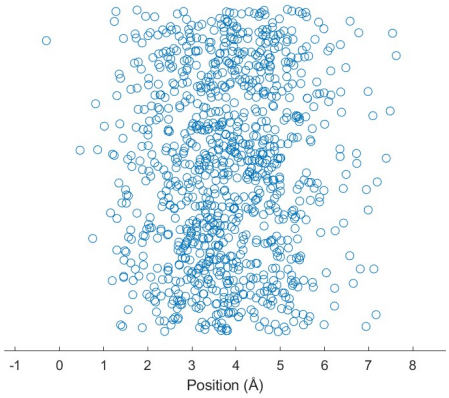
(b) Packet of particles with a gaussian spatial distribution at the begining.

List of Figure 3.1: Wave-function and gaussian packet of particles at the initial instant.

Alongside this, we also show a gaussian packet of particles with their positions as predicted by Bohm's interpretation, using the same initial wave-function to guide the particle evolution. The figures below illustrate how both interpretations evolve over time, allowing us to compare the smooth probabilistic spread of the wave-packet in the Copenhagen view with the distinguishable particle trajectories in Bohm's interpretation.



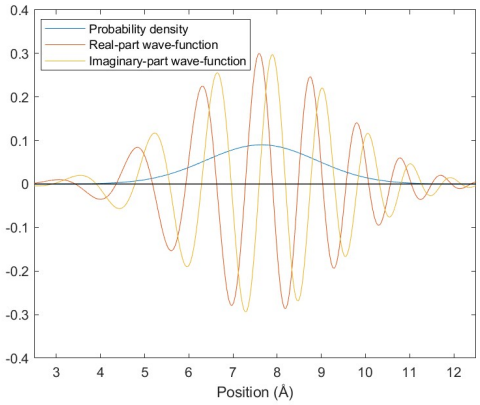
(a) Probability density, real and imaginary part of the gaussian wave-function at 0.75 units of time.



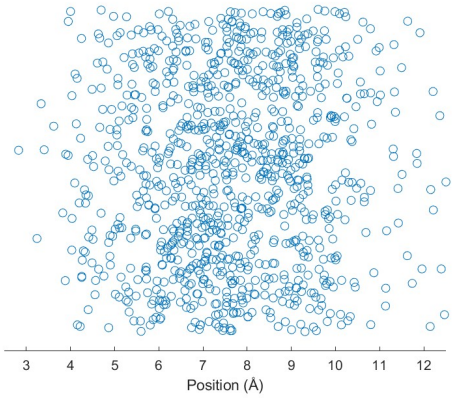
(b) Packet of particles with a gaussian spatial distribution past 0.75 units of time.

List of Figure 3.2: Wave-function and gaussian packet of particles past 0.75 units of time.

The x axis was moved to follow the center of the gaussian wave-function and packet of particles in order to see them centered, while the limits are the same to visualize the spread of the wave-function and particles. We can also observe that the real and imaginary part oscillate in **Figure** 3.2 while the wave-function propagates as we are changing its phase, which is why this particular instant of time was chosen. This is further appreciated in **Figure** 3.3 as the wave-function propagates while oscillating reaching the same phase as it had at the initial instant whereas it is enlarged as a result of the motion.



(a) Probability density, real and imaginary part of the gaussian wave-function at 1.5 units of time.



(b) Packet of particles with a gaussian spatial distribution past 1.5 units of time.

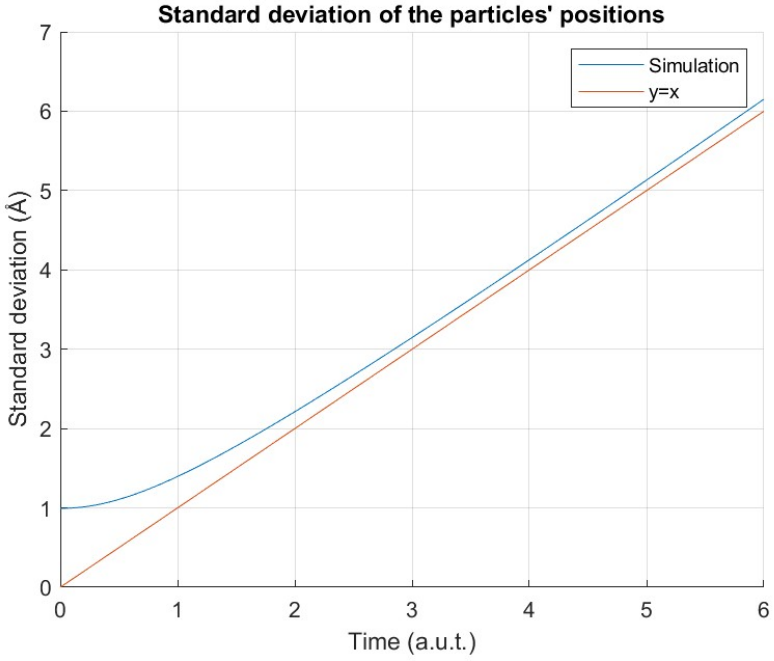
List of Figure 3.3: Wave-function and gaussian packet of particles past 1.5 units of time.

Notably, while the overall probability distributions show clear similarities such as the center and expansion of both the wave-function and gaussian packet of particles, the individual particle paths in Bohm's interpretation provide a more detailed and deterministic picture of the system's dynamics.

Uncertainty principle

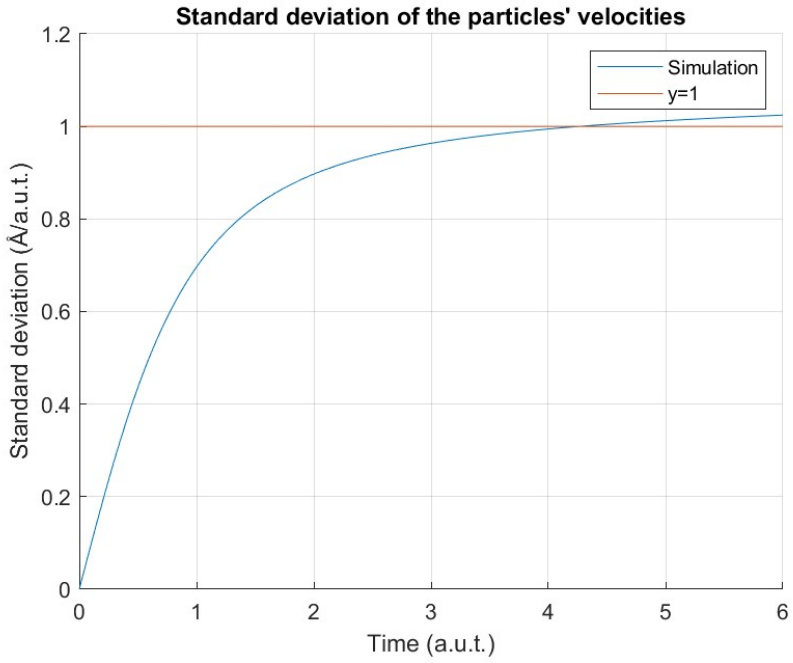
In the introduction chapter, we have analyzed how this principle manifests in both the Copenhagen interpretation and the Bohmian interpretation and the implications it has over the measuring processes in quantum mechanics. Now we will use our simulation to examine the evolution of standard deviations in position, velocity and the uncertainty over time.

In the Bohmian interpretation, particles follow well-defined trajectories guided by the wave function, and their statistical behavior can be analyzed dynamically. Our results in **Figure** 3.4 show that the standard deviation of the particles' positions tends to increase linearly over time once the system surpasses the first unit of time. Specifically, we observe that after this initial period, the standard deviation increases by $1\mathring{A}$ per unit of time, converging to a straight line with a slope of 1 with a 0 y-intercept. The only difference is that our result starts with a initial standard deviation of $1\mathring{A}$ (as it should be because our packet had that initial standard deviation on the position) and quickly tends to the line but its values are a little bit above the line at all times.



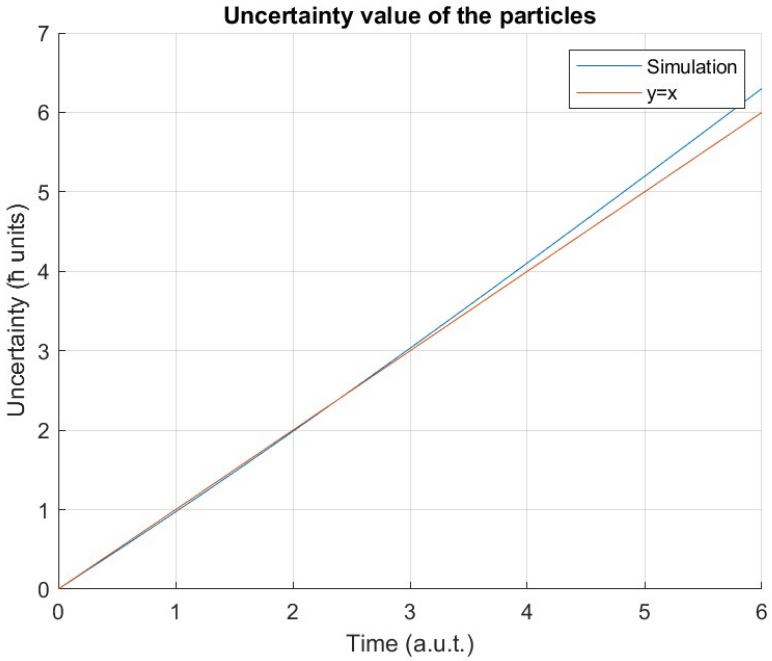
List of Figure 3.4: Standard deviation of the particles' position compared to a slope 1 line

Similarly, we have computed the standard deviation of the velocity of Bohmian trajectories in **Figure** 3.5, obtaining a trend where it grows quickly during the first unit of time and slows down the growth and stabilizes around a constant value of $1\mathring{A}/a.u.t.$ (the actual value is slightly higher but it can be approximated to 1) after some time units. This implies that the dispersion in velocity does not grow indefinitely but rather asymptotically approaches a characteristic value dictated by the system's wave function. From this result, the standard deviation of the momentum can be analyzed too because as we know, $p = mv$. Since we are simulating free electrons the mass will be m_e, but we chose it to be our basic mass unit. Hence, in our results the velocity and the momentum have the same value (with different units of measure as the velocity is measured in $\mathring{A}/a.u.t.$ and the momentum in $m_e\mathring{A}/a.u.t.$) as we would be multiplying the velocity by 1. This is not only applied to the relationship of the momentum and the velocity but also to the relation of their standard deviations, obtaining the same graph and results too.



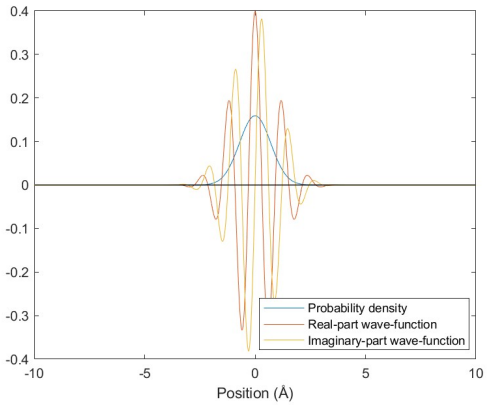
List of Figure 3.5: Standard deviation of the particles' velocity and a line of $1\mathring{A}/a.u.t.$

Finally, when analyzing the uncertainty relation given by the product of position and momentum standard deviations in **Figure** 3.6, we find that it increases linearly with time. Specifically, the uncertainty follows a straight-line trend with a growth rate of $1\hbar$ per unit of time and differing a little in the last instants (which could be due to the approximations made during the simulation or to accumulative rounding values when calculating parameters).

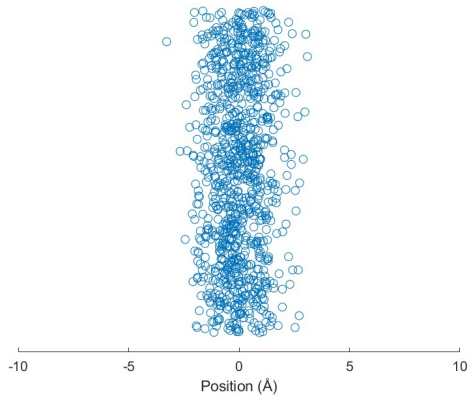


List of Figure 3.6: Uncertainty value compared to a slope 1 line

3.6.2. Time-reversal on both interpretations In this section, we present the results of applying time-reversal to both interpretations by simulating the evolution of a wave-function and a gaussian packet of particles as before. First, the wave-function as obtained from the time-dependent Schrödinger equation, evolves fordward in time, showing a spread of the probability density over time (**Figure** 3.7, **Figure** 3.8), which is consistent with what should happen as in the previous section. At the same time, the trajectories of the particles in Bohm's interpretation are shown, following the flow of the wave function.

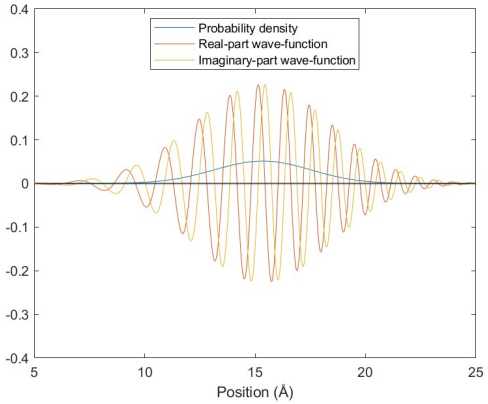


(a) Probability density, real and imaginary part of the gaussian wave-function at the begining.

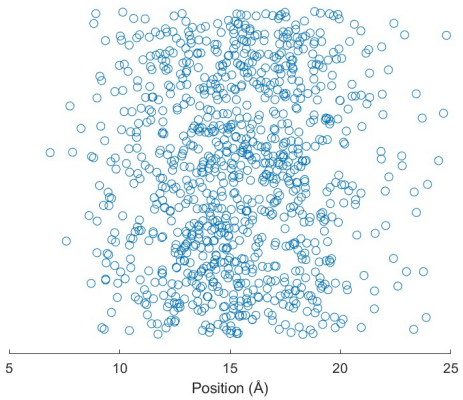


(b) Packet of particles with a gaussian spatial distribution at the begining.

List of Figure 3.7: Wave-function and gaussian packet of particles at the initial instant.



(a) Probability density, real and imaginary part of the gaussian wave-function at 2.99 units of time.

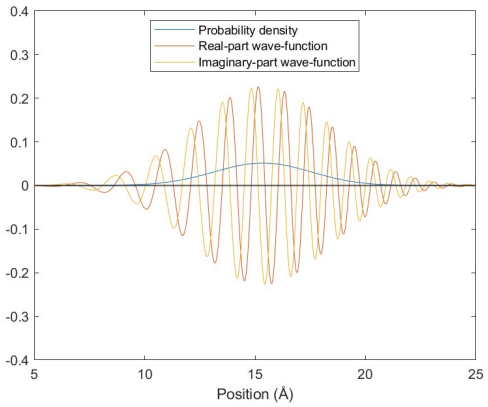


(b) Packet of particles with a gaussian spatial distribution past 2.99 units of time.

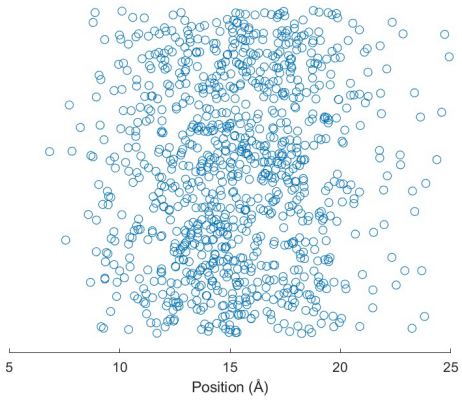
List of Figure 3.8: Wave-function and gaussian packet of particles past 2.99 units of time (before the temporal inversion).

Then, when we arrive at the moment of the time reversal, the wave-function as obtained from the time-dependent Schrödinger equation, will evolve backward in time, showing a reversal of the probability density's spread, consistent with the Copenhagen interpretation. Simultaneously, the trajectories of the particles in Bohm's interpretation also

reverse, following the flow of the time-reversed wave function as we will observe in the following figures.



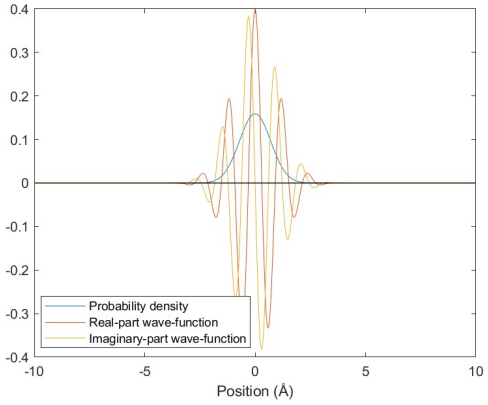
(a) Probability density, real and imaginary part of the gaussian wave-function at 3 units of time.



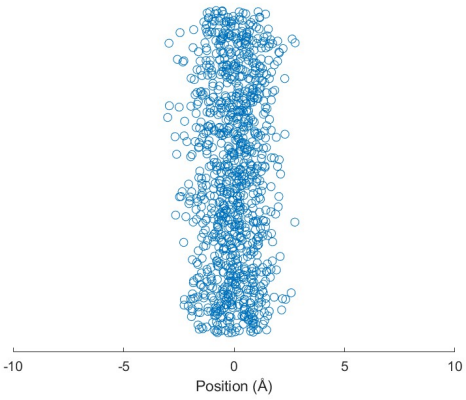
(b) Packet of particles with a gaussian spatial distribution past 3 units of time.

List of Figure 3.9: Wave-function and gaussian packet of particles past 3 units of time (after de temporal inversion).

In **Figure** 3.9, time inversion has been applied and as a result, the wavefunction has been transformed into its complex conjugate, but if we were to measure its position the probability density is unaltered. However, in the gaussian-distributed particle packet no visible change can be observed. This leads to the conclusion that this representation is not entirely complete, as it lacks information about the behavior of the particles.



(a) Probability density, real and imaginary part of the gaussian wave-function at 6 units of time.



(b) Packet of particles with a gaussian spatial distribution past 6 units of time.

List of Figure 3.10: Wave-function and gaussian packet of particles past 6 units of time.

This final figure (**Figure** 3.10) represents an important and intriguing result. It shows that not only does the center of the wavefunction and the Gaussian-distributed particle packet return to their original position, but they also recover their initial dispersion, demonstrating a remarkable symmetry in the system's evolution. However, we can esily detect that they are not the same graphs as in the case of the wave-function we have the complex conjugate of the initial value as explained before since the time reversal

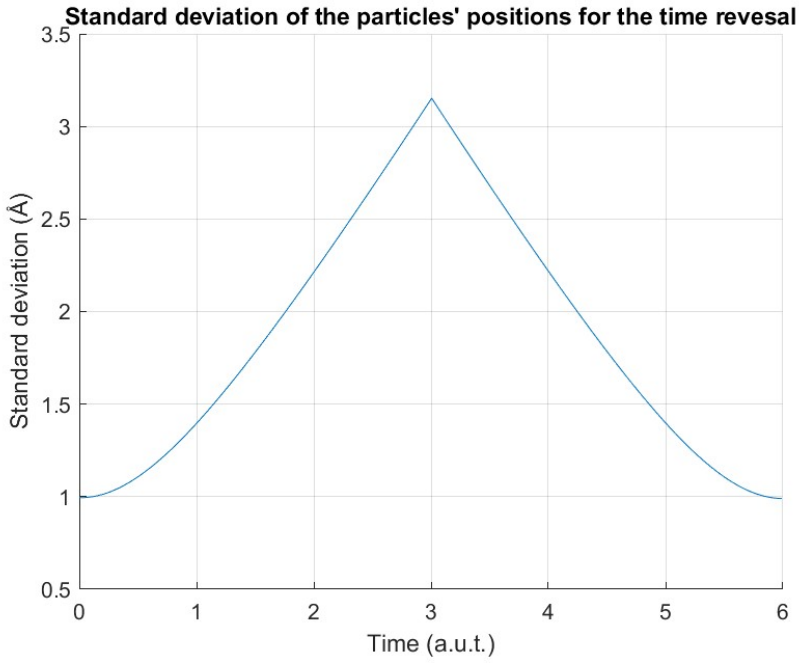
was a complex conjugation (if we don´t take into account spin). This is consistent with what should happen as this means that it if we let the system to continue evolving, bot simulations will proceed to follow their motion backwards over the x axis since we haven´t applied any other temporal inversion to make them evolve fordward again.

The figures above allow us to observe how both interpretations behave under time-reversal, highlighting the differences in how probability densities retrace their evolution versus the deterministic paths of individual particles in Bohm's theory. This comparison provides insights into the reversibility of quantum systems and the distinct ways each interpretation handles time symmetry.

Uncertainty principle

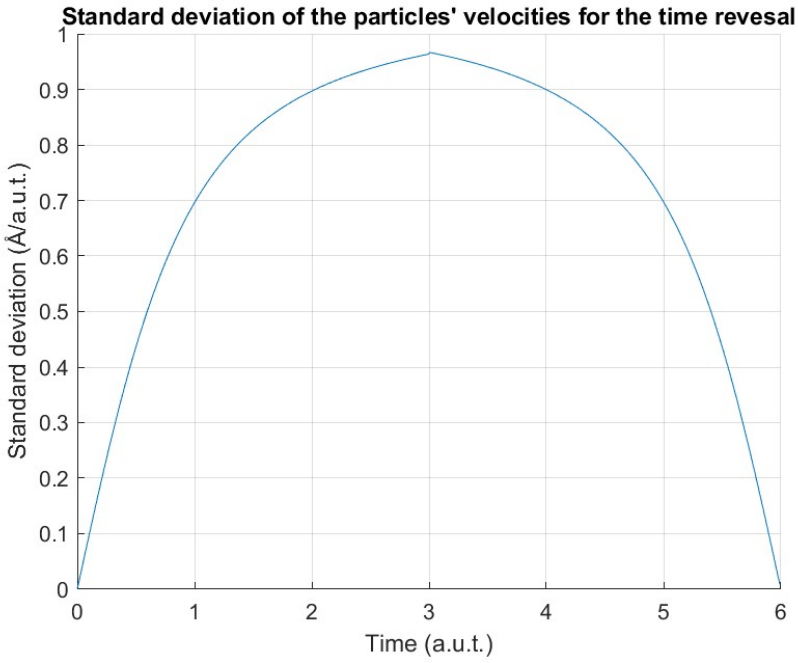
In the previous section, we analyzed the time evolution of the standard deviations of position, velocity, and the uncertainty relation within the Bohmian interpretation. Now, we introduce a time-reversal operation at $t = 3\,a.u.t.$ and examine how it affects these quantities.

As shown in **Figure** 3.11, the standard deviation of the particle positions initially follows the same linear increase observed before, growing by $1\mathring{A}$ per unit of time after the first time unit. However, once the time-reversal is applied, the trend inverts, and the dispersion decreases symmetrically as if reflecting the previous values with respect to a vertical line at $t = 3\,a.u.t.$. This behavior confirms that the time-reversed trajectories retain the deterministic nature of the Bohmian interpretation while fully adhering to the imposed inversion.



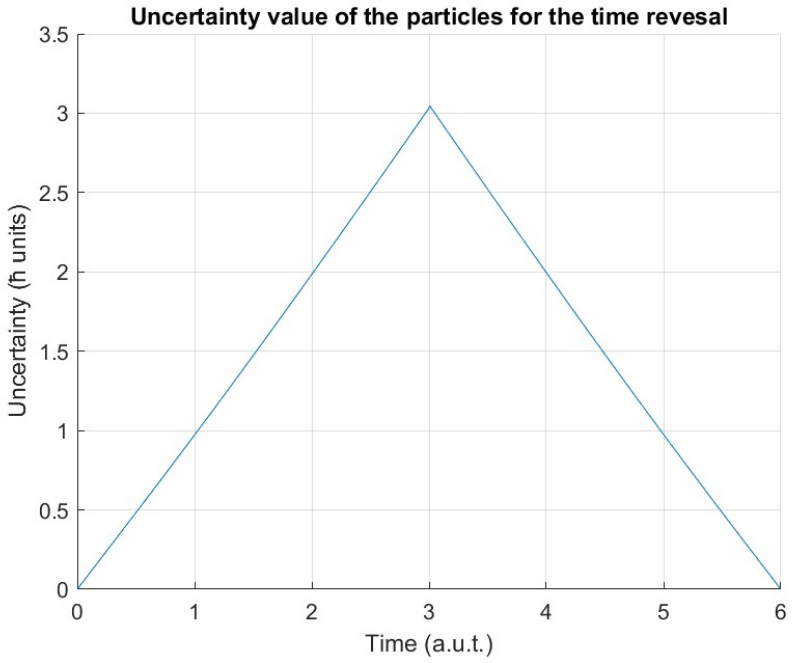
List of Figure 3.11: Standard deviation of the particles' position for the time reversal

A similar effect is observed for the standard deviation of velocities in **Figure** 3.12. Initially, the dispersion grows rapidly, stabilizing around $1\mathring{A}/a.u.t.$ after a few time units. However, upon applying time reversal, the values mirror those before the inversion point, effectively retracing the previous evolution in reverse. This suggests that the system exhibits full reversibility under time inversion, a key feature of the Bohmian framework.



List of Figure 3.12: Standard deviation of the particles' velocity for the time reversal

Finally, when analyzing the uncertainty relation given by the product of position and momentum standard deviations, we find that it increases linearly with time before the inversion, following a straight-line trend with a growth rate of $1\hbar$ per unit of time. As shown in **Figure** 3.13, after the time-reversal operation, this trend is also reflected symmetrically, decreasing in the same manner as it previously grew. This result highlights the compatibility of the uncertainty principle with time-reversed dynamics, reinforcing the idea that the Bohmian trajectories preserve information about past states in a predictable manner.



List of Figure 3.13: Uncertainty value for the time reversal

These findings illustrate that, under the Bohmian interpretation, time reversal does not disrupt the deterministic nature of particle trajectories but instead leads to an exact reversal of previous statistical trends.

Conclusiones

A lo largo de este trabajo, se han comparado las interpretaciones de Copenhague y Bohm en mecánica cuántica, analizando sus diferencias conceptuales y similitudes prácticas. Se estudiaron el movimiento de partículas libres, el cumplimiento del principio de indeterminación y la inversión temporal, permitiendo reflexionar sobre sus implicaciones en nuestra comprensión de la teoría cuántica.

En la interpretación de Copenhague, basada en el colapso de la función de onda, el principio de indeterminación se cumple en todo momento, reflejando su naturaleza probabilística. En contraste, la interpretación de Bohm, con su enfoque determinista mediante la onda piloto, muestra inicialmente una violación de este principio, aunque con el tiempo converge hacia los valores esperados. Para analizar estas diferencias, se desarrollaron simulaciones numéricas: en Copenhague, la evolución de la función de onda se resolvió con el método de Crank-Nicholson, mientras que en Bohm se modelaron trayectorias de partículas guiadas por la onda piloto. Los resultados confirmaron que, pese a las diferencias en su formulación, ambas interpretaciones predicen la misma evolución del sistema.

Además, se introdujo el concepto de inversión temporal en mecánica cuántica, definida mediante la reversión de los momentos lineales y angulares de las partículas sin alterar sus posiciones. En el contexto cuántico, esta operación se modeló mediante un operador que combina conjugación compleja y rotación del espín. Al aplicar la inversión a los sistemas estudiados, se observó que la expansión de la función de onda y la dispersión de las trayectorias en Bohm se revertían, restaurando el estado inicial del sistema. Este resultado demostró que ambas interpretaciones son equivalentes en la descripción de este fenómeno.

Cabe destacar que, aunque la interpretación de Bohm introduce trayectorias definidas y variables ocultas, no contradice los resultados de la mecánica cuántica estándar. Su comportamiento a lo largo de la evolución temporal sigue siendo consistente con la formulación de Copenhague, lo que refuerza la idea de que la diferencia entre ambas radica en la forma de describir los procesos cuánticos más que en sus predicciones experimentales.

En conclusión, aunque Copenhague y Bohm ofrecen enfoques distintos, convergen en los resultados físicos. La primera mantiene el principio de indeterminación en todo momento, mientras que la segunda permite trayectorias definidas, pero ambas describen con precisión la evolución de los sistemas cuánticos. Esta comparativa resalta la complementariedad de ambas interpretaciones, enriqueciendo nuestra comprensión de la mecánica cuántica y su evolución temporal.

Conclusions

Throughout this work, the Copenhagen and Bohmian interpretations of quantum mechanics have been compared, analyzing their conceptual differences and practical similarities. The study focused on the motion of free particles, the fulfillment of the uncertainty principle, and time reversal, allowing for a deeper reflection on their implications for our understanding of quantum theory.

In the Copenhagen interpretation, based on wave function collapse, the uncertainty principle holds at all times, reflecting its probabilistic nature. In contrast, the Bohmian interpretation, with its deterministic approach through the pilot wave, initially violates this principle, although it converges to the expected values over time. To analyze these differences, numerical simulations were developed: in Copenhagen, wave function evolution was solved using the Crank-Nicholson method, while in Bohmian mechanics, particle trajectories were modeled following guidance from the pilot wave. The results confirmed that despite their conceptual differences, both interpretations predict the same system evolution.

Additionally, the concept of time reversal in quantum mechanics was introduced, defined as the inversion of linear and angular momenta while keeping particle positions unchanged. In the quantum context, this operation was modeled through an operator combining complex conjugation and spin rotation. When applied to the studied systems, it was observed that both the wave function spreading and the dispersion of Bohmian trajectories were reversed, restoring the system to its initial state. This result demonstrated that both interpretations are equivalent in describing this phenomenon.

It is important to highlight that, although the Bohmian interpretation introduces well-defined trajectories and hidden variables, it does not contradict the results of standard quantum mechanics. Its behavior throughout time evolution remains consistent with the Copenhagen formulation, reinforcing the idea that the difference between them lies in how they describe quantum processes rather than in their experimental predictions.

In conclusion, while Copenhagen and Bohm offer different approaches, they converge in physical results. The former maintains the uncertainty principle at all times, whereas the latter allows for well-defined trajectories, yet both accurately describe the evolution of quantum systems. This comparison highlights the complementarity of both interpretations, enriching our understanding of quantum mechanics and its temporal evolution.

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