Study of Single Particle Bohmian Mechanics

Author: Pol Ureta Cañellas, Advisor: Artur Polls
Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.
(Dated: 16/01/2019)

Abstract: Bohmian Mechanics is an interpretation of quantum mechanics alternative to the Copenhagen interpretation introduced by D. Bohm in 1952. In this work we study two simple, time dependent, single particle problems to illustrate the concept of Bohmian trajectory and the physics behind it.

I. SINGLE PARTICLE BOHMIAN MECHANICS

Bohmian Mechanics is the name given to an alternative formulation and interpretation of quantum mechanics developed by Bohm in 1952 [1]. Altough it differs in interpretation and mathematical treatment from the Copenhagen interpretation, it can recover its results for the measured expected values, as shown by Bohm himself in his original papers. The historical and ontological discussion of the Bohmian interpretation will be put aside for the rest of the text. Details on the formulation and interpretation of Bohmian Mechanics can be found in the book *Applied Bohmian Mechanics* by X. Oriols and J. Mompart [2].

A. The Standard Formulation of Bohmian Mechanics

The most common way to formulate single particle Bohmian Mechanics is by using the following parametrization of the wave function:

$$\psi(x,t) = R(x,t)e^{iS(x,t)/\hbar} , \tag{1}$$

where R and S are real value functions. Using this parameterization in the Schrödinger equation,

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

we can derive the following equations for the $S(x,t)$ and $R(x,t)$:

$$\frac{\partial S(x,t)}{\partial t} + \frac{1}{2m}\left(\frac{\partial S(x,t)}{\partial x}\right)^2 + Q(x) + V(x) = 0 , \tag{3}$$

$$\frac{\partial R(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\frac{R(x,t)^2}{m}\frac{\partial S(x,t)}{\partial x}\right) = 0 . \tag{4}$$

Eq. (3) corresponds to a Hamilton-Jacobi equation, where S takes the role of the action. In contrast to the Hamilton-Jacobi equation found in classical mechanics, a new term appears: the quantum potential $Q(x,t)$,

$$Q(x,t) \equiv \frac{-\hbar^2}{2mR}\frac{\partial^2 R}{\partial x^2} . \tag{5}$$

On the other hand, Eq. (4) is the law of local conservation of probability density. In order to show that, one has to define the following two quantities:

$$v(x,t) \equiv \frac{1}{m}\frac{\partial S}{\partial x} , \tag{6}$$

$$\rho(x,t) \equiv R^2(x,t) = |\psi(x,t)|^2 \equiv e^{2C(x,t)} , \tag{7}$$

where $C(x,t)$ is called the C-amplitude. After substituting these quantities in Eq. (4) we obtain:

$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(v(x,t)\rho(x,t)\right) = 0 . \tag{8}$$

This equation is a conservation law, namely the law of probability density conservation. ρ is the probability density and v corresponds to the velocity as usually defined in Hamilton-Jacobi equations. Alternatively, the velocity can be defined through the current $J(x,t)$,

$$v(x,t) \equiv \frac{J(x,t)}{|\psi(x,t)|^2} , \tag{9}$$

$$J(x,t) \equiv i\frac{\hbar}{2m}\left(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x} - \psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right) , \tag{10}$$

which can be shown to be coincident with the previous definition [2]. Eqs. (3,8) lead to one of the main features of the Bohmian formulation: the focus on the Hamilton-Jacobi equation and not on the Schrödinger equation. This is because the Hamilton-Jacobi equation is interpreted, besides describing the evolution of the modulus and phase of the wave function, as the guiding equation for a particle, the Bohmian particle. This Bohmian particle is point-like and describes a trajectory as it moves governed by the Hamilton-Jacobi equation. This in turn re-introduces the concept of trajectory which is not found in the Copenhagen interpretation of quantum mechanics. To enlighten the physics behind Bohmian Mechanics and Bohmian particles we will consider two representative examples for which the trajectories will be explicitly calculated.

B. The Lagrangian Formulation of Bohmian Mechanics

Another way to study Bohmian Mechanics is by using a Lagrangian point of view. In this case, the observer follows an individual piece of fluid as it moves through space and time. In contrast, the Eulerian point of view is the way of looking at the fluid motion focusing on specific locations in the space through which the fluid flows as time passes.

In our case, instead of a fluid we consider the wave function, and we will apply a Lagrangian point of view to our expressions. We will focus on the movement of an infinitesimal piece of the wave function. The Bohmian particle will follow the path of that infinitesimal piece, so the trajectories of the wave function elements are identified with the trajectories of the Bohmian particles. To use the Lagrangian formulation, we

need to establish the relation between total (Lagrangian) and partial (Eulerian) derivatives respect to time:

$$\frac{dF(x,t)}{dt} = \frac{\partial F(x,t)}{\partial t} + v(x,t)\cdot\nabla F(x,t)\ , \qquad (11)$$

where F is the considered variable of the fluid (e.g. density) and v the velocity of the fluid. The relation between the total and the partial derivatives allows to write the probability density conservation (Eq. (8)) in Lagrangian form as:

$$\frac{d\rho}{dt} = -\rho\frac{\partial v}{\partial x}\ . \qquad (12)$$

Along with this approach, we introduce the Quantum Lagrangian $\mathcal{L}$,

$$\mathcal{L} \equiv \frac{dS}{dt} = \frac{1}{2}mv^2 - V - Q\ , \qquad (13)$$

where S is the action and Q the quantum potential. Using Eqs. (6, 8, 13) and $v = dr/dt$ we can describe the movement of the system. The state of the system will be fully defined by the position, the R-amplitude and phase S of every fluid element. Afterwards, the wave function could be constructed using Eq. (1). The velocity of each fluid element does not need to be specified, because it can be obtained from Eq. (6).

It is worth noting that this Lagrangian formulation is not exclusive of the Bohmian Mechanics, it has been also used in the Quantum Hydrodynamics treatment of the wave function introduced by E. Madelung in 1926 [3]. This formulation also introduces trajectories in quantum mechanics but without using the concept of Bohmian particle.

II. NUMERICAL COMPUTATIONS IN BOHMIAN MECHANICS

Once the basic equations of the Bohmian Mechanics have been introduced, let us explain how to simulate and compute properties of quantum systems within this formulation. The main focus will be in time-dependent scenarios, but that does not mean that time-independent cases can not be considered or studied. The algorithms that use the Bohmian formulation can be mostly split in two approches: analytic and synthetic [5].

A. The Analytic Approach

In the *analytic* approach one first obtains the wave function of the system by solving the Schrödinger equation and after computes the Bohmian trajectories. So in this method Eq. (2) is first solved in traditional ways and the wave-function at all points of space and time is obtained. Once the wave function is known, the trajectories of the Bohmian particles are computed using Eqs. (9, 10) and time-integrating the velocity. To compute the velocity we use a first order approximation of the spatial derivatives found in the definition of the current J. Then we calculate the trajectory of the particle using a first order approximation: $x\left[t+\Delta t\right] = x\left[t\right] + v\left[t\right]\Delta t$. Due to the fact that the velocity is only defined at the mesh points, the particle can be at a position where no velocity is defined. This difficulty is solved by linearly interpolating the velocity from the two closest points to the point considered.

In this approach, the trajectories are obtained from the wave function. This means that the knowledge of trajectories has no computational benefits to obtain the wave function. However, the visualization of the Bohmian trajectories can be useful to understand and to enlighten the time evolution of the wave function.

B. The Synthetic Approach

The *synthetic* approach is based on taking the Lagrangian approach to Bohmian Mechanics as described in sec. I B. In this approach, the system is treated as if we were solving a classical hydrodynamic problem, but with different equations: instead of solving the Navier-Stokes equation we will solve the Quantum-Hamilton Jacobi equation, the continuity equation and the equations introduced in Sec. I B. In R. E. Wyatt's book: *Quantum Dynamics with Trajectories* [5] a method using this point of view is introduced: the Quantum Trajectory Method. In this method we consider a moving mesh of space points $\{x_i\}$ and we define the variables R and S at each of them. The main idea is to use the trajectories of these points to compute the wave function wherever and whenever needed. The equations we need to solve the problem have already been introduced in Sec. I B: (6), (8), (13) and $v = dr/dt$. It is computationally very useful, though, to use the C-amplitude introduced in Eq. (7) instead of the R-amplitude or the ρ density, so equations (5) and (12) can be expressed as:

$$\frac{dC}{dt} = -\frac{1}{2}\frac{\partial v}{\partial x}\ , \qquad (14)$$

$$Q = -\frac{\hbar^2}{2mR}\frac{\partial^2 R}{\partial x^2} = -\frac{\hbar^2}{2m}\left[\left(\frac{\partial C}{\partial x}\right)^2 + \frac{\partial^2 C}{\partial x^2}\right]\ . \qquad (15)$$

Solving this system of coupled partial derivative equations is in general not easy. An Euler approximation to solve this system usually yields to very unstable results, so an implicit method is convenient. In this case we used a predictor-corrector method. In this method, we first have to identify our variables as a vector: $\mathbf{y} \equiv \{C, S, x\}$. Using this vector we can write the following equation:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, t)\ , \qquad (16)$$

where the rhs $\mathbf{f}$ is the rhs of equations (14), (13) and (6), respectively. Then, the predictor-corrector method can be written as:

$$\mathbf{y}^{pred}(t+\Delta t) = \mathbf{y}(t) + \Delta t\mathbf{f}(t, \mathbf{y}(t))\ , \qquad (17)$$

$$\mathbf{y}(t+\Delta t) = \mathbf{y}(t) + \frac{\Delta t}{2}\left(\mathbf{f}(t, \mathbf{y}(t)) + \mathbf{f}(t+\Delta t, \mathbf{y}^{pred}(t+\Delta t))\right)\ . \qquad (18)$$

This methods proves to be more stable than the Euler method.

On the other hand, there is a second computational difficulty: the evaluation of the spatial derivatives of the functions. As the mesh is not stationary, i.e. the mesh points are moving as Bohmian particles, the mesh points can be separated non-uniformly soon after the motion starts, forming an unstructured grid. In this case, one cannot use the usual approximations to calculate the derivative in a structured grid. The way out of this problem is to first compute a simple analytical function $g(x)$ which approximates to the value of the variable at the moving mesh and then derive explicitly this function.

In our numerical procedure we wanted to implement a fast and easy way to obtain $g(x)$. A good solution was to use a quadratic interpolation build with the Legendre formulas: we interpolated a parabolic function using three consecutive data points. From this function it is straight-forward to compute the first and second derivatives. However, this quadratic interpolation method can be too imprecise for some cases. Better solutions could be obtained using a cubic spline interpolator or by using a fitting procedure. However, these other methods are usually slower than the straight-forward method used in this work.

III. NUMERICAL SIMULATIONS OF COHERENT STATES OF HARMONIC OSCILLATOR

A. Analytical Study of the Coherent States

Let us now apply the methods presented to a well-known system: a single particle in a harmonic oscillator potential $V = \frac{1}{2}m\omega^2 x^2$. The *Coherent States* of the harmonic oscillator is a well-known example of a dynamically evolving wave function in a potential. As we are interested in computing the evolution of the wavefunction and the Bohmian trajectories, we will only present the main results [4]. We will from now on use the harmonic oscillator units.

A coherent state in a harmonic oscillator is the result of displacing the ground state wave function by an amount x_0. This displaced wave function will oscillate without changing shape from x_0 to $-x_0$ with the same frequency as the harmonic potential. This state is sometimes called the "semi-classical" state of the harmonic oscillator, due to the fact that its expected values of position and momentum are very similar to the classical harmonic oscillator:

$$\langle x(t)\rangle = \langle x(t=0)\rangle \cos(t) + \langle p(t=0)\rangle \sin(t)\ , \tag{19}$$

$$\langle p(t)\rangle = \langle p(t=0)\rangle \cos(t) - \langle x(t=0)\rangle \sin(t)\ . \tag{20}$$

It can also be shown that the coherent state wave functions have the following form:

$$\psi(x,t) = \exp(i\,\langle p(t)\rangle\, x)\left(\frac{1}{\pi}\right)^{\frac{1}{4}} \exp\left(\frac{-\left(x-\langle x(t)\rangle\right)^2}{2}\right)\ . \tag{21}$$

If we take the squared modulus of this result it is clear that the shape of the probability density does not change but it oscillates. One can also study the Bohmian formulation of this problem: First, let us use the previous results for this state to analytically compute the velocity and the trajectory of a Bohmian particle. From Eq. (21) we can identify the modulus R and the phase S in a straight-forward way. From the expression for the phase we can compute the velocity of a Bohmian Particle with Eq. (6):

$$v[t] = \frac{dr[t]}{dt} = \frac{\partial S}{\partial x} = \langle p(t)\rangle\ . \tag{22}$$

This means that any Bohmian particle in this system will have the same velocity as the expected value of the momentum of the state. As it can bee seen from Eq. (20) this coincides with the velocity in a classical harmonic oscillator. We can now time-integrate the solution to obtain the trajectory:

$$x[t] = x_0 - \langle x(t=0)\rangle + \langle p(t=0)\rangle \sin t + \langle x(t=0)\rangle \cos t\ . \tag{23}$$

Another interesting quantity is the quantum potential (Eq. (5)). Using the modulus of the wave function we can obtain the following expression for the quantum potential:

$$Q(x,t) = \frac{1}{2}\left(1 - \left(x - \langle x(t)\rangle\right)^2\right)\ . \tag{24}$$

This result for the quantum potential can be somewhat unexpected. As we have seen in Eq. (23) the trajectory of a Bohmian particle in a system resembles a lot the classical solution for the trajectory of a particle in a classical harmonic oscillator. The classical solution for the trajectory in a harmonic oscillator can be obtained from a Hamilton-Jacobi equation which is very similar to Eq. (3), but with the term corresponding to the $Q(x,t)$ set to 0. In this case, the solution takes the form $x[t] = x_0\cos(t+\phi)$. But, comparing this equation with Eq. (23) we can see that they are not equal: if we have two classical particles with different x_0 and $p_0 = 0$ they will cross their paths at $x = 0$ when $t + \phi = \pi/2$. However two Bohmian particles with different x_0, $\langle p(t=0)\rangle = 0$ and the same $\langle x(t=0)\rangle$ will never cross their paths, they will always describe parallel trajectories. This difference is due to the quantum potential.

B. Numerical Results for the coherent states

In order to check our numerical codes, let us first numerically recover the previous results for the harmonic oscillator. We first use the analytic approach with an implicit Crank-Nicolson method to solve the time evolution of a coherent state. The initial state coincides with the solution provided by Eq. (21) but taking $\langle p(t=0)\rangle = 0$.

The numerical procedure solves the Schrödinger equation with the mentioned potential and initial wave function. Then, it computes the velocity at every mesh point and from that the desired trajectories. In Fig. 1, we plot the probability density at different times. The initial coherent state corresponds to the ground state translated to $\langle x(t=0)\rangle = 1$. The shape of the coherent state remains constant along all the evolution with

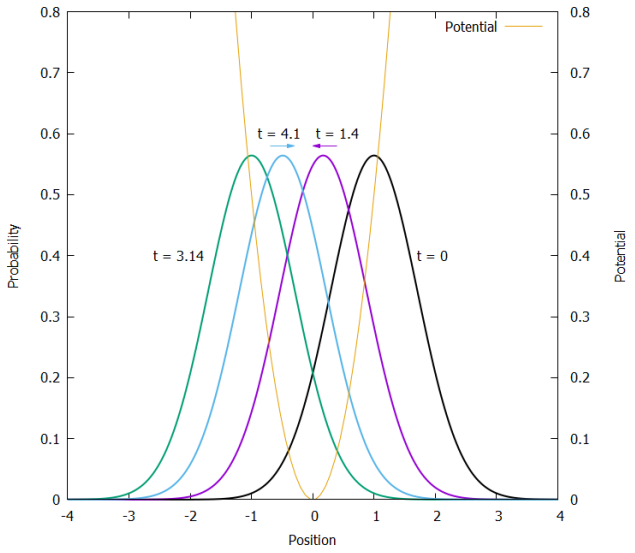

Fig. 1: Probability density of a coherent state at different times obtained by solving the Schrödinger equation. The arrows indicate the direction of the linear moment.

a period $T = 2\pi$. Our numerical procedure provide indistinguishable results from the analytic expressions (Eq. (21)), providing the reliability test of our numerical programs.

In Fig. 2 we plot several Bohmian trajectories, they described the same displaced sinusoidal function. The initial positions of the Bohmian particles were arbitrarily placed. The input parameters were $\langle x(t=0)\rangle = 1$ and $p(t=0)$. The Schrödinger equation was solved in a mesh of $N_x = 1200$ points between $x_i \in [-10, 10]$, while the time step, $\Delta t = 0.01$ until $T_{max} = 10$.

In the next step, we use the synthetic approach to solve the system. In this case we closely follow a numerical algorithm proposed in Appendix 1 of the book *Quantum Dynamics with Trajectories* from Wyatt [5]. This algorithm implements the mentioned synthetic approach of sec. II B using the Euler method to solve the differential equations.

This algorithm leaves us to our choice the procedure to compute the spatial derivatives of the action S and the C-amplitude. After trying different methods (Forsythe polynomials, spline interpolators and Taylor polynomials) the final solution was to use the quadratic interpolation introduced in sec. II B, which was successfully applied. However, the results obtained in the analytic approach were reproduced only for very short times and soon after the system became unstable and broke down. The cause of this instability can be assigned to the Euler method for solving the differential equations, which became unstable when using a lot of time steps. The solution to this problem was to use the predictor-corrector method described in sec. II B. In this case we have used the same initial wave function and the initial mesh points (were the Bohmian particles are located), $N_x = 100$ are taken in the representative interval $[-2, 4]$ while the time should be taken much smaller $\Delta t = 0.0005$ and $T_{max} = 10$. Notice that the initial interval in which the Bohmian particles are distributed

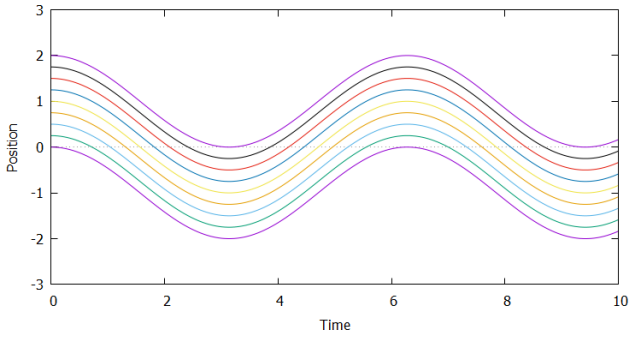

Fig. 2: Trajectories of nine Bohmian particles during the evolution of a coherent state

varies in time.

Now let us compare the results for these two approaches: analytic and synthetic with the exact results derived in the previous section. The first test is provided by the integral of the probability density N. The normalization integral in the analytic approach is obtained by using the Simpson rule. However, it is worth to notice that in the synthetic approach the points can be not equally space as the time evolves and the trapezoidal rule is used as the simplest quadrature to implement in nonuniform grids. We define the parameter $\beta = (N(t) - N(t=0))/N(t=0)$ as a measure of the norm conservation in the time evolution in the two approaches. In both cases, analytic and synthetic, the values of $\beta \leq 10^{-15}$ at any time step.

The next check is to compare the computed wave function against the exact one using the following parameter: $\gamma = |1 - \int |\psi_{Exac}\psi^*_{Comp}|dx|$. For the analytic approach we obtain that $\gamma \leq 10^{-5}$ and for the synthetic approach we obtained $\gamma \leq 3 * 10^{-6}$.

As a final test we compare the computed trajectories to the exact ones. To this end we define $\epsilon(t) = \max\left(x_{Num}(t) - x_{Ex}(t)\right)^2$, over the considered trajectories. For the analytic approach we find that $\epsilon \leq 10^{-5}$ for any time, while for the synthetic approach we obtain $\epsilon \leq 10^{-14}$.

It is worth noting the pros and cons of these two approaches. From the values of the test parameters, we can conclude that both approaches successfully integrate the Schrödinger equation. However, from the trajectory point of view, the synthetic approach proves to be more successful. This is probably due to the errors introduced in computing the velocity and obtaining the trajectories in the analytic method. It is interesting to mention that the analytic approach requires a lot of mesh points ($N_x^A = 1200$ in front of $N_x^S = 100$), while the synthetic approach needs more time steps ($N_t = 1000$ analytic in front of $N_t = 20000$ synthetic). The computing time turns out to be comparable. The most important difference, though, is the stability. The Crank-Nicolson method is very stable and does not require very small time steps to solve the Schrödinger equation, while the predictor-corrector method used in the synthetic approach is more unstable, $\Delta t \leq 0.005$ to get a reliable result.

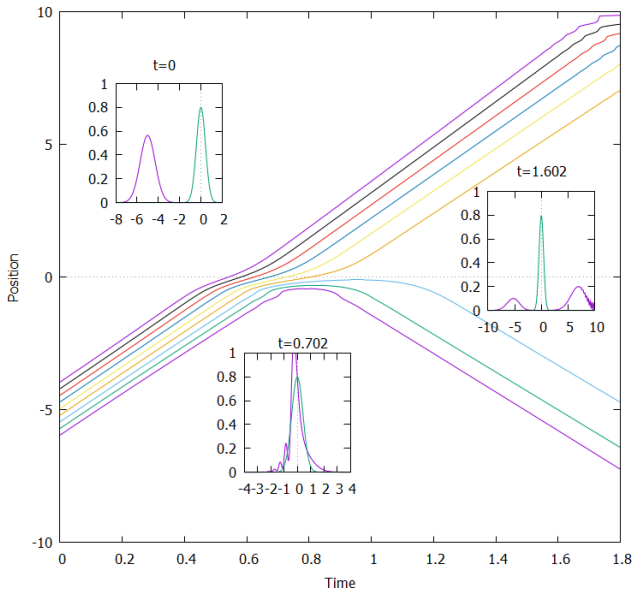

Fig. 3: Trajectories of nine Bohmian particles of a free wave packet which scatters with a potential barrier. The subfigures plot the probability density at different times

IV. NUMERICAL SIMULATIONS OF A FREE WAVE PACKET AND A POTENTIAL BARRIER

We can also use our numerical procedure to study another representative system. In particular, we will consider the scattering of a free wave packet with an exponential potential barrier. The gaussian wave packet of Eq. (21) was used as the initial wave function. The wave packet was located at $\langle x(t=0)\rangle = -5$ with an initial $\langle p(t=0)\rangle = 8$. The potential barrier is described by a gaussian located at the origin: $V(x) = 28.5\exp\left(\frac{-x^2}{(0.6)^2}\right)$. The initial wave packet will hit the barrier and split in two wave packets, one goes through the barrier and the other will be reflected. The Crank-Nicolson method was used to solve the system with $N_x = 600$ mesh points equally spaced between $[-10, 10]$. The time step was $\Delta t = 0.006$.

We computed the β parameter for this case and found that for the first 1.8 units of time $\beta \leq 10^{-10}$, so we assume that the Schrödinger equation integration was successful. The trajectories were calculated after obtaining the wave function. In Fig. 3, the resulting trajectories and some snapshots of the probability density are plotted.

It is worth to study the considered trajectories. From the nine Bohmian particles, initially equally spaced between $x = -6$ and $x = -4$, the closest six particles to the barrier crossed it while the other three did not. This result is to be somewhat expected, as the wave packet is split in two pieces and the transmitted part of the wave function is bigger than the reflected. In general the Bohmian particles that started at the right of the wave function center crossed the barrier while the ones on the left did not, but it is worth to notice that the particle that started at the center of the wave packet and one particle which started at the left of center crossed also the barrier. Apparently, the fact that a trajectory goes through the barrier mainly depends on the starting position of the Bohmian particle. It is also worth noting that after the scattering, both the reflected and transmitted trajectories are no longer equally spaced, but never cross each other.

V. CONCLUSIONS

One of the crucial concepts in the interpretation of Bohmian Mechanics are the Bohmian particles and their trajectories. To enlighten the physics behind these concepts we have calculated the trajectories of the Bohmian particles for two illustrative examples.

To this end, we have presented two numerical procedures, called analytic and synthetic, to simulate time evolving systems in the context of Bohmian mechanics. We have used both methods to study the coherent states of the harmonic oscillator and found that both methods were consistent with each other and with the exact results. We have also studied the scattering of a free wave packet against a gaussian potential barrier using the analytic procedure, which allowed us to visualize the Bohmian trajectories for this system.

It has been shown that the Bohmian trajectories, despite being part of an interpretation of Quantum Mechanics that differs from the Copenhagen interpretation, can be useful to visualize and to understand the quantum behavior of the time dependent Schrödinger equation.

Acknowledgments

I want to thank my advisors Profs. Artur Polls and Bruno Juliá-Díaz for their help and guidance during the project. I would also like to thank Prof. Jordi Mompart for introducing us to the Bohmian Mechanics. Lastly, I would like to thank my family and friends for all their support and help.

[1] D. Bohm. (1952). *A Suggested Interpretation of Quantum Theory in Terms of "Hidden Variables" I and II.* Phys. Rev. 85, 166.

[2] X. Oriols and J. Mompart. (2012). *Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology*. Pan Stanford Publishing Pte. Ltd.

[3] E. Madelung. (1926) *Quantentheorie in Hydrodynamischer Form.* Z. Physik, 40, 322-326.

[4] F. Salvat. (2017). *Notas de Mecánica Quántica*.

[5] R. E. Wyatt. (2005). *Quantum Dynamics With Trajectories*. Springer Science Inc, Interdisciplinary Applied Mathematics, Volume 28.