Evaluating Bohm’s quantum force in the scattering process by a classical potential

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Abstract

In this work, we show an application of the de Broglie–Bohm quantum theory of motion (QTM) as a powerful tool for evaluating Bohm’s quantum force in the scattering process of a Gaussian wavepacket by a classical Eckart potential. Our results show that in the absence of a classical potential, the system experiences quantum effects arising from an effective force, intrinsically related to the existence of the wavepacket itself. In contrast, in the scattering by the classical potential, it experiences a quantum force effect even in the absence of any classical force, reinforcing the fact that potentials can act without classical force fields. Thus, this application could be useful to introduce QTM, through the discussion of the concept of Bohm’s quantum force, as a classroom working tool instead of merely an alternative interpretation of the quantum theory.

Keywords: quantum force, quantum theory of motion, de Broglie–Bohm formulation

(Some figures may appear in colour only in the online journal)

1. Introduction

For a long time, the scientific community tried to preserve the classical determinism for quantum events, one of the most relevant and best-structured theories about this theme comes up with...
from the de Broglie–Bohm formulation of the quantum mechanics [1–9]. Based on the con-
ceptions of the pilot wave of de Broglie [8, 9], Bohm proposes a theoretical formulation for the
quantum mechanics [6, 7], in which the quantum events are driven according to an essentially
quantum potential, arising from the interaction between the particle and its wave-guide, being
responsible for the quantum nature of the events during the system dynamics [3, 10–17].

Recent works have proposed alternative applications to this formulation [2, 3, 10,18–20],
unravelling interesting properties and interpretations for the dynamics of quantum systems
[18, 20]. The existence of the quantum potential provides one path towards the under-
standing these dynamics in a Newtonian-like point of view, through the existence of the so-called
Bohm’s quantum force [18, 20, 21]. This is in the context of, recently, Becker et al [18]
observed the quantum force predicted by Shelankov [22], Berry [23] and Keating [24] for
an Aharonov–Bohm physical system, providing the experimental support for the evidence of
the quantum force in the Aharonov–Bohm effect [25].

In this context, we show in this paper an application of the de Broglie–Bohm QTM to esti-
mate Bohm’s quantum force in the quantum dynamics of a Gaussian wavepacket, with and
without the presence of a classical potential. For that, we consider two situations, the first one
associated with the free particle case [26], and the second one related to a system subjected
to the Eckart potential model [27]. The dynamic variables were analyzed through the tempo-
ral propagation technique, using the popular and easy to implement finite-difference method,
facilitating the reproduction of this analysis for most undergraduate and graduate quantum
mechanics students.

Our results show that in the absence of a classical potential, the system experiences quantum
effects arising from an effective force intrinsically related to the existence of the wavepacket
itself, while the classical determinism is preserved in some way. Moreover, strengthening the
fact that classical potentials can act without force fields and giving us indications that the
nature of the Aharonov–Bohm effect can be observed in different classical potentials, in the
scattering process by a classical potential the wavepacket experiences a quantum force effect
which depends on the presence of the potential, even in the absence of any classical force field,
perceiving it even before the explicit interaction.

Therefore, this application could be used as an example of the evaluation of Bohm’s quan-
tum force, presenting the QTM as a useful working tool for the study of quantum dynamics,
instead of merely an alternative interpretation of the quantum theory.

2. de Broglie–Bohm interpretation

The de Broglie–Bohm QTM presents an interesting interpretation for quantum mechanics, in
which the quantum system can be interpreted as two intrinsic counterparts: a wave and a point
particle [1, 3, 21]. In this context, an individual system comprises one wave, that propagates
into spacetime driving the motion of a punctual particle. The wave is mathematically described
by a function $\Psi(q_i; t)$, which is a solution of the Schrödinger’s equation, in such a way that

$$\Psi(q_i; t) = R(q_i; t) e^{iS(q_i; t)/\hbar},$$

where $R = R(q_i, t)$ and $S = S(q_i, t)$ are real functions given by:

$$R(q_i, t) = |\Psi(q_i, t)| \geq 0, \quad \forall \{q_i, t\},$$

$$\frac{S(q_i, t)}{\hbar} = \tan^{-1} \left( \frac{\text{Im}\{\Psi(q_i, t)\}}{\text{Re}\{\Psi(q_i, t)\}} \right).$$
Here \( S \) can be seen as an action having dimension of \( \hbar \).

Considering the functional form of \( \Psi(q_i; t) \), given in equation (1), the Schrödinger’s equation results on two coupled equations

\[
\frac{1}{2m} (\nabla S(q_i; t))^2 + V(q_i; t) - \frac{\hbar^2}{2m} \frac{\nabla^2 R(q_i; t)}{R(q_i; t)} = -\frac{\partial S(q_i; t)}{\partial t}, \tag{4}
\]

\[
\frac{\partial R^2(q_i; t)}{\partial t} + \nabla \cdot \left( R^2(q_i; t) \frac{\nabla S(q_i; t)}{m} \right) = 0 \tag{5}
\]

with \( V(q_i; t) \) being an external classical potential. Equations (4) and (5) describe the dynamic evolution of a particle in the classical theory and a continuity equation for the probability density, respectively, and the quantum nature of the events emerge from the coupled terms between these equations [1–3].

Equation (4) provides a total energy, \(-\frac{\partial S(q_i; t)}{\partial t}\), given by a sum of kinetic and potential energies, plus an additional term interpreted as a quantum potential [11–17], while equation (5) can be identified as a continuity equation, with the probability density \( R^2(q_i; t) \) and the current density given by

\[
J = R^2(q_i; t) \frac{\nabla S(q_i; t)}{m}. \tag{6}
\]

The uniqueness of \( \Psi(q_i; t) \) is immediately verified in \( R(q_i; t) \), for each pair \( \{q_i, t\} \); but not necessarily into \( S(q_i, t) \), since for each pair one can define a distinct set of these functions. However, if the functions \( S(q_i, t) \) differ from each other by integer multiples of \( \hbar \), then the wave function \( \Psi(q_i; t) \) will be unique, and the field \( p_i \) defined as

\[
p_i = \nabla S(q_i, t) \tag{7}
\]

shall have uniqueness assured for each point \( \{q_i, t\} \).

In QTM, the equations (4) and (5) control the dynamics of a system particles [11–17]. In this scenario, the term

\[
V(q_i; t) = \frac{\hbar^2}{2m} \frac{\nabla^2 R(q_i, t)}{R(q_i, t)} \tag{8}
\]

provides an effective potential in which the particle is submitted. Therefore, the equation (4) consists into the Hamilton–Jacobi equation [28], unless a so-called quantum potential term

\[
Q(q_i; t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R(q_i, t)}{R(q_i, t)}. \tag{9}
\]

This term arises from the interaction between the guiding wave \( \Psi(q_i, t) \) and the particle, and it is responsible for the quantum nature of the events during the evolution of the physical system [11–17].

Since \( R(q_i, t) \), equation (2), consists in a probability density, equation (5) provides a continuity equation associated to \( R(q_i, t) \). In this regard, the specification of \( q(t) \) and the guiding wave \( \Psi(q_i, t) \), at a certain instant \( t \), define the state of an individual system. As demonstrated from equation (4), \( Q(q_i, t) \) depends explicitly of \( R(q_i, t) \), and it is coupled with \( S(q_i, t) \) in such way that

\[
\frac{\partial S(q_i, t)}{\partial t} + \frac{1}{2m} (\nabla S(q_i, t))^2 + V(q_i, t) + Q(q_i, t) = 0. \tag{10}
\]
Thus, the quantum potential is not previously known, such as $V(q_i, t)$, but it depends on the state of the whole system, defining a wave-particle interaction that evolves according to the system dynamics, which is mediated by a force like effect [18, 20, 21, 24]. In this regard, the dynamic of the particle wavepacket can be described in terms of an effective force:

$$F_{\text{eff}} = \frac{dp}{dt} = F_C + F_Q,$$

in terms of the classical force ($F_C$), derived from the classical potential $V(q_i, t)$, and the so-called quantum force ($F_Q$) [18, 21]

$$F_Q(q_i, t) = -\nabla Q(q_i, t),$$

derived from the quantum potential, equation (9).

The quantum force acts on the de Broglie–Bohm trajectories [29], and it is not measurable [18, 29]. In an operational way, the presence of the quantum force can be observed in the presence of a deflection in the average trajectories [18, 29]. In this context, we propose a study of a free particle and a particle subjected to the Eckart potential, through the QTM, and so we compare the effect of a classical potential on the Bohm’s quantum force.

### 3. Temporal propagation through the finite-difference method

Most of the studies involving scattering in QTM search for descriptive and representative quantities of the dynamic process [13–15, 24, 30]. These quantities are obtained in terms of the functions $R(q_i, t)$ and $S(q_i, t)$. Thus, we can solve the Schrödinger equation, and obtain these functions in terms of $\Psi(q_i, t)$. In this work, we apply the quantum trajectory method [31, 32] on the field $\Psi$, in order to obtain the system dynamics through interactive processes at a given initial condition, with the proper adjustments to ensure the convergence criteria and stability. Additionally, we have limited our applications in one-dimensional problems: the free particle and with the presence of a classical Eckart potential.

Adopting the interactive finite-difference method [33, 34] since it is a common method to the students, being widely discussed in traditional undergraduate courses in physics, the one-dimensional time-dependent Schrödinger equation can be written as:

$$\frac{\Psi(q, t + \Delta t) - \Psi(q, t)}{\Delta t} = \frac{i}{2} \frac{\partial^2 \Psi(q, t)}{\partial q^2} - iV(q, t)\Psi(q, t),$$

where $\Delta t$ is a small finite time interval. We use the atomic units (a.u.) system\(^4\) [35], which is a ubiquitous unit system that simplifies the main equations in atomic physics and computational chemistry, ensuring reasonable performances without compromising the relevant theoretical aspects.

In order to make use of the propagation process, it is necessary to define the initial state of the quantum wave function. Here, we are choosing the Gaussian packet\(^5\) [26] at the

\(^4\)In this unit system, the numerical values of the electron mass (atomic unit of mass $m_e$), its elementary charge (atomic unit of charge $e$), the Bohr radius (atomic unit of length $a_0$), and the reduced Planck constant (atomic unit of action $\hbar$), are all unity by definition.

\(^5\)For a detailed account, see appendix G of reference [26], this text gives analytical solutions for the Gaussian wavepacket describing the differences between the classical and the de Broglie–Bohm trajectories.
instant \( t = 0 \):

\[
\psi(q, 0) = \left(\frac{2\gamma}{\pi}\right)^{\frac{1}{4}} \exp\left[-\gamma(q - q_0)^2 + ip_0(q - q_0)\right],
\]

(14)

where \( \gamma = 1/2\delta^2 \), with \( \delta \) being the packet’s width, and \( q_0 \) and \( p_0 \) are, respectively, the center of position and momentum of the packet.

Since the scalar fields \( R(q, t) \) and \( S(q, t) \) can be determined in terms of \( \Psi(q, t) \), equations (2) and (3), one may use them into equations (4) and (5), in order to obtain the dynamic of the system. Considering the problem under the influence of a time-independent potential \( V(q) \) and the equation (7), it is possible to determine the velocity distributions \( \dot{q}(t) \) and the associated trajectories, as well as the effective force related to the quantum potential. For determination of the trajectory, we use the temporal propagation by finite difference technique, making the necessary adjustments for the initial conditions,

\[
q(t_k + \Delta t) = q(t_k) + \frac{\partial S(q, t_k)}{\partial q} \Delta t.
\]

In addition, for determination of the mediating force, from equation (9) one can apply the finite differences approach upon the quantum potential \( Q \) as

\[
Q(q, 0) = \frac{1}{2R(q, 0)} \left[ \frac{R(q + \Delta q, 0) - 2R(q, 0) + R(q - \Delta q, 0)}{\Delta q^2} \right]
\]

(15)

in terms of the generalized coordinates. In the cases considered in this work, the implementation of the numerical calculus is with a discretization of 2500 points in the variable \( q \) and \( 10^7 \) points in the variable \( t \), in a way to guarantee a satisfactory description, without incurring significant divergences on the values, and assuring a relatively low computational cost\(^6\).

4. Results

4.1. Free particle wavepacket

Considering the propagation of a free \((V(q) = 0)\) Gaussian wavepacket, equation (14), centered on \( q_0 = -2.0 \text{ a.u.}, p_0 = 10 \text{ a.u.} \) and spatially distributed in the interval \([-10, 10]\). We obtain the propagation profile for this wavepacket, applying the temporal propagation through the finite-difference method, (see figure 1). According the figure 1, the scattering effect on the wavepacket is clearly perceived during the process of temporal propagation. Usual interpretations of the quantum mechanics also provide this result, and it is intrinsically connected to the uncertainty of observations in the Schrödinger representation for position.

In order to highlight the trajectories localized at the center and extremes of the wavepacket we select 19 points symmetrically distributed around the center of the wavepacket, \( q_0 = q_{10} \), which represent the initial configuration associated to the particles ensemble. In such way, each point is initially distributed around \( q_{10} \), as depicted in figure 2. Thus, through the dynamic variables we can observe what happens individually with the constituent elements of the distribution.

\(^6\)The template of the program is not provided, since the prior programming experience of the readers could vary, and finite-difference method can be easily implemented in the most popular programming platforms as C++, FORTRAN, Python (using NumPy), MATLAB and Mathematica, for instance.
Figure 1. Propagation profile of a free Gaussian wavepacket, obtained from the temporal propagation through the finite-difference method.

Figure 2. Trajectories associated to a set of 19 points distributed over the free wavepacket, highlighting trajectories localized at the center \(q_{10}\) (green dash-dotted line), left \(q_1\) (solid red line), and right \(q_{19}\) (dashed blue line) of the packet.

In the de Broglie–Bohm theory, despite the absence of a classical potential, the system is subjected to a quantum potential \(Q(q, t)\), which arises from the dual wave-particle nature, through the interaction between the particle and its wave-guide. In this approach, the statistical nature of the wave function associated with the particle, according to Max Born’s interpretation, is represented by a statistical distribution of accessible states. For each accessible state, we can associate a set of replicas of the particle occupying its corresponding movement configuration (an ensemble). The quantum nature of the problem is preserved, since the shape of this statistical distribution in the initial state, around the initial position of the particle, is determined by its interaction with the quantum potential. Thus, the wavepacket propagation acquires a different connotation, which is explained as being a direct consequence of the action of a field \(\Psi(q, t)\) on the ensemble of particles via potential \(Q(q, t)\), offering new prospects to the interpretation of the system dynamics. According to this representation, we calculate the quantum potential using equation (15). Figure 3 shows the quantum potential associated to the three representative trajectories of the ensemble at the center \(q_{10}\) and extremes \(q_1; q_{19}\) of the free wavepacket. Those trajectories correspond to initial points localized at the center and extremes of the wavepacket, as highlighted in figure 2.
Therefore, evidencing the non-classical nature of this process, from the quantum potential the ensemble experiences the action of a non-null effective force (equation (11)) consisting of elements intrinsically related to the initial conditions of the system, even in the absence of a classical potential. Using equation (12) we calculate the respective quantum force associated to the same trajectories described in the figure 3. In the absence of any classical potential, the effective force experienced by the wavepacket arises exclusively from the quantum potential being considered as a quantum force.

Figure 4 shows the effective quantum force as a function of the time and the generalized coordinate $q(t)$. As indicated, although the effective force being zero at the center of wavepacket, the dispersion on the trajectories at the extremes obeys the tendency that the quantum force acts over the elements distributed at the edges of the wavepacket, in such way that it accelerates$^7$ points on the left side of the wavepacket center (back), $q < q_{10}$, and slows down points on the right side (front), $q > q_{10}$.

Therefore, one can conclude that the center of the wavepacket experienced a classical free particle dynamics, because there is no classical or quantum force acting on it, whereas the edges experience a quantum dynamics from the quantum potential emergent from the interaction between the corpuscular and wave nature of the system. Therefore, the quantum force is strongly connected to the existence of the wavepacket itself, while the classical determinism of a physical system is in some way preserved, and the events of quantum nature are guided by a field of probabilistic nature, $\Psi$, which acts on the ensemble of particle modifying the system dynamics, as a wave-guide.

4.2. Particle subjected to the Eckart potential

In order to illustrate the effect of a classical potential on the quantum force$^8$ [27], we consider the propagation of the wavepacket, equation (14), scattered by one of the most applicable and

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$^7$ Although we have adopted the idea of an acceleration, the effective force does not consist of a Newtonian interaction between the wave-guide and the particle, so it is not possible to talk about a pair of action and reaction between them.

$^8$ The scattering process of Gaussian wavepackets from classical potentials has been extensively studied using the de Broglie–Bohm theory over many years in the specialized literature that discusses quantum tunneling through Bohm’s theory [14, 36, 37]. For a detailed account, see reference [27].
Figure 4. Effective force as a function of the time (a) and the generalized coordinate \(q(t)\) (b), for the trajectories localized at the center (green dash-dotted line), left (solid red line) and right (dashed blue line) of the free (Gaussian) wavepacket. Since there is no classical potential the effective force is only due to the existence of a quantum potential emergent from the interaction between the corpuscular and wave nature of the system.

Useful potentials for investigations about scattering parameters and bound states [36–44] the Eckart potential

\[
V(q) = V_0 \frac{\exp[\beta(q - q_v)]}{\{1 + \exp[\beta(q - q_v)]\}^2}, \tag{16}
\]

where \(V_0\), \(\beta\) and \(q_v\) are, respectively, amplitude, width and center of the potential.

Since, we have adopted atomic units, the coefficient \(\beta\) has the unit of inverse of the Bohr radius. For our analysis, we are assuming the potential with amplitude \(V_0 = 200\) a.u., width \(\beta = 20\) a.u., and centered at \(q_v = -2.0\) a.u. and \(p_v = 10\) a.u.

In figure 5(a), we depicted the wavepacket propagation scattered by the Eckart potential given in the equation (16), obtained from the finite-difference method. Even the initial average energy of the wavepacket being equal to the height of the barrier, one fraction of the
Figure 5. (a) Propagation profile of the Gaussian wavepacket subjected to the Eckart potential. (b) Trajectories of 19 points distributed around \( q_0 = -2.0 \) a.u., with \( E = 50.0 \) a.u. The highlighted trajectories are associated to the points placed at the center (green dash-dotted line), extremes left (solid red line) and right (dashed blue line) of the wavepacket.

The wavepacket is transmitted and the other one is reflected, with most of the amplitude being transmitted for present initial conditions, so it furnishes the behavior characteristic for that type of process, showing a distinction for effects of transmission and reflection on this potential barrier. The propagation of the wavepacket and the dispersion, during the scattering process, are illustrated in terms of the trajectories pictured in the figure 5(b). Those trajectories, represented in figure 5(b), allow us to conclude that the scattering process starts at \( t = 0.15 \) a.u. and any influence registered before this interval elapses without an explicit action of the classical potential.

As illustrated, the left (back) of the wavepacket \( \{q_1\} \) is reflected, whereas the center \( \{q_{10}\} \) and the right (front) \( \{q_{19}\} \) of the wavepacket are transmitted, tunneling the potential barrier. The same effect can also be observed by the plot of the quantum potential and the analysis of quantum forces acting in each trajectory.

Figure 6 shows the quantum potential \( Q(q, t) \) obtained from equation (15) for the wavepacket scattered by a classical Eckart potential, for the trajectories highlighted in figure 5(b), localized at the center \( \{q_{10}\} \) and extremes \( \{q_1; q_{19}\} \) of the wavepacket. As shown in figure 6, when the wavepacket approaches the potential barrier the quantum potential profile changes and even before the scattering the behavior is completely different from the one obtained in the case of
Figure 6. (a) Quantum potential $Q(t)$ represented at the time interval 0 a.u. and 0.15 a.u., with $E = 50.0$ a.u., subjected to the classical interaction of amplitude $V_0 = 200$ a.u. (b) Comparison between the quantum and classical potential. These profiles are associated to the three representative trajectories: center (green dash-dotted line), extremes left (solid red line) and right (dashed blue line) of the Gaussian wavepacket subjected to the Eckart potential.

A free particle, considering the same quantities (figure 3). Figure 6(b) shows the tunneling of the front and the center of the wavepacket in the potential barrier as previously discussed. The tunneling effect with the Eckart potential was discussed before in the literature in terms of the Bohmian total potential [14, 36].

Using equation (12) we calculate the quantum force for the same trajectories described in figure 6. Figure 7 shows the quantum force as a function of the time and the generalized coordinate $q(t)$, for the wavepacket scattered by a classical Eckart potential.

As the scattering occurs, different points of the wavepacket experience a variation on the interaction profile which they are subjected. That can be seen in figure 6(b) describing the quantum potential $Q(q)$ and the classical potential $V(q)$ in terms of their coordinates. As can be seen, the constituents of the ensemble perceive the classical potential even before the classical interaction, since the element localized to the left side of the packet ($q_l$) suffers a significant
change in its potential profile, even not interacting explicitly with the potential $V(q)$, but receiving this information through a correlation existing among the elements of the wavepacket. In other words, the particle experiences a quantum force effect which depends on the presence of the classical potential, even in the absence of any classical force field. In order to illustrate this effect we show in figure 8 comparison between the forces in the transmitted trajectory at the edge of the scattered wavepacket.

Therefore, this result can be interpreted analogously to that observed in the Aharonov–Bohm effect [25] since even in the absence of a force field, the quantum dynamics of the particle is altered by the presence of the classical potential. These results strengthen the fact that classical potentials can act without force-fields, giving us indications that the Aharonov–Bohm effect could be observed in other classical potentials.
5. Conclusions

In this work, we report an application of the de Broglie–Bohm QTM as a powerful tool for evaluating Bohm’s quantum force in the scattering process of a Gaussian wavepacket by a classical Eckart potential. In order to make our analysis easy to reproduce by undergraduate and graduate students of quantum mechanics courses, we adopt the temporal propagation method, which is an interactive technique of finite differences.

Firstly, we consider the free particle dynamics, where we observe that, in the absence of a classical potential, the edges of the wavepacket experience an effective force, intrinsically related to the existence of the quantum potential $Q(q,t)$, which emerges from the interaction between the corpuscular and wave nature of the system, while the center of the wavepacket shows a classical free particle dynamics. Thus, the quantum force is strongly connected to the existence of the wavepacket itself, while the classical determinism of a physical system is in some way preserved.

In the following, we illustrate the effect of a classical Eckart potential. In this example, the system experiences a quantum force effect, which depends on the classical potential, even in the absence of any classical force field. This result is analogous to that observed in the Aharonov–Bohm effect, giving indications that the nature of this effect can be observed in different classical potentials. Thus, the system experiences significant changes in its dynamics, even before the explicit interaction with the classical force, giving us evidence of the presence of the quantum force in the scattering process by a classical potential.

Therefore, these results show the potential of the de Broglie–Bohm formulation as a complementary picture for the quantum theory, being a useful classroom working tool for the study of quantum dynamics through the concept of Bohm’s quantum force, instead of merely an alternative interpretation of the quantum theory.

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