Effective quantum tunneling from semiclassical momentous approach

L. Aragon-Muñoz
Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Ciudad Universitaria, 04510 Coyoacán, Ciudad de México, México
E-mail: luis.aragon@correo.nucleares.unam.mx

G. Chacon-Acosta
Applied Mathematics and Systems Department, Universidad Autónoma Metropolitana-Cuajimalpa, Av. Vasco de Quiroga 4871, Ciudad de México, 05348, México
E-mail: gchacon@correo.cua.uam.mx

H. Hernandez-Hernandez
Facultad de Ingeniería, Nuevo Campus Universitario, Universidad Autónoma de Chihuahua, Chihuahua 31125, México
E-mail: hhernandez@uach.mx

Abstract. We study the quantum tunnel effect through a potential barrier employing a semiclassical formulation of quantum mechanics based on expectation values of configuration variables and quantum dispersions as dynamical variables. The evolution of the system is given in terms of a dynamical system for which we are able to determine effective trajectories for individual particles, in a total resemblance of the Bohmian description of quantum mechanics. We obtain a type of semiclassical confinement for particles in a similar way as with the quantum potential, and also determine a semiclassical transmission coefficient for the tunneling process.

1. Introduction

Quantum tunneling, the microscopic phenomenon where a particle can penetrate or pass through a potential barrier, can be considered as one of the defining phenomena of quantum mechanics; it is observed in general physical phenomena that appears whenever the system is described by a wave equation or a wavepacket scattering off some physical barrier, as in optics [1] for example. It has no classical analog: the passage of a particle trough a potential barrier when its maximum is higher than its kinetic energy is not allowed by the laws of classical dynamics: tunneling is a direct consequence of the matter wave structure of quantum mechanics.
Just after the appearance of Schrödinger’s equation and theoretical evidence of quantum tunneling was obtained the tunnel effect was proposed as the physical mechanism explaining both the field electron emission [2] and the alpha decay [3], which were the first successful applications of quantum theory to nuclear phenomena [4]. Several other remarkable applications of the tunnel effect followed: problems related to the spectra of molecules [5], molecular and condensed matter physics [6], the tunnel diode and electron tunneling in solids [7], superconductivity [8] engineering and manufacturing of aggregates on the nanoscopic and mesoscopic scale and many others. All of this has paved the way for a very fruitful exchange of experimental techniques and theoretical concepts in atomic, molecular, and condensed matter physics and chemistry (see [9]).

Analyzing the tunnel effect under general boundary conditions and interaction potentials, in one and several dimensions, is a complicated matter as one needs to solve the Schrödinger equation [10], which is not possible in a general analytical way. In such scenario the need of semiclassical techniques for studying the process of quantum tunneling is not only desirable but imperative, serving also as a direct path to implementing numerical methods and provide physical insight into the very complicated nature of quantum systems by exploiting the intuition gained from classical physics.

We analyze the quantum tunneling by means of a semiclassical approach of quantum mechanics [11] which resembles the description given by Bohm [12], in which the evolution of the system is given by an ensemble of trajectories. An appealing feature of the Bohmian description is that one can impose initial conditions for the trajectories, just as in any classical dynamical system, thus allowing the determination of several features of the system and its evolution, like the time of tunneling (or time of reaction in some application processes). As Bohm’s mechanics is based on an ensemble of trajectories the information of such system is subject to statistical fluctuations. We employ an alternative approach based on one-particle trajectories in an extended phase space given by expectation values of quantum observables and higher order moments. A similar method has been used in quantum chemistry [13] where ionization and chemical reactions are studied. The interaction between the expectation values, which can be interpreted as classical canonical dynamical variables, and the momenta and dispersions through the coupled equations of motion generically lower and modify the classical barrier, in this way one can interpret in a natural manner reflection, the crossing or even the “trapping” of the classical particle under such a potential, behavior not shown in the classical setting.

In this model one can study, for instance, which of the individual trajectories pass through the barrier even if at a later time it crosses back or even gets trapped, as we will show. Although quantum trajectories are not experimentally observable, one can still extract valuable information from this qualitative tunneling that could be used in several ways, for example, in designing quantum control experiments involving tunneling. This model has also been proved effective for a semiclassical description of several quantum cosmological models [14], and more recently it provides a very interesting tool in analyzing the concept of tunneling times [15].
Our manuscript is organized as follows: in section 2 we describe the momentous semiclassical description of quantum mechanics, the semiclassical effective description of a quantum system as a Hamiltonian dynamical system of expectation values and dispersions with infinitely many degrees of freedom. In section 3 we describe the model for which we want to study the tunnel effect, its description in terms of effective momenta and the classical potential barrier. In section 4 initial conditions for the evolution of the system are given whereas in section 5 we solve the system numerically and describe the behavior of the system in terms of effective trajectories and the interpretation of the transmission and reflection. In section 6 we provide a discussion of our results and propose several future extensions of our proposal.

2. Effective dynamics of quantum systems: Momentous quantum mechanics

Despite the successful impact of quantum mechanics in the development of science and technology, in the core of its very definition is the fact that it is probabilistic in nature. This fact, together with its intricate dynamics, make the study of general systems very involved, making the use of semiclassical approximations a very useful, and sometimes necessary tool. Semiclassical approximations are of importance in order to extract new effects or potentially observable phenomena in regimes in which quantum features are relevant. Several such approximations have been developed [9, 13], specially the one known as semiclassical momentous quantum mechanics [11].

This formulation provides a system of semiclassical equations that are equivalent to the full quantum description. One obtains an effective Hamiltonian from which equations of motion may be derived, treating expectation values of observables, their associated momenta and dispersions as classical configuration variables. Quantum fluctuations are introduced as a set of new semiclassical dynamical variables, defined as

$$G^{a,b} = \langle (\hat{x} - x)^a (\hat{p} - p)^b \rangle_{\text{Weyl}}, \quad a + b \geq 2$$

where $x = \langle \hat{x} \rangle$ and $p = \langle \hat{p} \rangle$, and the subscript indicates that the operators inside the brackets are Weyl ordered. We obtain, thus, a classical evolution that gets quantum back-reacted by the quantum variables (or dispersions) and therefore modified.

The quantum dispersions are not completely arbitrary, they are subject to generalized uncertainty relations such as

$$G^{2,0}G^{0,2} - (G^{1,1})^2 \geq \frac{\hbar^2}{4}. \quad (2)$$

$G^{2,0}$ and $G^{0,2}$ are the standard dispersions $\Delta x^2$ and $\Delta p^2$, and (2) simplifies to the usual uncertainty principle for pure states [10].

Evolution is obtained in the usual way, by evaluating Poisson brackets of variables and momenta with the quantum effective Hamiltonian, defined as the expectation value of the standard Hamiltonian operator

$$\langle \hat{H} \rangle \equiv H_Q = H(x, p) + \sum_{a,b} \frac{1}{a!b!} \frac{\partial^{a+b} H}{\partial x^a \partial p^b} G^{a,b}, \quad (3)$$
where $H(x,p)$ is the classical Hamiltonian. Equations of motion are obtained in the Hamiltonian formulation $\dot{f} = \{f, H_Q\}$. Quantum variables $G^{a,b}$ are now dynamical, as the classical ones $(x,p)$. It is evident that, for general systems, one gets an infinite-dimensional dynamical system that, however complicated, provides a full description of the system.

To obtain equations of motion for momenta we need to compute their Poisson brackets with the quantum-corrected Hamiltonian: for systems with one degree of freedom we get

\begin{align}
\{x,p\} &= 1, \\
\{x,G^{a,b}\} &= 0, \\
\{p,G^{a,b}\} &= 0.
\end{align}

The Poisson algebra for the moments was obtained in general in \cite{14}

\begin{align}
\{G^{a,b},G^{c,d}\} &= a d G^{a-1,b} G^{c-1,d} - b c G^{a,b-1} G^{c-1,d} + \\
&\quad + \sum_n \left(\frac{i\hbar}{2}\right)^{n-1} K^{n}_{abcd} G^{a+c-n,b+d-n},
\end{align}

where the sum runs over odd numbers from $n = 1 \ldots \tilde{N}$, with $1 \leq \tilde{N} < \min[a+c,b+d,a+b,c+d]$, and the coefficient is

\begin{align}
K^{n}_{abcd} &= \sum_{s=0}^{n} (-1)^{s} s!(n-s)! \binom{a}{s} \binom{b}{n-s} \binom{c}{n-s} \binom{d}{s}.
\end{align}

This method has been successfully applied to several interesting physical systems, most notably to the quantum harmonic oscillator, where it was shown that the ground state energy is added to the classical Hamiltonian \cite{11,16}, and also to anharmonic systems where adiabatic approximations were proven useful. It has also been applied to the isotropic and homogeneous model in loop quantum cosmology \cite{17,18}, and to study different cosmological models with matter \cite{19}, cosmological constant, among others.

It is also possible to generalize the above formulae for systems with more than one pair of canonical conjugate variables, however for the purposes of our analysis the description with one degree of freedom will suffice (see \cite{14}). We present this generalized analysis in the appendices.

### 3. Classical description of the tunnel effect

We want to analyze the tunnel effect for particles scattering off a potential barrier, a system with one degree of freedom, so we will describe the classical scenario. This will make clear different aspects we will exploit when we study the quantum case. We consider smooth potentials in our effective description (3), although general potentials can be used. The system consists of particles of mass $m$ in the presence of a family of potentials of the form
Effective quantum tunneling from semiclassical momentous approach

\[ V(q) = \frac{\alpha}{q^{2n} + a^{2n}}, \quad \alpha, a \in \mathbb{R}, \quad n \in \mathbb{N}. \quad (9) \]

with height \( \alpha/a^{2n} \) at \( q = 0 \), \( a \) being the width of the potential. It can bee seen in figure 1 that the larger \( n \) the more the potential looks like the standard potential barrier.

![Figure 1. Potential \( V(q) \) for \( a = 1, \alpha = 1 \), from \( n = 1 \) (green) to \( n = 10 \) (blue)](image)

As usual, classical dynamics is obtained from Hamilton equations

\[ \dot{q} = \{q, H\} = p/m; \quad (10) \]
\[ \dot{p} = \{p, H\} = -V', \quad (11) \]

with Hamiltonian \( H = \frac{p^2}{2m} + V(q) \). Classical return points are given by the condition

\[ V(q) = \frac{\alpha}{x^{2n} + a^{2n}} = E \rightarrow x = a(\gamma - 1)^{1/2n} \quad (12) \]

where \( \gamma = V_0/E \) and \( V_0 = \alpha/a^{2n} \).

Classically there exists no tunneling since a particle incoming from the left will bounce back from the potential whenever \( E < V_0 \) or pass over the barrier when \( E > V_0 \), in this form the particle does not go “through” the barrier. Even so we will discuss the classical evolution in this scenario in order to give more clarity to the quantum semiclassical treatment, as we mentioned above.

Equation (10) gives

\[ p = m\dot{q} = \left[ 2mE \left( \frac{x^{2n} - q^{2n}}{q^{2n} + a^{2n}} \right) \right]^{1/2}, \quad |x| \leq |q|; \quad (13) \]

for \( \gamma \geq 1 \). There are no analytic solutions to this equation for arbitrary values of \( n \) and \( \alpha \), so we perform a numerical analysis. It is possible, however, to obtain an approximate expression for \( q(t) \) in the limiting case when \( \gamma = 1 \) given by
Effective quantum tunneling from semiclassical momentous approach

\[
\left( \frac{q_\circ}{q_0} \right)^{n-1} \approx \frac{1 + \frac{1 - n}{2(1 + n)} q_\circ^{2n}}{\left( \frac{2V_0q_\circ^{2(1-n)}}{ma^2} \right)^{1/2} (n - 1) t + 2F_1 \left[ \frac{1-n}{2n}, \frac{1}{2}; \frac{1+2n}{2n}, q_0^4 \right]},
\]

(14)

where \( q_\circ = |q/a|, \) \( q_0 = |q_i/a|, \) \( q_i \) are the initial positions of the particle and \( 2F_1 \) is the hypergeometric function.

Classical evolution can be obtained by numerically solving the equations of motion above. In figures (2)-(5) we present trajectories for \( \gamma = 1 \) and \( \gamma > 1 \), keeping the other parameters fixed.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{\( \gamma = 1.00. \)}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{\( \gamma = 1.00. \)}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{\( \gamma = 1.46484. \)}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{\( \gamma = 1.46484. \)}
\end{figure}

Different classical behaviors for particles can be seen from the trajectories: for the critical case, \( (\gamma = 1 \iff V_0 = E) \) there is no barrier penetration, all the particles approach the return point and their momentum vanishes, both asymptotically. For the classical forbidden region, \( (\gamma > 1 \iff V_0 < E) \) the reflection is total, trajectories bounce back off the barrier and the momentum changes sign. It is dynamically irrelevant the initial position and the time it takes the particle to reach the potential, but at the quantum level it will prove essential. We will come back to this latter on.
4. Semiclassical evolution

4.1. Semiclassical description

We proceed to investigate the interaction, at the quantum level, of the particles and the potential barrier by analyzing their trajectories, as we did for the classical particle in section 3. To this end we use the formalism presented in section 2. First we write the quantum corrected Hamiltonian (3)

\[ H_Q = H_{\text{class}} + \frac{1}{2m} G^{0,2} + \sum_{n=2}^{\infty} \frac{1}{n!} \frac{d^n V}{dq^n} G^{n,0}. \] (15)

As we mentioned earlier, quantum dynamics is replaced by a Hamiltonian system with infinitely many variables, two conforming the classical phase space \((q, p)\) and infinitely many quantum dispersions acting as corrections in \(H_Q\). The equation of motion for \(p\), equation (11), gets corrected as follows

\[ \dot{p} = \{p, H_Q\} = -V' + \sum_{k=2}^{\infty} \frac{1}{k!} G^{k,0} \left\{ p, \frac{d^k V}{dq^k} \right\}, \] (16)

while the equation for \(q\) does not change.

The system conformed by equations (10), (16), those for the momenta \(G^{ab}\), and suitable initial conditions is what we require to study the evolution of the system and the tunnel effect. However, as we mentioned above, the dynamical system consists of infinitely-many differential equations which, given the form of the potential (9), it is impossible to solve analytically. In order to analyze the evolution we will perform consistent truncations in the dispersions and derive conclusions therein.

4.2. Second order truncation

Let us consider the second order‡ subsystem of (3). The effective Hamiltonian reads

\[ H_Q = \frac{p^2}{2m} + V(q) + G^{0,2} + \frac{1}{2} V'' G^{2,0}. \] (17)

From this we obtain the equations of motion

\[ \dot{q} = \frac{\dot{p}}{m}; \]
\[ \dot{G}^{2,0} = -\frac{2}{m} G^{1,1}; \]
\[ \dot{G}^{0,2} = 2 V'' G^{1,1}; \]
\[ \dot{p} = -V' - \frac{1}{2} V''' G^{2,0}; \]
\[ \dot{G}^{1,1} = -\frac{G^{0,2}}{m} + V'' G^{2,0}. \] (18)

As we mentioned earlier, the dispersions also satisfy the uncertainty relation (2)

\[ G^{2,0}(t) G^{0,2}(t) - (G^{1,1}(t))^2 \geq \frac{\hbar^2}{4}. \] (19)

‡ The order of the truncation is considered in terms of the dispersions, that is, order \(n\) for \(G^{a,b}\) with \(a + b \leq n\).
Effective quantum tunneling from semiclassical momentous approach

The effective Hamiltonian (17) generates a (semi) classical dynamical system, for one can show it is conserved

\[ \frac{d}{dt} \left( \frac{p^2}{2m} \right) = -\frac{dq}{dt} \left( \frac{dV}{dq} + \frac{1}{2} \frac{d}{dq} \left( V'' G^{2,0} \right) \right) \]

\[ = -\frac{dq}{dt} \left( \frac{dV}{dq} + \frac{1}{2} \frac{d}{dq} \left( V'' G^{2,0} \right) - \frac{1}{2} V'' \frac{dG^{2,0}}{dq} \right); \]

\[ \frac{d}{dt} \left( \frac{p^2}{2m} \right) = -\frac{dq}{dt} \left( V + \frac{G^{2,0}}{2} V'' \right) + \frac{1}{2} V'' \dot{G}^{2,0} \]

\[ = -\frac{d}{dt} \left( V + \frac{G^{2,0}}{2} V'' \right) - \frac{2 V''}{2m} G^{1,1}; \]

\[ \dot{H}_Q = \frac{d}{dt} \left( \frac{p^2}{2m} + V + \frac{1}{2} V'' G^{2,0} + \frac{G^{0,2}}{2m} \right) = 0. \]

It is possible to define an effective potential, as is customary in classical mechanics [20]

\[ V_{\text{eff}} = V + \frac{1}{2} V'' G^{2,0} + \frac{G^{0,2}}{2m}. \] (21)

The effective potential is convenient because one can interpret the various types of evolution for the system in terms of this dynamical, quantum-modified potential, in a similar way as in [21].

We can see that the quantum dispersions strongly back-react the dynamics of the classical system, making the evolution non trivial. Even though we were able to obtain a (semi)classical effective Hamiltonian with augmented degrees of freedom it is, even at this second order approximation, not analytically solvable, and a thorough numerical exploration is required, as we will describe.

4.3. Gaussian wavepacket

In order to perform a numerical evolution for the second order system (18) it is necessary to provide initial conditions for the dynamical system

\[ q_0 = \langle \hat{q} \rangle_{t=0}; \]

\[ p_0 = \langle \hat{p} \rangle_{t=0}; \]

\[ G^{2,0}_0 = G(0)^{2,0} = \langle \Delta q^2 \rangle_{t=0}; \]

\[ G^{0,2}_0 = G(0)^{0,2} = \langle \Delta p^2 \rangle_{t=0}; \]

\[ G^{1,1}_0 = G(0)^{1,1} = \text{Re} \left( \langle \Delta \hat{q} \Psi_0 | \Delta \hat{p} \Psi_0 \rangle \right). \] (22)
We propose, for the quantum dispersions $G^{a,b}$, an initial gaussian state from which we determine expectation values as needed [22]. That is
\begin{equation}
\Psi_0 = \frac{1}{(2\pi\sigma_0^2)^{1/4}} \exp \left( -\frac{(q-q_0)^2}{4\sigma_0^2} + i\frac{p_0}{\hbar}(q-q_0) \right),
\end{equation}
with $q_0$ its peak value and $\sigma_0 = \sqrt{G_0^{2,0}}$ its standard deviation. Its probability density is
\begin{equation}
\rho_0(q) = |\Psi_0|^2 = \frac{1}{\sqrt{2\pi\sigma_0^2}} \exp \left( -\frac{(q-q_0)^2}{2\sigma_0^2} \right).
\end{equation}

In this way initial conditions for the momenta $G^{0,2}$, $G^{2,0}$ and dispersion $G^{1,1}$ can be implemented from the parameters above
\begin{equation}
\Delta \hat{q} \Psi_0 = (q-q_0) \Psi_0; \quad \Delta \hat{p} \Psi_0 = \frac{i\hbar}{2\sigma_0^2}(q-q_0) \Psi_0 = \frac{i\hbar}{2\sigma_0^2} \Delta \hat{q} \Psi_0,
\end{equation}
thus
\begin{equation}
G_0^{0,2} = \langle \Delta \hat{p}^2 \rangle_{t=0} = |\Delta \hat{p} \Psi_0|^2 = \left( \frac{\hbar}{2\sigma_0^2} \right)^2 \langle \Delta \hat{q}^2 \rangle = \left( \frac{\hbar}{2\sigma_0} \right)^2;
\end{equation}
\begin{equation}
G_0^{1,1} = \text{Re} \left( \langle \Delta \hat{q} \Psi_0 | \Delta \hat{p} \Psi_0 \rangle \right) = \text{Re} \left( \frac{i\hbar}{2\sigma_0^2} \langle \Delta \hat{q}^2 \rangle \right) = \text{Re} \left( \frac{i\hbar}{2} \right) = 0.
\end{equation}

The simplest and physical way to fulfill the initial conditions above is by satisfying the lower bound for the uncertainty relation (2), that is
\begin{equation}
G_0^{0,2} G_0^{2,0} - G_0^{1,1} = \frac{\hbar^2}{4}.
\end{equation}

5. Numerical evolution

We are ready to analyze the evolution of the system at the order we are considering, driven by the system (18). For generic potential barriers of the form (9) it is not possible to obtain analytical solutions, as stated before, but we can implement a numerical evolution and study its behavior. We show that it is possible to determine not only the transmission coefficients in a very natural and direct way but we can also determine semiclassical trajectories at the same level of those in the Bohmian formulation of quantum mechanics [12].

Equipped with initial conditions (26) we generate trajectories for particles incident from the left at the barrier, with energy $E_0$. We also need initial conditions for the classical configuration variables $(q,p)$, discussed below. Evolution is restricted to physical trajectories, that is, those constrained by the uncertainty relation (2).

Tunneling is attained when the particle reaches points beyond the classical return points $x$ (12), for which we have two types: one where the particle goes beyond $x > 0$ on the right and can (potentially) be detected, and a second where the particle gets
“trapped” inside the potential, \( |q| < x \), as has been discussed in the literature (see for instance [21]). Initial conditions are obtained for quantum dispersions by preparing gaussian packets with parameters \((q_0, p_0, \sigma_0)\).

Transmission (and reflection) coefficient can be defined in an intuitive way: it is the fraction of trajectories passing through the points of return, that is

\[
T_{\text{eff}} \equiv \frac{\text{#Trajectories } q(t) > x}{\text{#Total trajectories}}.
\]  

(28)

We work in units of \( \hbar = 1 \).

5.1. Total reflection

Three different generic behaviors are obtained. The first one shows the evolution of particles that are totally reflected, just as in the classical case. In figures (6)-(14) we show classical trajectories (blue) and semiclassical ones (red) for fixed parameters.

![Figure 6. \(-3.72638 < q_0 < -1.36634\).](image)

![Figure 7. \(-3.33517 < q_0 < -1.2229\).](image)
Effective quantum tunneling from semiclassical momentous approach

Figure 8. $-3.0762 < q_0 < -1.23048$.

Figure 9. $-3.56824 < q_0 < -1.30835$.

Figure 10. $-3.26527 < q_0 < -1.19727$. 
Effective quantum tunneling from semiclassical momentous approach

Figure 11. $-3.06081 < q_0 < -1.22432$.

Figure 12. $-3.46656 < q_0 < -1.27107$.

Figure 13. $-3.21948 < q_0 < -1.18048$. 
Particles whose energy lies below the classical potential, $\gamma > 1$, get reflected at points to the left of the classical return point. It is so because they interact with the effective, time dependent, potential that gets widen from the classical one, as we will show in the next section.

5.2. Tunneling

A second distinctive behavior is when particles interact with the potential barrier and pass through to the right, displaying its true quantum behavior and effectively tunneling. It can be appreciated in figures 15 - 23.

Figure 14. $-3.05059 < q_0 < \pm 1.42361$.

Figure 15. $-2.26967 < q_0 < -2.22546$. 
Effective quantum tunneling from semiclassical momentous approach

Figure 16. $-2.31154 < q_0 < -2.24234$.

Figure 17. $-2.44686 < q_0 < -2.23783$.

Figure 18. $-2.05226 < q_0 < -2.00526$. 
Effective quantum tunneling from semiclassical momentous approach

Figure 19. \(-2.11565 < q_0 < -1.99645\).

Figure 20. \(-2.1548 < q_0 < -2.03283\).

Figure 21. \(q_0 = -1.87645\).
Effective quantum tunneling from semiclassical momentous approach

Once again the interaction with the effective potential seemingly occurs before the classical left turning point, as in the previous case.

In order to provide a more detailed comparison between the classical and quantum behavior we show the semiclassical trajectories bounded by its dispersion (shown here as a blue shadow), \( q(t) \pm \sqrt{G^{2,0}(t)} \), for \( n = 6 \).

**Figure 22.** \(-1.94039 < q_0 < -1.86215\).

**Figure 23.** \(-1.96661 < q_0 < -1.85093\).

**Figure 24.** Representative trajectory.
5.3. Trapping

In the previous subsections we showed particles whose trajectories are totally reflected, as in the classical case, and those tunneled, as only in the quantum regime can occur. There exists a third behavior though, a very particular one, when particles get “trapped”: nor reflected nor transmitted. These particles, classically, would be either reflected or remain at the turning point in an unstable equilibrium for the case $\gamma = 1$, however at the quantum level it appears as if they got trapped inside the barrier. Interestingly enough is the kind of trajectory they present, the bounce back and forth as if trapped inside a kind of harmonic potential, whose explanation can be given in terms of the effective potential defined above.

Figures (27)-(38) show the trajectories and the uncertainty in the position, contrasted with the classical behavior.
Figure 27. $-1.82511 < q_0 < -0.988603$.

Figure 28. $-2.07461 < q_0 < -0.923987$.

Figure 29. $-2.3251 < q_0 < -1.15495$. 
Effective quantum tunneling from semiclassical momentous approach

Figure 30. $-1.67086 < q_0 < -0.998675$.

Figure 31. $-1.86359 < q_0 < -0.931797$.

Figure 32. $-2.07107 < q_0 < -1.26833$. 
Figure 33. $-1.58551 < q_0 < -0.986111$.

Figure 34. $-1.75203 < q_0 < -0.967266$.

Figure 35. $-1.88186 < q_0 < -1.24902$. 
Although possible this kind of behavior is characterized by a high uncertainty making it very unstable. In the next subsection we explain what is the final faith of such particles.

An interpolating curve for the semiclassical transmission coefficient is also shown in Fig.39 by making use of (28) for $\alpha = 1$ and $E = 0.98$ ($\gamma = 1/E$)
Effective potential dynamics

The results obtained in this section can be interpreted, in the light of our semiclassical treatment, by analyzing the dynamics generated by the effective potential (21). We look specifically the case $n = 4$ since it is particularly illuminating and it contains all the features of higher order cases.

In fig. (40) we show the classical potential in dashed blue and some sections of $V_{\text{eff}}(q,t)$ at several constant times whereas in 3 dimensions

![Figure 41. Effective potential $V_{\text{eff}}(q,t)$ as a function of time and position.](image)

We can give an interpretation for the different trajectories shown in this work in following way: the classical potential (9) gets modified due to the quantum back-reaction
of the quantum dispersions, and $V_{\text{eff}}(q,t)$ moves away from the former. For $t = 0$ it is higher than the classical but it gets lower in height for a short period of time, then it bounces up in a symmetrical way and for later times it acquires two new regions of minimal potential where stability can be attained. Incident particles coming from the left encounter the potential at different heights depending on initial conditions in three possible ways

(i) Potential higher than the incident energy: the particle gets reflected;

(ii) Potential lower than the incident energy: if the particle travels the potential while it remains lower than its energy then the particle can go through the potential and emerge on the right and effective tunneling;

(iii) Potential lower than the incident energy: the particle penetrates the potential but, as the later increases its height the particle gets trapped in one of the two potential minima.

Indeed, there is a window for transmission if the particle penetrates the barrier and goes through it for a shorter period of time than that taken for the potential barrier to grow higher than the particle’s energy. This also explains the existence of trapping in between the two potential valleys where the particle bounces back and forth, the particle was able to penetrate the barrier from the left but the potential grew enough so that it bounces back from the right wall.
We illustrate this in the following density plots: In Fig.42 a particle incident from the left gets reflected by $V_{\text{eff}}(q,t)$ as the potential is higher than its energy, whereas in Fig.43 the particles tunnels through the effective potential whereas its peak is lower than $V_{\text{eff}}(0)$. Fig.44 and Fig.45 show the tunneling and trapping of particles inside the two valleys of $V_{\text{eff}}$. As can be seen, when the particles get trapped inside the potential they behave as classical dynamics dictates, they oscillate around the minimum of the potential.

**Figure 42.** Reflection near $V_0$

**Figure 43.** Tunneling at the beginning of $V_{\text{eff}}$.

**Figure 44.** Trapping inside $V_{\text{eff}}$, left potential valley.

**Figure 45.** Trapping inside $V_{\text{eff}}$, right potential valley.
The final faith of the particle is completely probabilistic, due to the uncertainty in the position it is not possible to tell exactly how it is behaving but it will reflect from the barrier if it was trapped in the left valley while it tunnels away if it was trapped in the right valley.

6. Discussion

The detailed physical process of tunneling, a genuinely quantum mechanical effect is usually studied in standard quantum mechanics by means of time-independent or semiclassical methods, such as the WKB, or in a numerical way by computing transmission-reflection coefficients for the system under scrutiny. In this work we have studied the tunneling under a more detailed semiclassical approach, momentous semiclassical mechanics, where one is able to obtain effective individual trajectories for particles thus providing a more intuitive description of the process. These “effective trajectories” resemble those generated in Bohmian approaches of quantum mechanics ([23, 24, 13]).

We were able to generate numerically trajectories of particles for general initial conditions as well as dispersions and momenta that back-react on the classical evolution. In this way one can determine which particles will tunnel through the barrier or reflect from it, but it is also possible, in principle, trace back the original preparation of the system or experiment by measuring or detecting the fraction of transmission, thus providing an interesting experimental tool. In our formulation the definition and determination of transmission and reflection coefficients is very natural an physical by counting those trajectories that actually get transmitted or reflected, there is no need of further assumptions. However, as attractive our results may appear, it is important to mention that we do not obtain a completely deterministic evolution for the particles, the behavior of individual particles is subjected to uncertainty due to the dynamical nature of quantum dispersions showing the ultimate quantum nature of the formulation.

Another noticeable result obtained from this effective formulation of quantum mechanics is that there are three different possibilities for a particle to evolve, they can tunnel the barrier, reflect from it or get trapped inside the potential. This last behavior is due to the fact that the classical potential barrier gets modified, lowered in particular, by the back-reaction of the quantum dispersions, rendering an effective quantum potential, in a total resemblance with the quantum potential obtained in the Bohm formulation [21]. At the beginning of the evolution the effective potential gets lower from its initial value, then it gets higher and modified in such a way that it acquires two valleys of potential; there exists a time interval for which a particle can actually live inside the potential. This behavior is short lived, due to quantum fluctuations the particle ultimately either tunnels away or gets reflected. Certainly this effective potential is worthy of further studies due to the possible implications in several fields [25].

It is possible to compute the time needed for a particle to effective go through the
barrier, the so called tunneling time, although further investigation needs to be done in this matter due to the existence of uncertainty in the evolution. A first discussion in this path has been done in a recent work for a type ionization experiments [15].

It is our opinion that this work may be an interesting starting point for research at an applied level. Even though quantum trajectories are not experimentally observable nor measurable the information our formulation provides can be used as a tool to study experimental processes and phenomena whenever quantum tunneling is present, fields such as quantum control experiments [26], multielectron and ionization experiments [27] among others. It was brought to our attention that the modification of the effective potential and the trapping of particles by the effective potential may have implications in resonant tunneling diodes where the capture of electrons between potential wells is an important feature [28]. Our description is not complete, however, it is an approximation in the sense that it is not possible to solve the whole system in general, even so we consider that it is interesting in its own right as a ground where some predictions or hypothesis could be tested.

Appendix A. Third order evolution

We show the evolution of the system with effective Hamiltonian (15) at third order in quantum dispersions \(G^{a,b}\). At this order the Hamiltonian reads

\[
H_Q = H_{\text{class}} + \frac{G^{0,2}}{2m} + \frac{1}{2} V'' G^{2,0} + \frac{1}{6} V''' G^{3,0},
\]

and now the system consists of classical configuration variables \((p,q)\), second order momenta \((G^{2,0}, G^{1,1}, G^{0,2})\) and third order momenta \((G^{3,0}, G^{2,1}, G^{1,2}, G^{0,3})\), with equations of motion

\[
\begin{align*}
\dot{q} &= p/m; \\
\dot{p} &= -V' - \frac{1}{2} V''' G^{2,0} - \frac{1}{6} V''' G^{3,0}; \\
\dot{G}^{0,2} &= 2 V'' G^{1,1} + V''' G^{2,1}; \\
\dot{G}^{2,0} &= -\frac{2}{m} G^{1,1}; \\
\dot{G}^{1,1} &= -\frac{m}{G^{0,2}} + V'' G^{2,0} + \frac{1}{2} V''' G^{3,0}; \\
\dot{G}^{1,2} &= -\frac{m}{G^{0,3}} + 2 V'' G^{2,1}; \\
\dot{G}^{2,1} &= -\frac{3m}{G^{1,2}} + V''' G^{3,0}; \\
\dot{G}^{3,0} &= -3 V'' G^{1,2}; \\
\dot{G}^{0,3} &= 3 V'' G^{1,2}.
\end{align*}
\]

Again initial conditions are obtained from the initial gaussian wavepacket as we did...
in section 4.3. Conditions (26) get complemented by the following

\[ G_{0}^{3,0} = \langle \Delta \hat{q}^{3} \rangle = 0; \]

\[ G_{0}^{0,3} = \langle \Delta \hat{p}^{3} \rangle = \frac{i \hbar}{2 \sigma_{0}^{2}} \langle \Delta \hat{p}^{2} \Delta \hat{q} \psi_{0} \rangle = -\frac{\hbar^{2}}{\sigma_{0}^{2}} p_{0} + \frac{i \hbar}{2 \sigma_{0}^{2}} p_{0}^{2} \langle \Delta \hat{q} \rangle = -\frac{\hbar^{2}}{\sigma_{0}^{2}} p_{0} \]

\[ G_{0}^{1,2} = \text{Re}(\langle \Delta \hat{q} \psi_{0} | \Delta \hat{p}^{2} \psi_{0} \rangle) = \text{Re}(\langle \Delta \hat{p}^{2} \Delta \hat{q} \psi_{0} | \psi_{0} \rangle) = \text{Re}(-i 2 \hbar p_{0}) = 0; \]

\[ G_{0}^{2,1} = \text{Re}(\langle \Delta \hat{p}^{2} \psi | \Delta \hat{q} \psi_{0} \rangle) = \text{Re}(\langle \psi | \Delta \hat{p}^{2} \Delta \hat{q} \psi_{0} \rangle) = \text{Re}(i 2 \hbar p_{0}) = 0. \]

Below we show trajectories for the three cases: reflection, tunneling and trapping, and trajectories with uncertainty for transmission and trapping.
Effective quantum tunneling from semiclassical momentous approach

Figure A3. Left trapping and reflection with uncertainty shadow

Figure A4. Tunneling and its uncertainty.

Notice that, at this order, the behavior is quite similar to that at second order. For the effective potential and the three semiclassical regimes we obtain, at third order

Figure A5. $V_{\text{eff}}(q)$ and $V_{\text{class}}$ in dashed blue, for some values of $t$. 
We obtain the same behavior for trajectories at third order in comparison to those at second order in momenta, under the same set of initial parameters, with an absolute error between them of the order of 5%. For the purpose of analyzing the tunnel effect within the effective momentous method presented here one can restrict the study to second order with a high order of accuracy.

References

[1] Main I.G. 1993, Vibrations and Waves in Physics, (Cambridge: University Press) 3rd ed.
[2] Fowler R. H. and Nordheim L. W. 1928, Proc. Roy. Soc. Lond. A 119 173
[3] Gamow G 1928 Z. Phys. 51 204
[4] Bethe H.A. 1937, Rev. Mod. Phys. 9, 161
[5] Heitler W. 1967, Int. J. Quantum Chem. 1, 37
[6] Kronig R. de L. 1932, Band Spectra and Molecular Structure, (Cambridge University Press)
[7] Esaki L. 1974, Proc. of the IEEE, 62, 825
[8] Giaever I. 1974, Science, 183, 1253
[9] Razavy M 2014, Quantum Theory of Tunneling (New Jersey: World Scientific), 2nd Ed;
    Ankerhold J 2007, Quantum Tunneling in Complex Systems, The Semiclassical Approach
    (Springer-Verlag Berlin Heidelberg);
    Wyatt R 2005, Quantum Dynamics with Trajectories, Introduction to Quantum Hydrodynamics
    (Springer Science+Business Media, Inc)
[10] Dirac P.A.M. 1958, The Principles of Quantum Mechanics (Oxford Univ. Press, London), 4th Ed
    Sakurai J.J. 1994, Modern Quantum Mechanics (Addison Wesley Pub, USA), Rev. Ed.
    Griffiths, D. 2017. Introduction to quantum mechanics. (Cambridge Univ. Press.) 1st Ed.
[11] Bojowald, M. and Skirzewski, A. 2006, Rev. Math. Phys. 18, 07.
[12] Bohm D. 1952, Phys. Rev. 85 166; Bohm D. 1952, Phys. Rev. 85 180
[13] Prezhdo O. V, Pereverzev Y. V. 2002, J. Chem. Phys. 116, 4450
    Prezhdo O. V, Brooksby C, 2001, Phys. Rev. Let. 86, 15
[14] Bojowald M, Brizuela D, Hernandez H. H, Koop M. J. and Morales-Tecotl H. A. 2011, Phys. Rev. D 84, 043514
[15] Baytas B, Bojowald M, Crowe S, 2018, Phys. Rev. A, 98 6, 063417
[16] Bojowald M. 2011, arXiv:1101.5592
[17] Bojowald M. 2007, Phys. Rev. D 75, 081301(R); Bojowald M, 2007, Phys. Rev. D 75, 123512
Effective quantum tunneling from semiclassical momentous approach

[18] Bojowald M. 2007, Nature Physics 3, 523
[19] Bojowald M. Hernández H. H. and Skirzewski A. 2007, Phys. Rev. D 76, 063511
[20] Goldstein H. 2002, Classical mechanics, (San Francisco: Addison Wesley) 1st Ed
[21] Dewdney C, Hiley B.J. 1982, Found. Phys. 12(1), 27-48.
[22] Brizuela, D. 2014, Phys. Rev. D. 90, 8
[23] Sanz A.S, Miret-Arts S. 2011, J. Phys. A: Math. Theo, 44(48), 485301
[24] Sanz A.S, Miret-Arts S. 2013, A Trajectory Description of Quantum Processes, A Bohmian Perspective. (Springer)
[25] Licata I, Fiscaletti D. 2014, Quantum potential: Physics, geometry and algebra. (New York: Springer)
[26] Ohmura H, Saito N, Morishita T. 2011, Phys. Rev. A, 83(6), 063407
[27] Shevelko V, Tawara H. 2013, Atomic multielectron processes, Vol. 23 (Springer Science and Business Media)
[28] Sun J.P, Haddad G.I, Mazumder P, Schulman J.N, J. N., 1998, Proc. IEEE, 86(4), 641-660