

Chapter 2

Some Selected Applications of Bohmian Mechanics

Abstract In this chapter, our purpose is to simply show that Bohmian mechanics is a powerful route to bring about new solutions to problems discussed by conventional quantum mechanical approaches, apart from allowing some striking correspondence between both frameworks. This goal is carried out by choosing some key quantum mechanical problems in the framework of Bohmian mechanics such as, for example, the so-called Ermakov–Bohm invariants, boundary conditions and uncertainty principle in tunneling, the quantum traversal time, Airy wave packets and Airy slits, the detection of inertial and gravitational masses with Airy wave packets, the geometric phase analyzing the Aharonov–Bohm effect and quantum vortices, the reformulation of the Gross–Pitaevskii equation within the hydrodynamical framework and, finally, the study of simple dissipative dynamics by using the well-known Caldirola–Kanai Hamiltonian. In this dissipative scenario, the motion of a free particle, the quantum interference of two wave packets and the dynamics in a linear potential as well as the corresponding of a damped harmonic oscillator (within the underdamped, critically damped and overdamped regimes) are finally analyzed for ulterior references.

2.1 Introduction

Recently, Bernstein has presented a pedagogically clear and historically brilliant review of the Bohmian theory [1] showing that it is sharp where the usual one is fuzzy and general where the usual one is special. Bell and Bernstein argued convincingly that the de Broglie–Bohm interpretation of quantum mechanics should be known from the very beginning and part of any college curriculum on the subject.

In this theory, the wave function provides only a partial description of the system. The description is completed by the specification of the actual positions of the particles which evolve according to the so-called guidance condition or guiding equation, Eq. (1.20). This equation provides the velocity of the particles in terms of the wave function. However, the trajectory of a particle is not at all classical; it is instead determined by the structure of the associated quantum wave which guides or pilots the particle along its path.

Comprehensive discussions of Bohmian mechanics can be found everywhere in the literature [2–6]. In this Chapter, we want to show that Bohmian mechanics is a powerful route to bring about new solutions to problems discussed by conventional quantum mechanical approaches, apart from allowing some striking correspondence between both frameworks. This goal is carried out by choosing some key quantum mechanical problems in the framework of Bohmian mechanics such as, for example, the so-called Ermakov–Bohm invariants, Airy wave packets and Airy slits, the geometric phase analyzing the Aharonov–Bohm effect and quantum vortices, reformulating the Gross–Pitaevskii equation within the hydrodynamical framework and, finally, the study of simple dissipative dynamics by using the well-known Caldirola–Kanai Hamiltonian. In this dissipative scenario, the motion of a free particle, the quantum interference of two wave packets and the dynamics in a linear potential as well as the corresponding of a damped harmonic oscillator (within the underdamped, critically damped and overdamped regimes) are finally analyzed for ulterior references.

2.2 Ermakov–Bohm Invariants for the Time-Dependent Harmonic Oscillator

A paradigmatic problem in classical and quantum mechanics is the one-dimensional harmonic oscillator. After Schrödinger developed wave mechanics, he tried very hard to make it into a classical theory. The wave packets describing the simple harmonic oscillator with constant frequency seemed like a good candidate. It is well known that the ground state of the oscillator has the minimum possible uncertainty, which suggests that wave packets associated with this state might show some classical behavior. A quite interesting extension of this problem is within the theory of invariants (constant of motion) for the time-dependent harmonic oscillator (TDHO) discovered by Ermakov [7–9]: it consists of demonstrating that for the corresponding equation of motion

$$\ddot{q}(t) + \omega^2(t)q(t) = 0 \quad (2.1)$$

there exists a time-dependent invariant

$$I = \frac{1}{2} \left[\left(\dot{q}(t)\delta(t) - \dot{\delta}(t)q(t) \right)^2 + \left(\frac{q(t)}{\delta(t)} \right)^2 \right] \quad (2.2)$$

provided that

$$\ddot{\delta}(t) + \omega^2(t)\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)}, \quad (2.3)$$

where $q(t)$, $\delta(t)$ and $\omega(t)$ represent the wave packet center of mass, width and frequency of the TDHO, respectively. Interestingly enough, this time-dependent invariant emerges naturally within Bohmian mechanics. It constitutes a natural connection between the classical to the quantum regime.

To demonstrate such an invariant, the associated Schrödinger equation can be written as

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + \frac{1}{2}m\omega^2(t)x^2\psi(x, t), \quad (2.4)$$

where m is the mass of the TDHO. Equation (2.4) can now be solved via the Bohmian formalism. To this end, the wave function is again expressed in polar form as

$$\psi(x, t) = \phi(x, t) \exp(iS(x, t)/\hbar). \quad (2.5)$$

Now, after substitution of Eq. (2.5) into (2.4), we obtain the following differential equation in partial derivatives

$$\begin{aligned} i\hbar \left[\frac{\partial \phi}{\partial t} + \frac{i}{\hbar} \frac{\partial S}{\partial t} \phi \right] = \\ = -\frac{\hbar^2}{2m} \left\{ \left[\frac{\partial^2 \phi}{\partial x^2} - \frac{\phi}{\hbar^2} \left(\frac{\partial S}{\partial x} \right)^2 \right] + \frac{i}{\hbar} \left[2 \frac{\partial S}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial^2 S}{\partial x^2} \right] \right\} + \frac{1}{2}m\omega^2 x^2 \phi. \end{aligned}$$

The equation above can be as usual separated into real and imaginary parts to give

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} = -\frac{1}{m} \frac{\partial}{\partial x} (Q + V), \quad (2.6)$$

and

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0, \quad (2.7)$$

with the following definitions for the quantum hydrodynamical density

$$\rho(x, t) = \phi^2(x, t), \quad (2.8)$$

the velocity

$$v = \frac{1}{m} \frac{\partial S}{\partial x}, \quad (2.9)$$

the quantum potential

$$Q = -\frac{\hbar^2}{2m\phi} \frac{\partial^2 \phi}{\partial x^2}, \quad (2.10)$$

and the interaction potential

$$V = \frac{1}{2} m \omega^2(t) x^2. \quad (2.11)$$

Equation (2.6) is an Euler-type equation describing trajectories of a fluid particle, with momentum $p = mv$, whereas Eq. (2.7) describes the evolution of the quantum fluid density ρ . This density is interpreted as the probability density of a particle being actually present within a specific region. Such a particle follows a definite space-time trajectory that is determined by its wave function through an equation of motion in accordance with the initial position, formulated in a way that is consistent with the Schrödinger time evolution. An essential and unique feature of the quantum potential is that the force arising from it is unlike a mechanical force of a wave pushing on a particle with a pressure proportional to the wave intensity.

By assuming now that the wave packet is initially centered at $x = 0$ and given by a Gaussian function, $\rho(x, 0) = [2\pi\delta^2(0)]^{-1/2} \exp[-x^2/2\delta^2(0)]$ then ρ vanishes for $|x| \rightarrow \infty$ at any time and we may rewrite

$$\rho(x, t) = |\psi(x, t)|^2 = [2\pi\delta^2(t)]^{-1/2} \exp\left(-\frac{[x - q(t)]^2}{2\delta^2(t)}\right), \quad (2.12)$$

$\delta(t)$ being the total width of the Gaussian wave packet and $q(t)$ a classical trajectory. Equation (2.12) can be readily used to demonstrate that

$$\int_{-\infty}^{+\infty} ([x - q(t)]^2) \rho(x, t) dx = \delta^2(t). \quad (2.13)$$

Substitution of Eq. (2.12) into (2.7) yields

$$\frac{\partial \rho}{\partial t} = \left[-\frac{\dot{\delta}}{\delta} + \frac{(x - q)}{\delta^2} \dot{q} + \frac{1}{\delta^3} (x - q)^2 \dot{\delta} \right] \rho, \quad (2.14)$$

and

$$\frac{\partial(\rho v)}{\partial x} = \left(\frac{\dot{\delta}}{\delta}\right)\rho + \left[\left(\frac{\dot{\delta}}{\delta}\right)(x - q) + \dot{q}\right]\left(-\frac{(x - q)}{\delta^2}\right)\rho, \quad (2.15)$$

which implies that

$$v(x, t) = \left(\frac{\dot{\delta}}{\delta}\right)(x - q) + \dot{q}. \quad (2.16)$$

Analogously, substitution of Eq. (2.16) into (2.6) yields

$$\left(\ddot{\delta}(t) + \omega^2(t)\delta - \frac{\hbar^2}{4m^2\delta^3(t)}\right)(x - q)^1 + (\ddot{q} + \omega^2(t)q)(x - q)^0 = 0, \quad (2.17)$$

leading to Eqs. (2.1) and (2.3).

In 1880, Ermakov [10] was the first to describe a relationship between nonlinear differential equations of second order such as Eq. (2.3) and a particular type of the linear equation (2.1). At the beginning of the thirties, Milne [11] developed a method quite similar to the WKB technique where the same nonlinear equation found by Ermakov occurred, and applied it successfully to several model problems in quantum mechanics. Further, in 1950, the solution to this nonlinear differential equation was given by Pinney [12]. It is worth pointing out that the term on the right side of Eq. (2.3) depends on $\hbar$ in contrast to a similar nonlinear equation studied by Ermakov, Milne and Pinney which contains an arbitrary constant. This $\hbar$ -term emerges naturally from the presence of the quantum potential $\mathcal{Q}$ given by Eq. (2.10).

By eliminating $\omega^2(t)$ between the two equations above, one obtains the invariant in Eq. (2.2). Inasmuch as this invariant connects the classical and quantum regimes, we call it an *Ermakov–Bohm invariant*. Further, from Eqs. (2.6) and (2.7), we can construct the relations for the energy density U , energy density flux $\mathcal{Q}$, momentum J and momentum flux P , respectively

$$\frac{\partial U}{\partial t} + \frac{\partial \mathcal{Q}}{\partial x} = 0, \quad (2.18)$$

$$\frac{\partial J}{\partial t} + \frac{\partial P}{\partial x} + \frac{\rho}{m} \frac{\partial V}{\partial x} = 0, \quad (2.19)$$

where

$$U = \rho \left(\frac{1}{2} m v^2 + V + \mathcal{Q} \right), \quad (2.20)$$

$$\mathcal{Q} = vU + \frac{\hbar^2}{2m^2} \left[\sqrt{\rho} \frac{\partial^2 \sqrt{\rho}}{\partial x \partial t} - \frac{\partial \sqrt{\rho}}{\partial t} \frac{\partial \sqrt{\rho}}{\partial x} \right], \quad (2.21)$$

$$J = \rho v \quad (2.22)$$

and

$$P = \rho v^2 - \frac{\hbar^2}{4m^2} \left[\frac{\partial^2 \rho}{\partial x^2} - \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 \right]. \quad (2.23)$$

Next, the wave packet dynamics will be completely determined by the solutions to Eqs. (2.3) and (2.1), which describe the time evolution of the width and center of the packet.

Integration of Eqs. (2.3) and (2.1) are subject to the general initial conditions [13]

$$\delta(0) = \delta_0, \quad \dot{\delta}(0) = d_0, \quad (2.24)$$

and

$$q(0) = q_0, \quad \dot{q}(0) = V_0. \quad (2.25)$$

In the following, we show that the general solution to the quantum Eq. (2.3) can be obtained with the help of just one particular solution to the classical Eq. (2.1). To this end, let us now substitute

$$\delta(t) = r(\theta) \alpha(t) \quad (2.26)$$

where we define [13]

$$d\theta = dt/\alpha^2(t) \quad (2.27)$$

and substitute into Eq. (2.26) to obtain the first Ermakov–Bohm invariant of motion

$$I_1 = [r(\theta)]^2 + \frac{\hbar^2}{4m^2} \left(\frac{1}{r(\theta)} \right)^2, \quad (2.28)$$

provided that

$$\ddot{\alpha} + \omega^2(t)\alpha = 0. \quad (2.29)$$

Upon a second integration Eq. (2.28) can be recast with the help of Eq. (2.26) as

$$\delta^2(t) = \left(\frac{\hbar^2}{4m^2 I_1} + I_1 I_2^2 \right) \alpha_1^2(t) + I_1 \alpha_2^2(t) + 2I_1 I_2 \alpha_1(t) \alpha_2(t) \quad (2.30)$$

where α_1 and α_2 are two independent solutions to the classical Eq. (2.29). The two constants I_1 and I_2 represent two Ermakov–Bohm invariants of motion of the problem. In addition, the two independent solutions to Eq. (2.29) can be obtained in general from just one particular solution to the same equation, namely,

$$\alpha_1(t) \equiv \alpha(t) \quad (2.31)$$

and

$$\alpha_2(t) \equiv \alpha(t) \int^t \frac{dt}{\alpha^2(t)}. \quad (2.32)$$

If initial conditions are imposed as follows

$$\alpha(0) = 1 \text{ and } \dot{\alpha}(0) = 0 \quad (2.33)$$

we are led to

$$\alpha_1(0) = 1, \alpha_2(0) = 0, \dot{\alpha}_1(0) = 0, \text{ and } \dot{\alpha}_2(0) = 1. \quad (2.34)$$

These initial conditions allow us to find that the two *Ermakov–Bohm* invariants of motion are given by:

$$I_1 = d_0^2 + (\delta_0^2/\tau^2), \quad (2.35)$$

and

$$I_2 = \delta_0 d_0 / [d_0^2 + (\delta_0^2/\tau^2)]. \quad (2.36)$$

Thus, the complete dynamics of the TDHO can be found with the help of Eqs. (2.31), (2.32), (2.35) and (2.36): the generalized squeezed states for the TDHO wave packet is finally written as

$$\delta(t) = \delta_0 \alpha(t) \left\{ 1 + \left(\frac{2\varsigma}{\tau} \right) \left[\int^t \frac{dt}{\alpha^2(t)} \right] + \left(\frac{(1+\varsigma^2)}{\tau^2} \right) \left[\int^t \frac{dt}{\alpha^2(t)} \right]^2 \right\}^{1/2} \quad (2.37)$$

where $\tau = 2m \delta_0^2/\hbar$, and $\varsigma = 2m \delta_0 d_0/\hbar$. In turn, the packet center of gravity evolves according to

$$q(t) = \alpha(t) \left\{ q_0 + V_0 \int^t \frac{dt}{\alpha^2(t)} \right\}. \quad (2.38)$$

Now, the full wave packet can be written in its final, general form as

$$\psi(x, t) = (2\pi\delta^2(t))^{-1/4} \exp \left[-\frac{[x - q(t)]^2}{4\delta^2(t)} + \frac{i}{\hbar} [S_1(x, t) + S_0(t)] \right] \quad (2.39)$$

where

$$S_1(x, t) = \frac{m\dot{\delta}(t)}{2\delta(t)} [x - q(t)]^2 + m\dot{X}(t)[x - q(t)] \quad (2.40)$$

and

$$S_0(t) = \int_0^t dt' \left(\frac{1}{2} m \dot{q}^2(t') - \frac{1}{2} m \Omega^2 q^2(t') - \frac{\hbar^2}{4m\delta^2(t')} \right). \quad (2.41)$$

The wave packet surrounds the position of the classical particle and the center of gravity of the packet follows the classical trajectory: its time evolution is completely determined by the quantum and classical solutions (2.37) and (2.38), respectively.

At the moment of observation, the packet is moving with an initial velocity V_0 and spreading with an initial rate d_0 . The associated variance of x [squared uncertainty] can be written as $[\Delta x(t)]^2 = \delta^2(t)$, which exhibits generalized squeezed states for the TDHO. Above all, our method gives a general solution to the quantum TDHO from just one particular solution $\alpha(t)$ to the classical time-dependent oscillator (2.29) in terms of two Ermakov–Bohm invariants of motion [13].

Finally, the associated Bohmian trajectories of an evolving i th particle of the ensemble with an initial position x_{0i} can be calculated via Eq. (2.16)

$$\dot{x}_i(t) = \dot{q}(t) + [x_i(t) - q(t)] \frac{\dot{\delta}(t)}{\delta(t)} \quad (2.42)$$

or

$$\int_0^t \frac{d}{dt'} (\ln[x_i(t') - q(t')]) dt' = \int_0^t \frac{d}{dt'} [\ln \delta(t')] dt' \quad (2.43)$$

leading to

$$x_i(t) = q(t) + (x_{0i} - q_0) \frac{\delta(t)}{\delta_0}, \quad (2.44)$$

where $\delta(t)$ and $q(t)$ are given by (2.37) and (2.38), respectively. Furthermore, Eqs. (2.16) and (2.44) also reproduce the dressing scheme of the quantum trajectory (velocity and position, respectively) mentioned in Chap. 1. In this scheme, the

quantum or nonlocal contribution is governed by the time evolution of the Gaussian wave packet width. This pattern is going to be also reproduced along this chapter as well as in the remaining chapters dealing with open quantum systems.

2.3 Boundary Conditions in Tunneling

A commonly used assumption in quantum mechanics [14–17] is that the boundary conditions at a surface where the potential undergoes a finite jump reduce to the requirement that both the wave function ψ and its derivative $(\partial\psi/\partial x)$ be continuous at the surface. It is illustrative to show through Bohmian mechanics how more general boundary conditions follow from the continuity of mass, momentum and energy densities. With this new boundary conditions, a novel approach to tunneling through sharp-edged potential barriers is presented.

Let us consider the dynamics of a quantum particle described by the coupled hydrodynamical equations (2.6) and (2.7), as previously defined. The momentum density ρv appearing in the hydrodynamical equations can be the real part of a more general quantum mechanical local momentum field P defined from the momentum-density operator as

$$P = \frac{\hbar}{i} \psi^* \frac{\partial \psi}{\partial x} = m\rho(v + iu), \quad (2.45)$$

where $u = -(\hbar/2m\rho)(\partial\rho/\partial x)$. So, it follows that the boundary conditions for the continuity of mass, momentum and energy are [18]

$$\rho, \rho v, \rho u, \rho \left(\frac{1}{2}mv^2 + V + Q \right). \quad (2.46)$$

In terms of the wave function, these boundary conditions become $(\psi^*\psi)$, $[\psi^*(\partial\psi/\partial x)]$ and $\partial S/\partial t = -(\frac{1}{2}mv^2 + V + Q)$.

Next, let us apply these boundaries conditions to the following quantum tunneling problem. Consider a particle with incident energy E striking a potential barrier of height V and width L : $V(x) = V$ for $0 < x < L$ and zero elsewhere. In what follows $a, b, c, d, \alpha, \beta$ and δ are constants to be determined and $k^2 = 2mE/\hbar^2$ and $\bar{q}^2 = 2m(V - E)/\hbar^2$. In a polar form, the wave function for $x < 0$ (incident region 1) is

$$\psi_1(x, t) = \sqrt{\rho_1} \exp(iS_1/\hbar), \quad (2.47)$$

where – detailed calculations can be found in Ref. [19] and Sect. 2.5,

$$\rho_1 = 1 + a^2 + 2a \cos(2kx - \alpha) \quad (2.48)$$

and

$$S_1/\hbar = -\omega t + \frac{\alpha}{2} + \tan^{-1} \left[\frac{1-a}{1+a} \tan \left(kx - \frac{\alpha}{2} \right) \right]. \quad (2.49)$$

For $0 < x < L$ (tunneling region 2), the wave function reads

$$\psi_2(x, t) = \sqrt{\rho_2} \exp(i S_2/\hbar) \quad (2.50)$$

where

$$\rho_2 = \frac{1}{\bar{q}} \left[c^2 e^{2\bar{q}x} + d^2 e^{-2\bar{q}x} + 2dc \cos(\beta - \delta) \right] \quad (2.51)$$

and

$$S_2/\hbar = -\omega t + \frac{\beta + \delta}{2} + \tan^{-1} \left[\frac{ce^{\bar{q}x} - de^{-\bar{q}x}}{ce^{\bar{q}x} + de^{-\bar{q}x}} \tan \left(\frac{\beta - \delta}{2} \right) \right]. \quad (2.52)$$

For $x > L$ (transmission region 3), the wave function is given by

$$\psi_3(x, t) = \sqrt{\rho_3} \exp(i S_3/\hbar), \quad (2.53)$$

where

$$\rho_3 = b \quad (2.54)$$

and

$$S_3/\hbar = -\omega t + kx + \beta, \quad (2.55)$$

The boundary conditions from Eq. (2.46) where the potential undergoes a finite jump read

$$\rho_1(0) = \rho_2(0), \quad (2.56)$$

$$\rho_2(L) = \rho_3(L), \quad (2.57)$$

$$\rho_1'(0) = \rho_2'(0), \quad (2.58)$$

$$\rho_2'(L) = \rho_3'(L), \quad (2.59)$$

$$\rho_1(0)v_1(0) = \rho_2(0)v_2(0), \quad (2.60)$$

$$\rho_2(L)v_2(L) = \rho_3(L)v_3(L), \quad (2.61)$$

$$\left(\frac{\partial S_1}{\partial t}\right)_0 = \left(\frac{\partial S_2}{\partial t}\right)_0, \quad (2.62)$$

$$\left(\frac{\partial S_2}{\partial t}\right)_L = \left(\frac{\partial S_3}{\partial t}\right)_L. \quad (2.63)$$

By applying the above boundary conditions on the wave functions (2.47), (2.50) and (2.53), we then obtain

$$1 + a^2 + 2a \cos \alpha = \frac{c^2 + d^2 + 2cd \cos(\beta - \delta)}{\bar{q}}, \quad (2.64)$$

$$\frac{c^2 e^{2\bar{q}L} + d^2 e^{-2\bar{q}L} + 2cd \cos(\beta - \delta)}{\bar{q}} = b^2, \quad (2.65)$$

$$2ak \sin \alpha = (c^2 - b^2), \quad (2.66)$$

$$c = d e^{-2\bar{q}L}, \quad (2.67)$$

$$1 - a^2 = \frac{2d^2 e^{-2\bar{q}L} \sin(\beta - \alpha)}{k}, \quad (2.68)$$

$$\frac{2d^2 e^{-2\bar{q}L} \sin(\beta - \alpha)}{k} = b^2. \quad (2.69)$$

From Eqs. (2.65) and (2.67), we have

$$b^2 = \frac{2d^2 e^{-2\bar{q}L} [1 + \cos(\beta - \alpha)]}{\bar{q}}, \quad (2.70)$$

which combined to Eq. (2.69) yields

$$\tan\left(\frac{\beta - \delta}{2}\right) = \frac{k}{\bar{q}}, \quad (2.71)$$

$$\sin(\beta - \delta) = \frac{2k\bar{q}}{\bar{q}^2 + k^2}, \quad (2.72)$$

$$\cos(\beta - \delta) = \frac{\bar{q}^2 - k^2}{\bar{q}^2 + k^2}. \quad (2.73)$$

Equations (2.69) and (2.73) allow us to write Eq. (2.70) as

$$b^2 = \left(\frac{4\bar{q}}{\bar{q}^2 + k^2} \right) d^2 e^{-2\bar{q}L}, \quad (2.74)$$

which, in turn, combined with Eqs. (2.67) and (2.73), reduces Eq. (2.64) to

$$1 + a^2 + 2a \cos \alpha = b^2 \left(\frac{\bar{q}^2 - k^2}{2\bar{q}^2} \right) \left(1 + \frac{\bar{q}^2 + k^2}{\bar{q}^2 - k^2} \cosh 2\bar{q}L \right). \quad (2.75)$$

Equations (2.68) and (2.69) imply that

$$a^2 = 1 - b^2 \quad (2.76)$$

which inserted into Eq. (2.75) gives

$$a \cos \alpha = b^2 \left(1 + \left[\frac{\bar{q}^2 + k^2}{2\bar{q}^2} \right] \sinh^2 \bar{q}L \right) - 1. \quad (2.77)$$

By the same procedure above, Eq. (2.66) can be rewritten as

$$a \sin \alpha = - \left[\frac{\bar{q}^2 + k^2}{4k\bar{q}} \right] b^2 \sinh 2\bar{q}L. \quad (2.78)$$

Combination of Eqs. (2.76), (2.77) and (2.78) leads to

$$b^{-2} = \frac{\left[1 + \left(\frac{\bar{q}^2 + k^2}{2\bar{q}^2} \right) \sinh^2 \bar{q}L \right]^2 + \left(\frac{\bar{q}^2 + k^2}{4k\bar{q}} \right) \sinh 2\bar{q}L}{\left[1 + \left(\frac{\bar{q}^2 + k^2}{2\bar{q}^2} \right) \sinh^2 \bar{q}L \right]}. \quad (2.79)$$

Using the identity $\sinh^2 2\bar{q}L = 4(\sinh^2 \bar{q}L + \sinh^4 \bar{q}L)$ and after dividing the numerator by the denominator of Eq. (2.79), we arrive at the known result

$$b^{-2} = 1 + \left(\frac{\bar{q}^2 + k^2}{2k\bar{q}} \right)^2 \sinh^2 \bar{q}L. \quad (2.80)$$

2.4 Quantum Potential and Uncertainty Principle in Tunneling

Quantum tunneling is an important effect in many physical phenomena, such as the rate of nuclear fusion, many chemical reactions, and a lot of technology, for example, scanning tunneling microscopy. The basic physics of fusion has been known for some time, and a key element of understanding it is quantum tunneling. Nuclei have a positive electric charge, and since like charges repel, there is an energy barrier to be overcome. Once the barrier is overcome, the strong nuclear force takes over. One way of overcoming the barrier is quantum tunnelling. There is even a possibility that the universe itself might at some point tunnel through to a lower energy state, depending on what the mass of the Higgs boson is exactly.

The role of the quantum potential on the tunneling of a Gaussian wave packet through a rectangular potential barrier is studied here by solving numerically the time-dependent Schrödinger equation via a computer simulation [20–23]. The algorithm used was originally developed by Goldberg et al. [21] and further developed by Koonin [20]. It is assumed that the barrier was confined in a finite region of a one-dimensional space $(0, L)$. At $x = 0$ and L , the wave function is set equal to zero, corresponding to a rigid barrier. The initial wave packet is established in the region to the left of the barrier, just far enough so that initially it does not interact or overlap the barrier. The time-dependent Schrödinger equation is solved numerically to determine the wave function at each time step, with small time increments and parameters used are the same as in Koonin's work [20]. As the time evolves, the wave packet travels to the right, and interacts with the barrier; part of the packet is reflected and part tunnels through, and then emerges from the other side of the barrier.

The familiar picture of a Gaussian wave packet prior to tunneling through a rectangular potential barrier is depicted in Fig. 2.1. The factors δ_i , L , V_0 represent the initial width of the packet, the width of the barrier and the barrier potential energy, respectively.

By analyzing the role of the quantum potential, we demonstrate an unfamiliar aspect of the tunneling rate as the initial wave packet width increases. We begin by recalling that the total energy of the quantum particle is given by: $E_T = \frac{1}{2}mv^2 + V + Q$, where m , v , $V = V_0$ and Q are the mass, velocity, potential-barrier height and

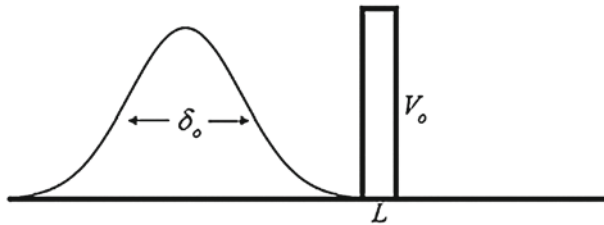


Fig. 2.1 Gaussian wave packet prior to the tunneling through a rectangular potential barrier

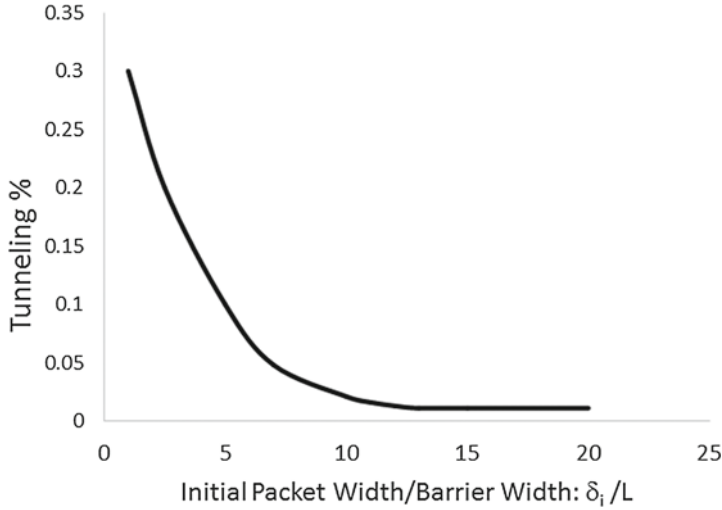


Fig. 2.2 Tunneling versus initial wave packet width

the quantum potential, respectively. In the tunneling case of an initially free-particle wave packet through a potential barrier, the wave packet width before the packet strikes the barrier must have a minimum initial value so that the energy uncertainty $\frac{1}{2}mv_i^2 + Q_i < V_0$ needs to be fulfilled in order to guarantee tunneling through and not hopping over the barrier. The quantum potential, for a free particle, decreases as δ_i increases. This fact can be verified for a free-particle where

$$Q_i = \frac{\hbar^2}{4m\delta_i^2[1 + (t/\tau)^2]} \left[1 - \frac{[x - x_0 - v_i t]^2}{2\delta_i^2[1 + (t/\tau)^2]} \right] \quad (2.81)$$

with $\tau \equiv 2m\delta_i^2/\hbar$. Choosing $\hbar = m = 1$, $E_i/V_0 = 0.8$, $(2mV_0/\hbar)^{1/2}L = 3.1$ and $\delta_i/L = 1$, Fig. 2.2 above indicates that initially the tunneling rate decreases as the incident wave packet width increases until it reaches a plateau (at $\delta_i/L \simeq 13$)— due to the uncertainty principle, for a minimum (or greater) value of the incident wave packet width the tunneling remains the same, i.e., the quantum potential is reduced to a minimum (since it depends inversely on the width of the packet). Consequently, above a critical initial wave packet width the tunneling rate is no longer dependent of the width of the wave packet. This point has been overlooked in the literature in light of another issue: the tunneling time. Many authors have advocated that the tunneling time through an opaque barrier is independent of the thickness of the barrier (the Hartman effect) [22, 24]. The quantum potential and the uncertainty principle then demand that the spatial extent of the packet be much greater than the barrier width. As a result, the duration of the tunneling event will be the temporal extent of the wave packet, assumed propagating at its initial velocity [25].

2.5 Scattering via Invariants of Bohmian Mechanics

We present here a new application of the theory of invariants to the problem of scattering within Bohmian mechanics. Within this formalism [26], we derive a formula for the transmission coefficient of a steady flux of fluid particles scattered by an arbitrary shaped potential well, and discuss the possibility of exact and approximate solutions for some particular cases.

The quantum potential is a responsible, crucial determining factor for the unbroken transition from microscopic to macroscopic levels. Quantum-wave phenomena, such as diffraction and interference, are precluded from a scattering process in the semiclassical regime [14] and therefore it becomes necessary to improve such approximations if the de Broglie wavelength is comparable with the potential dimensions. In the framework of Bohmian mechanics, this implies that the quantum potential can still be significant and its complete neglect is not desirable. So, let us consider again the dynamics of a quantum-fluid particle described previously by the pair of coupled hydrodynamical equations (2.6) and (2.7).

The stationary solution to the coupled Eqs. (2.6) and (2.7) ($\dot{\rho} = \dot{v} = 0$) can be found by expressing

$$\psi(x, t) = \phi(x) \exp(i [S(x) - Et] / \hbar) \quad (2.82)$$

which substituted into Eqs. (2.6) and (2.7) gives

$$\phi'(x)S'(x) + S''(x)\phi(x) = 0, \quad (2.83)$$

$$\phi''(x) + \lambda^2(x)\phi(x) = \left[\frac{S'(x)}{\hbar} \right]^2 \phi(x) \quad (2.84)$$

where for an arbitrarily shaped potential well $V(x)$, we have

$$\lambda^2(x) = 2m[E + V(x)]/\hbar^2. \quad (2.85)$$

Integration of Eq. (2.83) implies that

$$\rho(x)S'(x) = I_1, \quad (2.86)$$

which is the *first invariant*: the fluid-particle density current ($J(x) = \rho(x)v(x)$) is spatially conserved. Then, by inserting Eq. (2.86) into (2.84), and defining the dimensionless quantity

$$\tilde{\phi}(x) = \sqrt{\frac{k}{I_1}} \phi(x), \quad (2.87)$$

we have

$$\tilde{\phi}''(x) + \lambda^2(x)\tilde{\phi}(x) = \frac{\hbar^2 k^2}{\tilde{\phi}^3(x)}, \quad (2.88)$$

which is of the form of the so-called Ermakov-Pinney equation [10–12]. Noticeably, the term on the right side of Eq. (2.88) depends on $\hbar$ in contrast to the similar nonlinear equation studied by Ermakov, Milne and Pinney which contains an arbitrary constant and analyzed previously. This $\hbar$ -term emerges naturally from the presence of the quantum potential. A complete solution to this equation can be found by successive transformations. By following Reid and Ray [27], we express $\tilde{\phi}(x) = r(\theta)\alpha(x)$ and $d\theta = dx/\alpha^2(x)$, yielding $\ddot{r}(\theta) = k^2\hbar^2/r^3(\theta)$ and the second invariant

$$I_2 = [\dot{r}(\theta)]^2 + \frac{k^2\hbar^2}{r^2} \quad (2.89)$$

or

$$I_2 = \left[\tilde{\phi}\alpha' - \tilde{\phi}'\alpha \right]^2 + \frac{k^2\hbar^2}{\left(\alpha/\tilde{\phi} \right)^2}, \quad (2.90)$$

provided that α obeys

$$\alpha''(x) + \lambda^2(x)\alpha(x) = 0. \quad (2.91)$$

The overdot denotes differentiation with respect to θ . Upon integration, Eq. (2.90) leads to

$$\tilde{\rho}(x) = \left(\frac{k^2\hbar^2}{I_2} + I_2 I_3^2 \right) \alpha_1^2(x) + I_2 \alpha_2^2(x) + 2I_2 I_3 \alpha_1(x) \alpha_2(x) \quad (2.92)$$

where

$$\alpha_1(x) \equiv \alpha(x) \quad (2.93)$$

and

$$\alpha_2(x) \equiv \alpha(x) \int^x \frac{dx}{\alpha^2(x)}. \quad (2.94)$$

Because α_1 and α_2 are linearly independent functions and, therefore, cannot be zero simultaneously, $\tilde{\rho}(x)$ can never be zero. As justified in Lutzky's work [28], Eqs. (2.93) and (2.94) can be expressed as

$$\alpha_1(x) = \tilde{\phi}_P(x) \cos \beta(x) \quad (2.95)$$

and

$$\alpha_2(x) = [\tilde{\phi}_P(x)/k] \sin \beta(x), \quad (2.96)$$

where $\tilde{\phi}_P(x)$ is *any* particular solution to (2.88) and

$$\beta(x) = k \int \frac{dx}{\tilde{\rho}_P(x)}, \quad (2.97)$$

such that we obtain after some manipulations

$$\tilde{\rho}(x) = \tilde{\rho}_P(x) \left\{ a + \sqrt{a^2 - 1} \cos[2(\beta(x) - b)] \right\}, \quad (2.98)$$

where a and b are two (redefined) constants, which will be determined below. An advantage of having α_1 (and α_2) expressed in terms of $\tilde{\rho}_P$ is that while α_1 may vary rapidly (through $\cos \beta$), $\tilde{\rho}_P$ can be a slowly varying function, and therefore its corresponding equation is more suitable for approximations: $\tilde{\rho}_P$ can also be seen as a modulation of the total amplitude $\tilde{\rho}$.

Moreover, it is worth noting that a complete solution to (2.88) can be obtained from any (just one) particular solution to another equation of the same form as that of (2.88). This is the central point towards an exact and/or approximate solution without having to neglect its quantum potential term.

For a bound-state energy case, after some manipulations, we find that condition

$$\oint mv(x, t) dx = 2\pi n \hbar \quad (2.99)$$

is sufficiently satisfied if $\Delta\beta = n\pi$,

Now, consider the scattering of a steady flux of particles with energy E ($k^2 = 2mE/\hbar^2$) by an arbitrarily shaped potential well $V(x) = V$ for $0 \leq x \leq L$ and 0 elsewhere. For an incident flux of particles from the left ($x < 0$), with wave function given by

$$\psi_L(x) = e^{ikx} + Ae^{-ikx}, \quad (2.100)$$

and a transmitted flux to the right ($x > L$), with wave function

$$\psi_R(x) = Be^{ikx}, \quad (2.101)$$

the boundary conditions are now matched as follows at $x = 0$

$$1 + A = \phi(0)e^{iS(0)/\hbar}, \quad (2.102)$$

$$ik(1 - A) = \left(\phi'(0) + i \frac{S'(0)\phi(0)}{\hbar} \right) e^{iS(0)/\hbar}, \quad (2.103)$$

at $x = L$

$$\phi(L)e^{iS(L)/\hbar} = Be^{ikL}, \quad (2.104)$$

$$\left(\phi'(L) + i \frac{S'(L)\phi(L)}{\hbar} \right) e^{iS(L)/\hbar} = ikBe^{ikL}. \quad (2.105)$$

Eliminating A between Eqs. (2.102) and (2.103), the real and imaginary parts of the resulting expression are

$$2k \sin\left(\frac{S(0)}{\hbar}\right) = \phi'(0), \quad (2.106)$$

$$2k \cos\left(\frac{S(0)}{\hbar}\right) = \phi(0) \left(k + \frac{S'(0)}{\hbar} \right). \quad (2.107)$$

Likewise, elimination of B between Eqs. (2.104) and (2.105) leads to

$$\frac{S'(L)}{\hbar} = k \Rightarrow \tilde{\rho}(L) = 1, \quad (2.108)$$

$$\tilde{\rho}'(L) = 0. \quad (2.109)$$

Now, with the help of Eq. (2.108), the scattering transmission coefficient stems from Eq. (2.105)

$$T = |B|^2 = \rho(L) = I_1/k. \quad (2.110)$$

Squaring Eqs. (2.106) and (2.107) and adding, one finds

$$4k^2 = [\phi'(0)]^2 + \phi^2(0) \left(k + \frac{S'(0)}{\hbar} \right)^2. \quad (2.111)$$

With the help of Eqs. (2.86) and (2.87), we recast Eq. (2.111) as

$$T = 4k^2(C_1 + C_2 + C_3)^{-1} \quad (2.112)$$

where

$$C_1 = 2k^2 - k\sqrt{a^2 - 1} \frac{\tilde{\rho}'_P(0)}{\tilde{\rho}_P(0)} \sin(2[\beta(0) - b]), \quad (2.113)$$

$$C_2 = \frac{k^2}{\tilde{\rho}_P(0)} \frac{1 + (a^2 - 1)\sin^2(2[\beta(0) - b])}{a + \sqrt{a^2 - 1} \cos(2[\beta(0) - b])}, \quad (2.114)$$

$$C_3 = \tilde{\rho}_P(0) \left(k^2 + \frac{[\tilde{\rho}'_P(0)]^2}{4\tilde{\rho}_P^2(0)} \right) \left(a + \sqrt{a^2 - 1} \cos(2[\beta(0) - b]) \right), \quad (2.115)$$

where the constants a and b can be determined through the boundary conditions (2.108) and (2.109), namely,

$$a = \frac{\tilde{\rho}_P(L)}{2} \left(1 + \frac{1}{\tilde{\rho}_P^2(L)} + \frac{[\tilde{\rho}_P(L)]^2}{4k^2 \tilde{\rho}_P^2(L)} \right), \quad (2.116)$$

$$b = \beta(L) - \frac{1}{2} \sin^{-1} \left(\frac{\tilde{\rho}'_P(L)}{2k\sqrt{a^2 - 1}\tilde{\rho}_P(L)} \right), \quad (2.117)$$

and $\beta(x)$ is given by Eq. (2.97). All quantities above are given in terms of $\tilde{\rho}_P(x)$, and, therefore, any (just one!) particular solution for $\tilde{\rho}_P$ completes the problem. A large class of analytic, closed-form solutions for $\tilde{\rho}_P$, for different choices of $\lambda(x)$, can be found in the literature [26].

2.5.1 Quantum Traversal Time

The question of the duration of a tunneling process of a particle through a potential barrier has been debated considerably in the literature [19]. Let us consider the dynamics of a quantum particle described by the coupled hydrodynamical equations (2.6) and (2.7) recast in the form [19]

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}(vu) - \frac{\hbar}{2m} \frac{\partial^2 v}{\partial x^2} \quad (2.118)$$

and

$$\frac{\partial v}{\partial t} = -\frac{1}{m} \frac{\partial V}{\partial x} - v \frac{\partial v}{\partial x} + u \frac{\partial u}{\partial x} + \frac{\hbar}{2m} \frac{\partial^2 u}{\partial x^2} \quad (2.119)$$

such that for each quantum state with the wave function given by Eq. (2.5) we associate the velocity (2.9) and

$$u = (\hbar/2m)(\partial \ln \rho / \partial x). \quad (2.120)$$

We consider a particle with energy E scattering (tunneling) by a static potential well of depth V_o (or barrier) for $0 \leq x \leq L$ and 0 elsewhere [19]. The particle's forward (backward) drift velocity $v_+(v_-)$ can be written as the sum of (difference) of the current velocity v and the osmotic velocity u : $v_{\pm} = v \pm u$. Both the forward and backward velocities of the particle contribute to the traversal kinetic energy

$$KE = (m/2)(v^2 + u^2) = (m/2)[(v_+^2 + v_-^2)/2] \quad (2.121)$$

where

$$v_{\pm}(x) = \frac{\hbar}{m} \frac{[2k(q/k)^2 \pm q[1 - (q/k)^2] \sin 2q(x - L)]}{[1 + (q/k)^2] - [1 - (q/k)^2] \cos 2q(x - L)}. \quad (2.122)$$

For tunneling ($E < V_o$), we replace $q = \sqrt{2m(V_o + E)/\hbar}$ by $i\bar{q} = i\sqrt{2m(V_o - E)/\hbar}$ and $k = \sqrt{2mE/\hbar}$. We define for the stationary regime the quantum traversal time across a square barrier of width L as

$$\tau = \int_0^L \frac{dx}{\sqrt{(2/m)KE}}. \quad (2.123)$$

With the help of Sect. 2.5, we find that for the thin-barrier tunneling problem, the traversal time is given by $\tau = (m/\hbar k)L$, whereas for the opaque-barrier case, $\tau = (m/\hbar \bar{q})L$ [19].

In contrast, for an opaque rectangular barrier, the stationary-phase method [24] yields a traversal time that is independent of the barrier width. This result depends strongly on the form of the wave packet, and is sound only if the wave packet is characterized by a narrow momentum distribution. If a wave packet with a wide momentum distribution strikes a barrier, the transmitted wave packet will exhibit a distribution displaced to higher momenta since the high-energy components of the wave packet tunnel more easily. Thus, the transmitted wave packet moves faster and the reflected wave packet moves slower than the incident one. In contrast, our traversal time definition is that, while working in the configuration space, we avoid the restricted condition on the initial momentum distribution width. As remarked by Büttiker [29], the stationary-phase method does not distinguish between particle which at the end stay in the interaction region and are subsequently reflected and those that are transmitted. This yields the average dwell time of a particle in the barrier and not the traversal time, if most particles are reflected.

2.6 Wave Propagator for the Guiding Wave Function

Via the de Broglie-Bohm approach to quantum mechanics, we develop here a protocol to obtain a propagator for the guiding wave function as defined by the integral equation

$$\psi(x, t) = \int_{-\infty}^{+\infty} dx_0 K(x, x_0, t) \psi(x_0, 0). \quad (2.124)$$

The primary concept is introduced that a particle has a definite path which is determined by a suitable equation of motion and that this path is fundamentally affected by a guiding wave function [30]. Accordingly, the connection between the particle and wave properties can be obtained by writing the wave function in the polar form as in Eq. (2.5), and from Eqs. (2.6) and (2.7), the paths of a particle with velocity is given by

$$\frac{dx}{dt} = v(x, t)|_{x=x(t)} = \frac{1}{m} \frac{\partial S}{\partial x} \Big|_{x=x(t)} \quad (2.125)$$

as in Eq. (2.9) and subject to an arbitrary external potential V and the quantum potential Q . With the help of Eq. (2.125), we can readily obtain

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\frac{\partial S}{\partial x} \right)^2 + V + Q = 0, \quad (2.126)$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \quad (2.127)$$

is the hydrodynamical derivative. Equation (2.126) has the form of Newton's second law, in which the particle is subject to a quantum potential Q in addition to the classical potential V . A set of paths is obtained by considering the case when the amplitude of the wave function is a slowly varying function of position. In what follows, we develop a protocol to obtain a propagator for the wave function by retaining explicitly some of the features of the quantum potential. This procedure attempts to generalize that developed by Feynman and Hibbs [31], since their procedure is viewed as a method for obtaining the wave function from the set of classical paths, for which $Q = 0$.

We investigate the quantum hydrodynamical evolution of the Gaussian guiding wave packet given by Eq. (2.12). We now expand $S(x, t)$, $V(x, t)$ and Q around $q(t)$ up to second order

$$S(x, t) = S[q(t)] + S'[q(t), t][x - q(t)] + \frac{S''[q(t)]}{2}[x - q(t)]^2, \quad (2.128)$$

$$V(x, t) = V[q(t)] + V'[q(t), t][x - q(t)] + \frac{V''[q(t)]}{2}[x - q(t)]^2, \quad (2.129)$$

$$Q(x, t) = Q[q(t)] + Q'[q(t), t][x - q(t)] + \frac{Q''[q(t)]}{2}[x - q(t)]^2. \quad (2.130)$$

Next, substituting Eq. (2.12) into (2.7), we find again Eq. (2.16). Now, a connection to Eqs. (2.16) and (2.125) can be established by collecting terms in $[x - q(t)]^0$ and $[x - q(t)]^1$

$$S'[x(t), t] = m\dot{q}(t), \quad (2.131)$$

$$S''[x(t), t] = m \frac{\dot{\delta}(t)}{\delta(t)}. \quad (2.132)$$

Then, by substituting Eq. (2.12) and the previous Taylor expansions into Eq. (2.126) and again collecting terms in $[x - q(t)]^0$ and $[x - q(t)]^1$, we have

$$\dot{S}_0 = \frac{1}{2}m\dot{q}^2(t) - V[q(t), t] - \frac{\hbar^2}{4m\delta^2(t)}, \quad (2.133)$$

$$\ddot{q}(t) = -\frac{1}{m}V'[q(t), t], \quad (2.134)$$

$$\ddot{\delta}(t) + \frac{1}{m}V''[q(t), t]\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)}, \quad (2.135)$$

where we have denoted $\dot{S}_0 \equiv S[q(t), t]$. It is worth noticing the presence of the quantum potential in the last terms of Eqs. (2.133) and (2.135). These equations have the initial conditions

$$q(0) = x_0, \quad \dot{q}(0) = v_0, \quad (2.136)$$

$$\delta(0) = \delta_0, \quad \dot{\delta}(0) = 0, \quad (2.137)$$

and

$$S_0(0) = m v_0 x_0. \quad (2.138)$$

Now, the wave packet can be fully written as

$$\begin{aligned} \psi(x, t) = [2\pi\delta^2(t)]^{-1/4} \exp \left[\left(\frac{im\dot{\delta}(t)}{2\hbar\delta(t)} - \frac{1}{4\delta^2(t)} \right) [x - q(t)]^2 \right] \\ \times \exp \left[\frac{im\dot{q}(t)}{\hbar} [x - q(t)] + \frac{imv_0x_0}{\hbar} \right] \\ \times \exp \left[\frac{i}{\hbar} \int_0^t dt' \left(\frac{1}{2} m \dot{q}^2(t') - V[q(t')] - \frac{\hbar^2}{4m\delta^2(t')} \right) \right]. \end{aligned} \quad (2.139)$$

Next, we turn to finding the propagator $K(x, x_0, t)$ as defined by the integral Eq. (2.124). Let us first define the normalized quantity

$$\Phi(v_0, x, t) = (2\pi\delta_0^2)^{1/4} \psi(v_0, x, t), \quad (2.140)$$

which satisfies the completeness relation

$$\int_{-\infty}^{+\infty} dv_0 \Phi^*(v_0, x, t) \Phi(v_0, x', t) = \frac{2\pi\hbar}{m} \delta(x - x') \quad (2.141)$$

where $\delta(x - x')$ denotes the well-known delta function. From Eq. (2.7), it follows that

$$\frac{\partial(\Phi^*\psi)}{\partial t} + \frac{\partial(\Phi^*\psi v)}{\partial x} = 0 \quad (2.142)$$

which after integration yields

$$\frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dx \Phi^*\psi = 0, \quad (2.143)$$

whence

$$\int_{-\infty}^{+\infty} dx' \Phi^*(v_0, x', t) \psi(x', t) = \int_{-\infty}^{+\infty} dx_0 \Phi^*(v_0, x_0, t) \psi(x_0, t). \quad (2.144)$$

Multiplying Eq. (2.144) by $\Phi^*(v_0, x, t)$, integrating with respect to v_0 , and using Eq. (2.141), we have

$$\psi(x, t) = (m/2\pi\hbar) \int_{-\infty}^{+\infty} dv_0 \Phi(v_0, x, t) \int_{-\infty}^{+\infty} dx_0 \Phi^*(v_0, x_0, 0) \psi(x_0, 0), \quad (2.145)$$

whence the propagator reads

$$K(x, x_0, t) = (m/2\pi\hbar) \int_{-\infty}^{+\infty} dv_0 \Phi(v_0, x, t) \Phi^*(v_0, x_0, 0). \quad (2.146)$$

With the help of Eqs. (2.136)–(2.140), we have explicitly

$$\begin{aligned} K(x, x_0, t) = & \frac{m}{2\pi\hbar} \int_{-\infty}^{+\infty} dv_0 \left(\frac{\delta(t)}{\delta_0} \right)^{-1/2} \exp \left[\left(\frac{im\dot{\delta}(t)}{2\hbar\delta(t)} - \frac{1}{4\delta^2(t)} \right) [x - q(t)]^2 \right] \\ & \times \exp \frac{i}{\hbar} \left[m\dot{q}(t)[x - q(t)] + \int_0^t dt' \left(\frac{1}{2}m\dot{q}^2(t') - V[q(t'), t'] - \frac{\hbar^2}{4m\delta^2(t')} \right) \right]. \end{aligned} \quad (2.147)$$

Equation (2.147) shows that the quantum-mechanical information given by the propagator can be found in the guiding wave function. Besides, the quantum propagator can be viewed as an expansion of the guiding wave function over the v_0 -space (and not in just over the ordinary position space). It is a merit of the formalism of the de Broglie-Bohm quantum theory to bring this out so explicitly that it cannot be ignored.

2.7 Bohmian Trajectories of Airy Packets

The discovery of Berry and Balazs in 1979 [32] that the Schrödinger equation for a free particle of mass m allows a non-dispersive and accelerating Airy wave packet solution has taken the folklore of quantum mechanics by surprise. They have shown that for the Schrödinger equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}, \quad (2.148)$$

a unique solution is given by

$$\psi(x, t) = \text{Ai}^2 \left[\frac{B}{\hbar^{2/3}} \left(x - \frac{B^3 t^2}{4m^2} \right) \right] \exp \left[i \left(\frac{B^3 t}{2m\hbar} \right) \left(x - \frac{B^3 t^2}{6m^2} \right) \right]. \quad (2.149)$$

This is easily verified by direct substitution and use of the Airy function's differential equation [33]. Here Ai is the Airy function and B is an arbitrary constant. Airy packets continue to propagate without spreading even when a spatially uniform and time-varying force $F(t)$ acts. Over the years, this intriguing class of wave packets has sparked a considerable resurgence on research on diffraction theory and experiments on a classical analogue in optics of nondiffracting beams [34–42]. Despite its numerous applications in electrodynamics, optical theory, solid state physics, radiative transfer, semiconductors in electric fields, Airy functions have found to be a distinctive solution in quantum mechanics but only for force-free and for linear potentials [42–44].

Within the Bohmian mechanics framework, new features of Airy wave packet solutions to Schrödinger equation with time-dependent quadratic potentials can be introduced. In particular, we provide some insights to the problem by calculating its Bohmian trajectories. It is shown that by using general space-time transformations, these trajectories can display a variety of cases depending upon the initial position of the individual particle in the Airy wave packet. These results suggest some mathematical similarities between Schrödinger equation and the paraxial equation of diffraction and pave the way toward the discovery of new experimental observations notwithstanding the fact that the paraxial equation has solutions in terms of Airy functions with complex arguments. Numerous experimental configurations of optics and atom physics have shown that the dynamics of Airy beams depends significantly on initial parameters and configurations of the experimental set-up.

The simplest problem is defined by two evolution equations: the Schrödinger equation with time-dependent quadratic and linear potentials for the wave function $\psi(x, t)$

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + \left(\frac{1}{2} m \omega^2(t) x^2 - F(t)x \right) \psi(x, t) \quad (2.150)$$

and the first-order guiding equation for $x(t)$

$$\dot{x}_i(t) = \frac{\hbar}{m} \text{Im} \left(\frac{\partial}{\partial x} \log \psi(x, t) \right) \bigg|_{x=x_i(t)} \quad (2.151)$$

which constitutes the simplest first-order evolution equation for the position of the particle that is compatible with the Galilean and time-reversal covariance of the Schrödinger evolution. In Eq. (2.150), $\omega(t)$ and $F(t)$ represent the time-dependent harmonic-oscillator frequency and linear force, respectively. Thus, the main objective is to solve Eq. (2.151) for the Bohmian trajectories of an evolving i th particle of the Airy wave packet ensemble with an initial position x_{0i} .

A general solution to Eq. (2.150) can be found through a proper time rescaling of the space variables and introducing new times [45–47]. This new group of transformations reduce Eq. (2.150) to the case of the problem of a free-particle type motion. Although different techniques have been used, the scale and phase transformations presented here yield a simpler physical meaning to the mathematical protocol [48]. To this end, the extended space-time transformations is introduced as

$$\psi(x, t) = \frac{1}{\sqrt{\delta(t)}} \exp\left(\frac{i\phi_1(x, t)}{\hbar}\right) \psi_1(x, t), \quad (2.152)$$

$$x' = \frac{1}{\delta(t)} (x - q(t)), \quad (2.153)$$

and

$$t' = \int_0^t \frac{d\tau}{\delta^2(\tau)}. \quad (2.154)$$

These transformations represent a scale and phase transformation on the wave function and a scale transformation on space and time along with a space translation. In particular, Eq. (2.153) is a Galilean-type transformation. After lengthy but straightforward calculations is found that Eq. (2.150) reduces to

$$i\hbar \frac{\partial \psi_1(x', t')}{\partial t'} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_1(x', t')}{\partial x'^2} + f_1(t') \psi_1(x', t') \quad (2.155)$$

where

$$f_1(t') = \frac{m}{2} [\dot{\delta}^2 q^2 + \delta^2 \dot{q}^2 - 2q\dot{q}\delta\dot{\delta}]. \quad (2.156)$$

By performing the phase change

$$\psi_1(x', t') = \psi_2(x', t') \exp\left(-\frac{i}{\hbar} \int_0^{t'} f_1(t'') dt''\right), \quad (2.157)$$

Equation (2.155) reduces further to

$$i\hbar \frac{\partial \psi_2(x', t')}{\partial t'} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_2(x', t')}{\partial x'^2}. \quad (2.158)$$

Thus, the general solution to Eq. (2.150) then reads

$$\psi(x, t) = \frac{1}{\sqrt{\delta(t)}} Ai \left\{ \frac{B}{\hbar^{2/3}} \left[\frac{[x - q(t)]}{\delta(t)} - \frac{B^3}{4m^2} \left(\int_0^t \frac{d\tau}{\delta^2(\tau)} \right)^2 \right] \right\} \exp \frac{i}{\hbar} \phi_{total}(x, t), \quad (2.159)$$

where

$$\phi_{total} = \phi_1(x, t) + \phi_2(x, t) + \phi_3(x, t) \quad (2.160)$$

and

$$\phi_1 = - \int_0^{t'} f_1(\tau) d\tau, \quad (2.161)$$

$$\phi_2 = \frac{mx^2 \dot{\delta}(t)}{2\delta} - \left[\frac{mq(t) \dot{\delta}(t)}{\delta(t)} - m\dot{q}(t) \right] x, \quad (2.162)$$

$$\phi_3 = \frac{B^3}{2m} \left(\int_0^t \frac{dt'}{\delta^2(t')} \right) \left[\frac{x - q(t)}{\delta(t)} - \frac{B^3}{6m} \left(\int_0^t \frac{dt'}{\delta^2(t')} \right)^2 \right], \quad (2.163)$$

$$f_1 = \frac{1}{2} m [\dot{\delta}^2 q^2 + \delta^2 \dot{q}^2 - 2q\dot{q}\delta\dot{\delta}]. \quad (2.164)$$

In turn, the auxiliary functions $q(t)$ and $\delta(t)$ obey

$$\ddot{q}(t) + \omega^2(t)q(t) = \frac{F(t)}{m} \quad (2.165)$$

and

$$\ddot{\delta}(t) + \omega^2(t)\delta(t) = 0. \quad (2.166)$$

Now, with the help of Eqs. (2.160), (2.151) yields

$$\begin{aligned} \dot{x}_i(t) &= \frac{1}{m} \left(\frac{\partial \phi_{total}(x, t)}{\partial x} \right) \Big|_{x=x_i(t)} \\ &= \dot{q}(t) + [x_i(t) - q(t)] \frac{\dot{\delta}(t)}{\delta(t)} + \frac{B^3}{2m^2 \delta(t)} \int_0^t \frac{dt'}{\delta^2(t')}. \end{aligned} \quad (2.167)$$

Equation (2.167) can be integrated as follows. First, we recast it as

$$\frac{[\dot{x}_i(t) - \dot{q}(t)] \delta(t) - [x_i(t) - q(t)] \dot{\delta}(t)}{\delta^2(t)} = \frac{B^3}{2m^2 \delta^2(t)} \int_0^t \frac{dt'}{\delta^2(t')} \quad (2.168)$$

or

$$\frac{d}{dt} \left[\frac{x_i(t) - q(t)}{\delta(t)} \right] = \frac{B^3}{2m^2 \delta^2(t)} \int_0^t \frac{dt'}{\delta^2(t')} \quad (2.169)$$

which upon integration becomes

$$x_i(t) = q(t) + (x_{0i} - q_0) \frac{\delta(t)}{\delta_0} + \frac{B^3}{2m^2} \delta(t) \int_0^t \frac{dt'}{\delta^2(t')} \int_0^{t'} \frac{d\tau}{\delta^2(\tau)}, \quad (2.170)$$

where $q_0 = q(0)$ and $\delta_0 = \delta(0)$. Thus, Eq. (2.170) gives the associated Bohmian trajectories of the Airy wave packet that satisfies Eq. (2.150). In particular, if $\delta(t) = 1$, $\omega(t) = 0$, Eq. (2.159) yields the result found by Berry and Balazs in Eq. (2.148) [32]. Furthermore, Eq. (2.170) displays still a myriad of nontrivial Airy packet trajectories. For example, if x_{0i} is positive, then the particles distributed in the right half of the initial ensemble are accelerated whereas the particles distributed in the left half of the initial ensemble are decelerated. Besides, Eq. (2.170) implies that deviations from classical trajectories $\Delta x_i(t) = x_i(t) - X(t)$ are entirely dependent on the solution of Eq. (2.166) (which is a generalization of the Mathieu and Hill-Poschl-Teller equations) [13, 49, 50]. Two independent solutions to Eq. (2.166) can be obtained in general from just one particular solution to the same equation, namely,

$$\delta_1(t) \equiv \delta(t) \quad (2.171)$$

and

$$\delta_2(t) \equiv \delta(t) \int_0^t \frac{dt'}{\delta^2(t')}. \quad (2.172)$$

If initial conditions are imposed as follows: $\delta(0) = 1$ and $\dot{\delta}(0) = 0$ we are led to the orthogonal conditions $\delta_1(0) = 1$, $\delta_2(0) = 0$, $\dot{\delta}_1(0) = 0$ and $\dot{\delta}_2(0) = 1$. This constitutes a large set of general, nontrivial Bohmian trajectories associated to the Airy wave packet subject to time-dependent quadratic potentials.

These new features are worth introducing to the subject's theoretical folklore in light of the fact that the evolution of a quantum mechanical Airy wave packet, governed by the Schrödinger equation, is analogous to the propagation of a finite energy Airy beam satisfying the paraxial equation notwithstanding the fact that the paraxial equation has solutions in terms of Airy functions with complex arguments. As previously mentioned, numerous experimental configurations of optics and atom physics have shown that the dynamics of Airy beams depends significantly on initial parameters and configurations of the experimental set-up. The use of Airy beams for particle manipulation in nonlinear media remains a topic of intense theoretical and experimental research [33, 34]. The results discussed here could be extended in order to be applicable to physically realizable situations.

2.8 Airy and Gaussian Slits. Quantum Focal Point

It is well known that the Schrödinger equation describing a free particle can exhibit a remarkable, nonspreading wave packet solution in terms of an Airy function [32]. A remarkable feature of Airy packets is their ability to remain diffraction-free over long distances while they tend to freely accelerate during propagation in the absence of any external potential. They constitute nontrivial, unusual solutions to Schrödinger equation describing a free particle that remains invariant with time.

Another remarkable feature of Airy packets is worth discussing. We show that Young's two-slit quantum interference of two initially separated Airy wave packets (or *Airy slits*) yields a prominent focal point in the interference pattern. This point of maximum intensity resembles Fresnel's focal point in optics. We also show that Airy slits display a more robust interference pattern when compared to the case of two Gaussian slits. The results discussed here could be tested experimentally since Airy beams have been realized in both one- and two-dimensional configurations [34].

For comparison, let us recall that it is well-known that the solution for the free-particle Schrödinger equation [14–17]

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}, \quad (2.173)$$

can be described by a Gaussian wave packet

$$\psi_{Gauss}(x, t) = A(t) \exp \left[-\frac{[x - q(t)]^2}{4\tilde{\delta}(t)\delta(0)} + i\frac{mv[x - q(t)]}{\hbar} + i\frac{Et}{\hbar} \right] \quad (2.174)$$

where

$$A(t) = [2\pi\tilde{\delta}^2(t)]^{-1/4}, \quad (2.175)$$

the complex time dependent spreading is

$$\tilde{\delta}(t) = \delta(0) \left(1 + \frac{i \hbar t}{2m\delta^2(0)} \right), \quad (2.176)$$

where

$$\delta(t) = \delta(0) \sqrt{1 + \left(\frac{\hbar t}{2m\delta^2(0)} \right)^2}, \quad (2.177)$$

$$q(t) = q(0) + vt \quad (2.178)$$

and

$$E = \frac{1}{2}mv^2. \quad (2.179)$$

On the other hand, as seen in the previous Section, Berry and Balazs [32] showed that for the free-particle Schrödinger equation (2.173) a unique solution is given by Eq. (2.149). Now the initial total wave function can be written as

$$\psi(x, 0) = N \left[\psi_1 \left(x - \frac{d}{2}, 0 \right) + \psi_2 \left(x + \frac{d}{2}, 0 \right) \right] \quad (2.180)$$

where N is a normalization constant. The functions $\psi_{1,2}$ correspond to two widely separated wave packets (Gaussian or Airy slits), each located $x = \pm d/2$ so that the wavepackets are separated by a distance d . The general solution to Eq. (2.173) is given by [16]

$$\psi(x, t) = \sqrt{\frac{m}{2\pi i \hbar t}} \int_{-\infty}^{\infty} dx' \exp \left\{ -\frac{m(x - x')^2}{2i \hbar t} \right\} \psi(x', 0). \quad (2.181)$$

For comparison, the absolute squared value of expression above is plotted in Figs. 2.3, 2.4, 2.5 and 2.6 for the Young's two-slit quantum interference of two initially separated wave packets (Airy and Gaussian wave packets, respectively). It is clear seen a focal point in the corresponding interference patterns. This point of maximum intensity is analogous to Fresnel focal point in optics.

It is clearly observed that Airy slits display a more robust interference pattern and exhibit a unique point of maximum intensity in the preceding part of the pattern. These results could be easily tested experimentally in light of the successful experimental realization of finite energy Airy beams (one and two-dimensional) obtained by Siviloglou et al. in 2007 [34]. These new features are worth introducing to the subject's theoretical folklore in light of the fact that the evolution of a quantum mechanical Airy wave packet governed by the Schrödinger equation is analogous

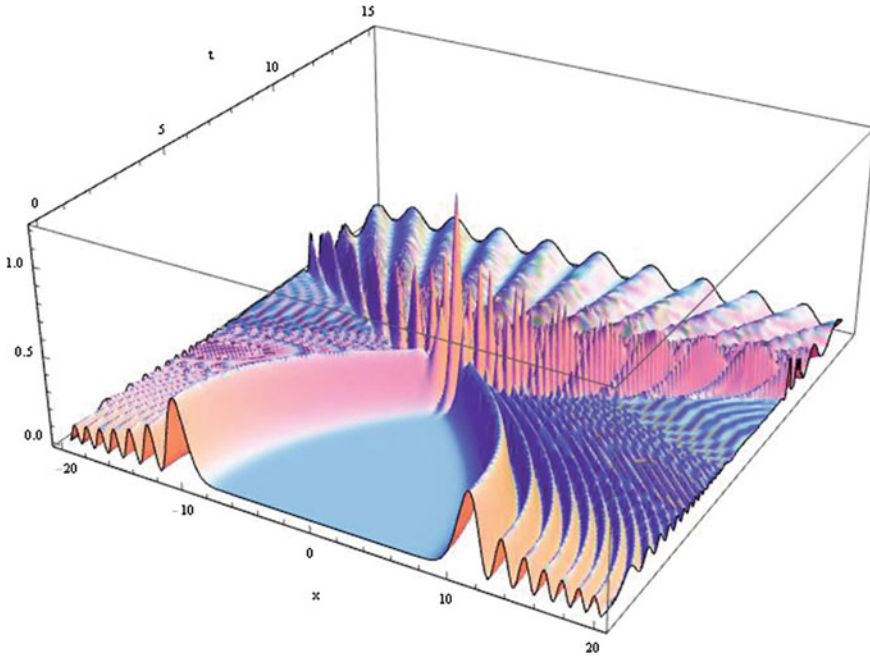


Fig. 2.3 Interference of two initially, widely separated Airy wave packets

to the propagation of a finite energy Airy beam satisfying the paraxial equation. Numerous experimental configurations of optics and atom physics have shown that the dynamics of Airy beams depends significantly on initial parameters and configurations of the experimental set-up.

2.9 Detection of Inertial and Gravitational Masses with Airy Wave Packets

The problem of how the inertial and gravitational mass enter in classical and quantum mechanics is of utmost interest. The first investigations on the equivalence of inertial and gravitational mass relied on pendulum experiments and can be traced back to Newton and Bessel [51]. Tests of higher accuracies were realized by the classical torsion balance experiments of Eötvös [52] and Roll et al. [53].

In quantum mechanics, tests of the universality of free fall have recently been carried out with atom interferometry in the context of the coherence of an atom laser or in connection with the so-called atom trampoline, or also known as the quantum bouncer. Matter wave interferometry with freely falling ^{85}Rb and ^{87}Rb isotopes has

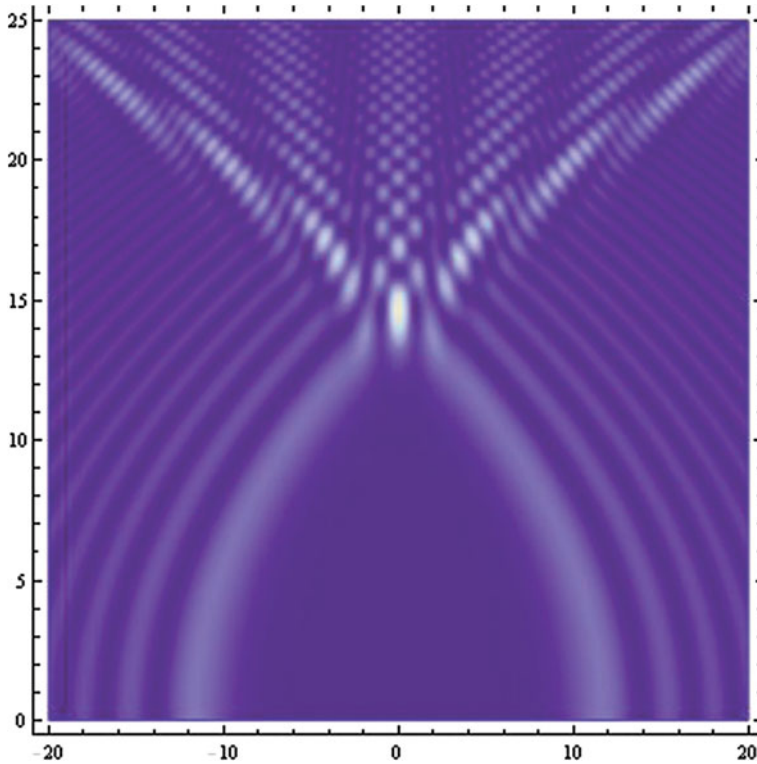


Fig. 2.4 Density plot of the interference of two initially, widely separated Airy wave packets: Quantum focal point

already been performed, and several other experiments worldwide using different species of atoms are in preparation [54–67].

In particular, the universality of the free fall problem has been reviewed and addressed for a quantum mechanical particle in a linear gravitational potential within the Wigner phase space formulation by Kajari et al. [54]. Their conclusion is three-fold: (i) The quantum dynamics reduces to classical dynamics and therefore can only involve the ratio of the inertial mass m_i and the (passive) gravitational mass m_g , (ii) the spatial modulation of the energy eigenfunctions depends on the third root of the product of the two masses, and (iii) the energy eigenvalues of the gravitational atom trampoline are proportional to $(m_g^2/m_i)^{1/3}$.

Here we show that the dynamics of a quantum particle in a linear gravitational potential can be readily described using Airy wave packets within the framework of Bohmian mechanics. It is clearly shown that the dynamics of a particle in a linear gravitational potential involves the gravitational mass (m_g) and the inertial mass (m_i) by the third root of the product of the two masses. This noteworthy feature may offer another avenue in quantum tests of the universality of free fall and experiments

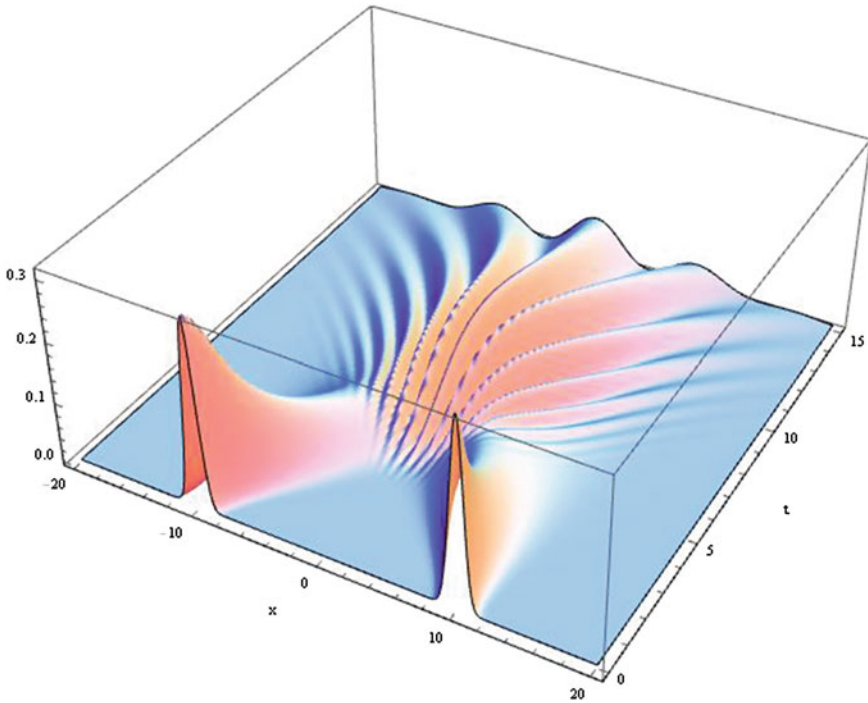


Fig. 2.5 Interference of two initially, widely separated Gaussian wave packets

capable of measuring the Airy-function shaped probability density would yield information about $\sqrt[3]{m_i m_g}$. Over the years, this intriguing class of Airy wave packets has sparked a considerable resurgence on research on diffraction theory and experiments on a classical analogue in optics of nondiffracting beams [33–38, 40]. Despite its numerous applications in electrodynamics, optical theory, solid state physics, radiative transfer, semiconductors in electric fields, Airy functions have found to be a distinctive solution in quantum mechanics not only for force-free and for linear potentials but for a large class of time-dependent quadratic potentials (see Sect. 2.7). The solution to the problem is sought in terms of Airy wave packets within the framework of Bohmian mechanics. Also, we show that the wave packet remains nonspreading and nonaccelerating if the well-known Berry-Balazs constant B is given specifically by $B = (2m_i m_g g)^{1/3}$. Therefore, B is not devoid of any physical meaning – a fact overlooked in the literature.

Our problem is defined by two evolution equations: the Schrödinger equation with a linear gravitational potential for the wave function $\psi(x, t)$

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m_i} \frac{\partial^2 \psi(x, t)}{\partial x^2} - (m_g g x) \psi(x, t) \quad (2.182)$$

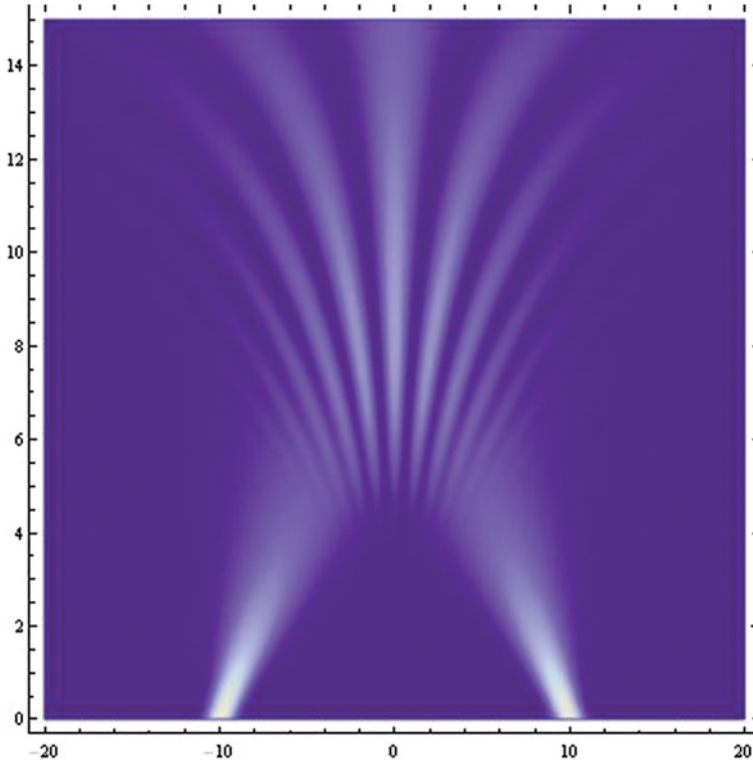


Fig. 2.6 Density plot of the interference of two initially, widely separated Gaussian wave packets: Quantum focal point

and the first-order de Broglie guiding equation for $x(t)$

$$\dot{x}_i(t) = \frac{\hbar}{m_i} \text{Im} \left(\frac{\partial}{\partial x} \log \psi(x, t) \right) \Big|_{x=x_i(t)} \quad (2.183)$$

which constitutes the simplest first-order evolution equation for the position of the particle that is compatible with the Galilean and time-reversal covariance of the Schrödinger evolution. We now solve Eqs. (2.182) and (2.183). To this end, a solution to Eq. (2.182) can be again found by introducing the space-time transformation

$$\psi(x, t) = \exp \left(\frac{i\phi_1(x', t)}{\hbar} \right) \psi_1(x', t), \quad (2.184)$$

$$x' = x - q(t), \quad (2.185)$$

and

$$t' = t. \quad (2.186)$$

These transformations represent a scale and phase transformation on the wave function and a scale transformation on space and time along with a space translation. Experiments have verified the validity of these transformation laws for noninertial frames also in the quantum limit. Equation (2.185) is a Galilean-type transformation which reduces Eq. (2.182) to

$$i\hbar \frac{\partial \psi_1(x', t')}{\partial t'} = -\frac{\hbar^2}{2m_i} \frac{\partial^2 \psi_1(x', t')}{\partial x'^2} + f_1(t') \psi_1(x', t') \quad (2.187)$$

where

$$f_1(t') = \frac{1}{2} m_i \dot{q}^2. \quad (2.188)$$

By performing the phase change

$$\psi_1(x', t') = \psi_2(x', t') \exp \left(-\frac{i}{\hbar} \int_0^{t'} f_1(t'') dt'' \right), \quad (2.189)$$

Equation (2.187) reduces further to

$$i\hbar \frac{\partial \psi_2(x', t')}{\partial t'} = -\frac{\hbar^2}{2m_i} \frac{\partial^2 \psi_2(x', t')}{\partial x'^2}. \quad (2.190)$$

Thus, the wave packet solution to Eq. (2.182) then reads

$$|\psi_2(x, t)| = Ai \left\{ \frac{B}{\hbar^{2/3}} \left[[x - q(t)] - \frac{B^3 t^2}{4m_i^2} \right] \right\}, \quad (2.191)$$

with

$$f_1(t) = \frac{1}{2} \frac{m_g^2}{m_i} g^2 t^2, \quad (2.192)$$

and

$$m_i \ddot{q}(t) = -m_g g. \quad (2.193)$$

Now, the Bohmian trajectories are found to be

$$x_i(t) = q(t) + (x_{oi} - q_o) + \frac{B^3 t^2}{2m_i^2}. \quad (2.194)$$

Thus, we can summarize our main results as follows

$$|\psi(x, t)|^2 = Ai^2 \left[\frac{B}{\hbar^{2/3}} \left(x - \frac{1}{2} \frac{m_g}{m_i} g t^2 + \frac{B^3 t^2}{4m_i^2} \right) \right] \quad (2.195)$$

and

$$x_i(t) = -\frac{1}{2} \frac{m_g}{m_i} g t^2 + (x_{oi} - q_o) + \frac{B^3 t^2}{4m_i^2}. \quad (2.196)$$

Further, we find that if B is given by the third root of the product of the inertial and gravitational mass, namely

$$B = \sqrt[3]{2m_i m_g g}, \quad (2.197)$$

the non-spreading Airy wave packet is also stationary [$x_i(t) = (x_{oi} - q_o)$] in the uniform gravitational field.

The transformation to the free fall system changes the argument of the wave function by introducing a phase factor. This means that the laws of quantum physics are the same in a frame with gravitational potential $-m_g g x$ as in a corresponding frame lacking this potential but having acceleration $-g$ instead. Experiments have verified the validity of these classical transformation laws for noninertial frames also in the quantum limit [57, 63].

It has been assumed so far in the literature that B is a completely arbitrary constant devoid of any special physical meaning. Classically, when the inertial mass m_i and the gravitational mass m_g are equated, the mass drops out of Newton's equations of motion, implying that particles of different mass with the same initial conditions follow the same trajectories. However, in Schrödinger's equation (2.182) the masses do not cancel. Now, Eq. (2.183) defines the Bohmian trajectories of an evolving i th particle of the wave packet ensemble with an initial position x_{oi} . In general, the Bohmian trajectories imply mass-dependent differences in motion, except when the well-known Berry-Balazs constant B is given by $B = (2m_i m_g g)^{1/3}$. For atoms from a condensate ⁸⁷Rb [62, 63] this quantity can be related to an inverse scale related to the wave number $k \approx 3.3 \times 10^6 \text{ m}^{-1}$ (k has the same physical units as the familiar wave vector of a plane wave) [54–61, 63–67].

$$B = \hbar^{2/3} k \approx 7.34 \times 10^{-17} (\text{mkg/s})^{1/3}. \quad (2.198)$$

This result might offer another avenue in quantum tests of the universality of free fall. The use of Airy beams for particle manipulation in nonlinear media remains a topic of intense theoretical and experimental research [33, 34]. Above all, experiments capable of measuring the Airy-function shaped probability density would yield information about $\sqrt[3]{m_i m_g}$.

2.10 The Geometric Phase

The time evolution of a quantum system is governed by differential equations, namely the Schrödinger equation, the Heisenberg or interaction picture equation of motion in the standard approach of quantum mechanics. The Hamiltonian operator plays an important role in this dynamics. Usually, this Hermitian linear operator is considered to be time-independent. However, there are many physical situations where the corresponding Hamiltonians are time-dependent due to the fact that some parameters are determined by external or environmental factors varying with time. The so-called geometric phase is a very important aspect of this type of dynamics [68–71]. The classical counterpart of the phase of the wave function is the phase of the quasi-periodic motion and is called Hannay’s angle.

Around thirty years ago, Berry [72] noticed that the standard description of adiabatic processes in quantum mechanics missed something important. We should remember that the notion of adiabaticity lies on the border of statics and dynamics; in other words, dynamical effects are taken into account but in the limit of infinitely slow changes. If a set of parameters are varied adiabatically during the time evolution, a *cyclic variation* (or periodical evolution in time) of such parameters leads to a change of the wave function by an additional phase factor, being completely ignored more than half a century. This phase factor, apart from the usual dynamical phase, contains a purely geometric part independent on the duration of such an evolution. Berry’s phase was derived in the adiabatic formalism and, therefore, this phase could only be an approximation of the true quantum phase. The latter was introduced for general unitary cyclic evolution by Aharonov and Anandan [73] and subsequently generalized to arbitrary, not necessarily unitary or cyclic, evolutions by Samuel and Bhandari [74]. In 1928, Fock [75] showed that such a phase could be redefined in non-cyclic evolutions and thought to be unimportant. Bortolotti [76] and Rytov [77] papers ignored by the optical community were pioneers in the rotation of the polarized vector of light travelling along the coiled ray. It turns out to be that the corresponding rotation can be simply interpreted in terms of the geometric phase. In 1956, Pancharatnam discovered an analog to the geometric phase when using polarized light [78] by defining the relative phase between two light beams in different polarization states. The same phase was reported in molecular physics when dealing with the Jahn-Teller effect by Longuet-Higgins et al. [79]. Aharonov and Bohm showed the importance of the electromagnetic vector potential in the interference pattern of electrons and the shift observed with respect to a normal interference pattern was coined the Aharonov–Bohm effect [80]. The first derivation of a geometric phase and the corresponding gauge potential is due to Mead and Truhlar when studying the well-known chemical reaction $H + H_2 \rightarrow H_2 + H$ [81]. Nowadays, geometric phases are been observed in many different fields going from magnetic resonance to condensed matter systems such as, for example, the anomalous Hall effect. The dynamics of quantized vortices is also a field where such a phase is relevant.

Soon after Berry reported his adiabatic geometric phase, Simon [82] realized that it could be interpreted as the holonomy of a fiber bundle and the corresponding

gauge potential played the role of a connection in this fiber bundle. It seems like this mathematical theory was waiting for nice and important application in quantum phase factors susceptible to be measured in interference experiments. Mukunda and Simon [83] proposed a new approach consisting of deriving the geometric phase from the so-called quantum kinematic approach instead of the Schrödinger equation.

The geometric phase has also been considered within the Bohmian formalism [84–86] and quantum vortices can be regarded as a manifestation of it.

2.10.1 The Aharonov–Bohm Effect

As is well known [2, 87], the Schrödinger equation is form invariant with respect to a gauge transformation, where the wave function undergoes a suitable unitary transformation. Unlike classical physics, the electromagnetic potentials (scalar, A_0 , and vector, $\mathbf{A}$, potentials) play a fundamental role in quantum processes involving charge interactions. In fact, both potentials enter in that equation instead of the electric and magnetic field strengths themselves.

The wave function of a particle with mass m and charge e in the presence of an electromagnetic field is governed by the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left\{ -\frac{\hbar^2}{2m} \left[\nabla - \frac{ie}{\hbar c} \mathbf{A} \right]^2 + eA_0 + V \right\} \Psi \quad (2.199)$$

where c is the speed of light. Under the gauge transformation in the configuration space

$$\Psi'(\mathbf{r}, t) = e^{ie\varphi(\mathbf{r}, t)/\hbar} \Psi(\mathbf{r}, t) \quad (2.200)$$

φ being an arbitrary single-valued function of $\mathbf{x}$ and t , the particle is governed by the same Schrödinger equation by replacing $\Psi \rightarrow \Psi'$, $\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} - \nabla\varphi$ and $A_0 \rightarrow A'_0 = A_0 + (1/c)\partial\varphi/\partial t$.

Analogously, in the Bohmian formalism, it is a quite straightforward exercise to show that the probability density, the velocity field and the quantum potential are gauge invariant quantities (as well as the quantum trajectories) unlike the total energy [2]. The particle momentum field is given by

$$\mathbf{p}(\mathbf{r}, t) = \nabla S - \frac{e}{c} \mathbf{A} \quad (2.201)$$

and the quantum Newton equation (or quantum Lorentz equation) can be expressed as

$$m \frac{d\mathbf{v}}{dt} = \frac{e}{c} \mathbf{v} \times (\nabla \times \mathbf{A}) - \nabla Q \quad (2.202)$$

when no electric field is present. Again, there is a quantum force even when the magnetic field is zero. The paths are no longer orthogonal to the surface $S = \text{constant}$

$$\oint_C dS = \oint_C \mathbf{p} \cdot d\mathbf{r} + \frac{e}{c} \oint_C \mathbf{A} \cdot d\mathbf{r} = n\hbar \quad (2.203)$$

where n is an integer number and the electromagnetic flux is expressed as

$$\Phi = \int_S \mathbf{B} \cdot d\mathbf{S} = \oint_C \mathbf{A} \cdot d\mathbf{r} \quad (2.204)$$

along the circuit or closed path C encircling the surface $\mathbf{S}$. The magnetic and electric fields are given by $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla A_0 - (1/c)\partial\mathbf{A}/\partial t$, respectively.

The so-called Aharonov–Bohm (AB) effect consists of the influence of the vector potential on charged particles in interference patterns. In particular, consider a collimated electron beam from a source reaching a beam splitter. The two resulting beams go round a line of flux and are recombined again to meet in a screen. When the flux is zero, a certain interference pattern is observed. However, when the flux is not zero, the corresponding interference pattern is shifted with respect to the original one. This line of flux can be seen as an infinite cylindrical solenoid. A steady current in the solenoid generates a flux given by Eq. (2.204), the magnetic field vanishes outside but the vector potential is not zero. Following Holland [2], the total wave function when the field is switched on is given by

$$\Psi = N[\Psi_A + \Psi_B e^{ie\Phi/\hbar c}] e^{(ie/\hbar c) \int_A \mathbf{A} \cdot d\mathbf{r}} \quad (2.205)$$

since each wave is multiplied by a phase factor due to the open path going from the beam splitter to the screen. The closed path C is formed by the sum of path A and path B and the total flux, Φ , is expressed by Eq. (2.203). The normalization factor N is chosen depending on the type of slit assumed (Gaussian, etc.). The total intensity is then given by

$$|\Psi|^2 = N^2\{|\Psi_A|^2 + |\Psi_B|^2 + 2|\Psi_A||\Psi_B|\cos[(S_A - S_B)/\hbar - (e\Phi/c\hbar)]\} \quad (2.206)$$

where, as usual, the total wave function as well as the partial waves have been expressed in polar form. The observable AB shift is given by $e\Phi/c\hbar$, the total flux being a gauge invariant quantity. The AB phase is a particular example of Berry's geometric phase; namely, a topological phase. This phase is independent of the details of the dynamics and is even insensitive to the shape of the close path C . The latter argument is precisely the main feature distinguishing topological phases from the more general geometric phases.

The so-called bound-state Aharonov–Bohm effect [88] has also been studied in terms of Bohmian trajectories [86]. In this problem, a particle with a given mass is confined to a motion on a ring of a finite radius around a magnetic flux. This flux is concentrated in a line through the origin perpendicular to the plane of the ring.

Twenty five years after the prediction of the AB effect, Aharonov and Casher [89] predicted a *dual* effect, the so-called Aharonov-Casher effect, the particle is neutral but has a magnetic moment, and the tube contains a line of charge. Experiments in neutron [90], vortex [91], atom [92], and electron [93] interferometry bear out the prediction of Aharonov and Casher.

2.10.2 Quantum Vortices

Consider a wave function in the three-dimensional configuration space and an arbitrary open or closed path $\mathbf{r}(t)$ on this space. The variation of the wave function along this path as time evolves originates a one-dimensional curve labelled by t . The inner product of this function at two different times is a complex number and the total phase, measuring the relative phase of the final point with respect to the initial point of the curve, is given by its argument. This total phase, $\varphi_{tot} = \arg[\langle \psi(t_1), \psi(t_2) \rangle]$, is defined modulo 2π and, after Aharonov and Anandan [73], is expressed as the sum of the so-called dynamical phase and the geometric phase. The dynamical phase measures the phase change locally accumulated along the path and is defined in Bohmian mechanics as [86]

$$\varphi_{dyn} = \frac{1}{\hbar} \int_{t_1}^{t_2} \frac{dS(\mathbf{r}(t), t)}{dt} dt. \quad (2.207)$$

Therefore, the geometric phase is then written as

$$\varphi_g = \frac{1}{\hbar} [S(\mathbf{r}(t_2), t_2) - S(\mathbf{r}(t_1), t_1)] - \varphi_{dyn} \quad (2.208)$$

where the total phase is now expressed in terms of the difference of the wave function phases. The single valuedness of the wave function implies that the phase difference at the final position of the path must be zero or $2\pi n$, n being an integer number. Thus, $\varphi_g = 2\pi n$ along an arbitrary path (closed or open). Even more, for stationary states, this phase along a closed path is proportional to the circulation integral

$$\varphi_g = \frac{1}{\hbar} \oint_C \mathbf{p} \cdot d\mathbf{r}. \quad (2.209)$$

This integral is quantized to be an integer multiple of $\hbar$. Thus, quantum vortices can be regarded as a manifestation of the geometric phase [86].

2.11 Bohmian Formulation of the Gross–Pitaevskii Equation

The so-called Gross–Pitaevskii Equation has been successfully used to discuss the behavior of Bose-Einstein condensates up to first order at zero temperature [94–97]

$$i \hbar \frac{\partial \Psi(x, t)}{\partial t} = - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V \Psi(x, t) - G |\Psi(x, t)|^2 \Psi(x, t). \quad (2.210)$$

This equation is effectively a mean-field approximation for the interparticle attractive interactions where m is an effective mass of the system, V is a constant potential and G a parameter that regulates the strength of the nonlinearity. It has a well-known solution in terms of a soliton

$$\Psi(x, t) = \left(\frac{k}{2}\right)^{1/2} \text{sech}[k(x - x_o - vt)] \times \quad (2.211)$$

$$\times \exp\left[\frac{imv}{\hbar}(x - x_o - v't)\right]. \quad (2.212)$$

where

$$k = \frac{mG}{2\hbar^2} \quad (2.213)$$

and

$$v' = \frac{V_e + m v^2/2 - \hbar^2 k^2/2}{m v}. \quad (2.214)$$

An additional, attractive characteristic of this equation can be demonstrated within the framework of Bohmian mechanics. In particular, we find a most remarkable solution: existence of exact soliton-like solutions of Gaussian form (gausson). To this end, from the polar form of the wave function given by Eq. (2.5), we have that

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0, \quad (2.215)$$

and

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} = -\frac{1}{m} \frac{\partial}{\partial x}(Q + V_{gp}), \quad (2.216)$$

where ρ , v , Q are defined as usual and $V_{gp} = -G\phi^2(x, t)$ is the so-called Gross–Pitaevskii potential. With the help of Eq. (2.216), it is readily obtained that

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\frac{\partial S}{\partial x} \right)^2 + V + Q + V_{gp} = 0. \quad (2.217)$$

A semiclassical solution to the Gross–Pitaevskii equation in terms of a Gaussian wave packet is easily reached. Thus, if we start again from Eq. (2.12), $S(x, t)$, V_{gp} and Q can be again expanded around $q(t)$ up to second order according to Eqs. (2.128), (2.129) and (2.130).

Next, substituting Eq. (2.12) into (2.215), we again find Eq. (2.16) for the velocity. Now, as previously carried out in Sect. 2.6, by collecting terms in $[x - q(t)]^0$ and $[x - q(t)]^1$, we have

$$S'[x(t), t] = m\dot{q}(t), \quad (2.218)$$

$$S''[x(t), t] = m \frac{\dot{\delta}(t)}{\delta(t)}. \quad (2.219)$$

Then, by substituting Eq. (2.12) and the previous Taylor expansions (2.128), (2.129) and (2.130) into (2.217) and again collecting terms in $[x - q(t)]^0$ and $[x - q(t)]^1$, it is reached that

$$\dot{S}_0 = \frac{1}{2}m\dot{q}^2(t) - \frac{\hbar^2}{4m\delta^2(t)} + \frac{G}{\sqrt{2\pi}\delta(t)}, \quad (2.220)$$

$$\ddot{q}(t) = 0, \quad (2.221)$$

$$\ddot{\delta}(t) = \frac{\hbar^2}{4m^2\delta^3(t)} - \frac{G}{\sqrt{2\pi}m\delta^2(t)}, \quad (2.222)$$

where have denoted $\dot{S}_0 \equiv \dot{S}[q(t), t]$. It is worth noticing the presence of the quantum and Gross–Pitaevskii potentials in the last terms of Eqs. (2.220) and (2.222). For linear and quadratic potentials, we note a remarkable feature: the existence of exact soliton-like solutions of Gaussian form (gaussons). We find a non-spreading width if

$$\delta_0 = \frac{\sqrt{2\pi}\hbar^2}{4mG}. \quad (2.223)$$

2.12 Dissipation in the Caldirola-Kanai Model

An effective description of dissipation can be achieved from explicitly time-dependent Lagrangians and/or Hamiltonians, thus avoiding to deal with the environment degrees of freedom. This approach allows one to preserve the canonical formalism, which

can be a good starting point to find out the quantum analogue of the corresponding dissipative dynamics [98, 99]. The so-called Caldirola-Kanai model [100, 101] can be considered a Hamiltonian formulation of the Langevin equation with zero fluctuations, that is, the Brownian-like thermal fluctuations due to the environment are neglected and the system undergoes a gradual decay until its total energy is completely and irreversibly lost by dissipation (leading to the stopping of the corresponding dynamics). This model can provide us a nice illustration of the dynamics of a particle on a quantum viscid media.

Consider first the classical equation of motion for a damped particle of mass m under the action of a one-dimensional external potential $V(x)$ and a mean friction γ . The corresponding Langevin equation can be written as

$$m\ddot{x} + m\gamma\dot{x} + V'(x) = 0, \quad (2.224)$$

where overdots on the position variable indicate the order of the total time derivatives, and primes for different orders of derivation of the external potential with respect to the position variable. Now, by multiplying this equation by $e^{\gamma t}$, we have

$$\frac{d}{dt} (me^{\gamma t}\dot{x}) + V'(x)e^{\gamma t} = 0. \quad (2.225)$$

If we consider the change of variable $X = x$ and

$$P \equiv me^{\gamma t}\dot{x} = pe^{\gamma t}, \quad (2.226)$$

where $p = m\dot{x}$ is the physical momentum, we readily notice that (2.225) is just the Lagrange equation satisfied by the time-dependent Lagrangian function

$$L = \frac{P^2}{2m} e^{-\gamma t} - V(X)e^{\gamma t}, \quad (2.227)$$

where P plays the role of a canonical momentum with $P = \partial L / \partial \dot{X}$. This equation allows us to obtain straightforwardly the corresponding Hamiltonian function

$$H = \dot{X}P - L = \frac{P^2}{2m} e^{-\gamma t} + V(X)e^{\gamma t}, \quad (2.228)$$

which is a function of the canonical variables X and P satisfying the Hamilton equations

$$\dot{X} = \frac{\partial H}{\partial P}, \quad \dot{P} = -\frac{\partial H}{\partial X}. \quad (2.229)$$

Thus, the energy of the classical system can be expressed as

$$E = \frac{p^2}{2m} + V(x) = He^{-\gamma t}. \quad (2.230)$$

which exhibits the typical exponential decay due to the dissipative dynamics.

The quantum analog of (2.228) can be now obtained by considering the (canonical) momentum operator $P = -i\hbar\partial/\partial X$ ($= -i\hbar\partial/\partial x$) leading to the standard commutation rule, $[X, P] = i\hbar$. Notice that the same commutation relation for the physical operators of position and momentum is written as $[x, p] = i\hbar e^{-\gamma t}$. The quantum Hamiltonian operator reads as

$$H = -\frac{\hbar^2}{2m} e^{-\gamma t} \nabla_x^2 + V(X)e^{\gamma t}, \quad (2.231)$$

leading to the generalized, dissipative Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} e^{-\gamma t} \nabla_x^2 \Psi + V(x)e^{\gamma t} \Psi \quad (2.232)$$

in terms of the physical coordinate. Thus, as long as the momentum operator is not acting, the use of the wave equation in the physical coordinate is formally correct.

In the Bohmian formalism [102], the polar form of the wave function is again used, $\Psi(x, t) = \rho^{1/2}(x, t)e^{iS(x, t)/\hbar}$. When substituting into (2.232), the following coupled partial differential equations are reached

$$\frac{\partial \rho}{\partial t} + \nabla_x J = 0, \quad (2.233)$$

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \nabla_x^2 S e^{-\gamma t} + V_{\text{eff}}(x, t) = 0, \quad (2.234)$$

where $J = (1/m)\rho \nabla_x S e^{-\gamma t}$ is the associated probability density current and $V_{\text{eff}}(x, t) = V(x)e^{\gamma t} + Q(x, t)$ is an effective potential, which includes the quantum potential

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla_x^2 \rho^{1/2}}{\rho^{1/2}} e^{-\gamma t} = -\frac{\hbar^2}{4m} \left[\frac{\nabla_x^2 \rho}{\rho} - \frac{1}{2} \left(\frac{\nabla_x \rho}{\rho} \right)^2 \right] e^{-\gamma t}. \quad (2.235)$$

The time-dependent decaying factor, $e^{-\gamma t}$, also manifests in the corresponding dissipative Bohmian trajectories, which are derived from the equation of motion

$$\dot{x} = \frac{J}{\rho} = \frac{\nabla_x S}{m} e^{-\gamma t} = \frac{\hbar}{2mi\rho} (\Psi^* \nabla_x \Psi - \Psi \nabla_x \Psi^*) e^{-\gamma t}. \quad (2.236)$$

In this expression, the Bohmian momentum also holds a similar relationship to (2.226), i.e., $P_B = \nabla_x S = me^{\gamma t} \dot{X}$, with $X(t) = x(t)$ being the corresponding Bohmian trajectory.

For simple problems such as, for example, free propagation, interference dynamics, linear potentials or the harmonic oscillator, analytical solutions are available. Usually, the initial wave function is described by a Gaussian wave packet written as [102]

$$\Psi(X, t) = e^{(i/\hbar)[\alpha_t(X-X_t)^2 + P_t(X-X_t) + f_t]}, \quad (2.237)$$

where the subscript t is used to denote explicit time-dependence of the parameters characterizing the wave function (the subscript 0 is found when $t = 0$). If the wave function (2.237) is normalized, then

$$f_0 = \frac{i\hbar}{4} \ln \left[\frac{\pi\hbar}{2\text{Im}\{\alpha_0\}} \right], \quad (2.238)$$

with $\text{Im}\{\alpha_0\} \neq 0$. In such a case, the position and momentum expectation values (and therefore the wave-packet centroid) follow a classical trajectory, i.e., $\langle \hat{X} \rangle(t) = X_t$ and $\langle \hat{P} \rangle(t) = P_t$, with (X_t, P_t) being obtained by integrating the Hamilton equations of motion (2.229), i.e.,

$$\dot{X}_t = \frac{P_t}{m} e^{-\gamma t}, \quad (2.239)$$

$$\dot{P}_t = -\frac{\partial}{\partial X_t} V(X_t) e^{\gamma t}. \quad (2.240)$$

Moreover, the physical dispersion of the wave packet is found to be

$$\Delta x(t) = \Delta X(t) = \sqrt{\langle X^2 \rangle(t) - [\langle X \rangle(t)]^2} = \sqrt{\frac{\hbar}{4\text{Im}\{\alpha_t\}}} = \sigma_t, \quad (2.241)$$

where σ_t is the instantaneous wave-packet spreading. The expectation value of its (also physical) energy,

$$\bar{E} = \langle \hat{H} \rangle e^{-\gamma t} = \frac{P_t^2}{2m} e^{-2\gamma t} + V_t + \frac{\hbar}{2m} \frac{|\alpha_t|^2}{\text{Im}\{\alpha_t\}} e^{-2\gamma t} + \frac{\hbar V_t''}{8\text{Im}\{\alpha_t\}}, \quad (2.242)$$

where the primes mean derivation with respect to X . Clearly, two contributions are present: one coming from the translational motion along the classical centroidal trajectory (E_t) and another one related to the wave-packet spreading. This second contribution contains information about the spatial variations of both the wave packet and the potential.

Concerning the shape parameters α_t and f_t , their equations of motion can be readily obtained as follows. Let us recast $V(X)$ as a Taylor series expansion around the centroidal position X_t up to the second order, i.e.,

$$V(X) = V_t + V_t'(X - X_t) + \frac{1}{2} V_t''(X - X_t)^2. \quad (2.243)$$

By substituting Eq. (2.237) and the expansion (2.243) into the dissipative Schrödinger equation (2.232), and then collecting the coefficients associated with the same power of $(X - X_t)$, it is easily found that

$$\dot{\alpha}_t = -\frac{2\alpha_t^2}{m} e^{-\gamma t} - \frac{1}{2} V_t'' e^{\gamma t}, \quad (2.244)$$

$$\dot{f}_t = \frac{i\hbar\alpha_t}{m} e^{-\gamma t} + L_t, \quad (2.245)$$

with L_t given by (2.227) evaluated along the classical trajectory (X_t, P_t) —since this term is only time-dependent and does not have any space dependance, it will not influence the Bohmian dynamics and therefore we will not consider its explicit functional form. Thus, integrating the set of coupled ordinary differential equations (2.239), (2.240), (2.244) and (2.245), the wave function (2.237) is completely specified at any time. By substituting this wave function into the Bohmian equation of motion (2.236), the following expression for the velocity is reached

$$\dot{X} = \left[\frac{P_t}{m} + \frac{2\text{Re}\{\alpha_t\}}{m} (X - X_t) \right] e^{-\gamma t}, \quad (2.246)$$

which after integration renders the corresponding dissipative Bohmian trajectory $x(t) = X(t)$. From Eq. (2.246), it is clearly seen that if the second term vanishes, the Bohmian trajectory exactly coincides with the classical one given by (2.240). Accordingly, the condition to recover the classical equations does not require necessarily of the limiting procedure of $\hbar \rightarrow 0$, but that the wave packet remains relatively localized (i.e., $1/\text{Re}\{\alpha_t\} \rightarrow 0$), in agreement with the hypothesis of Ehrenfest's theorem. Furthermore, if $\text{Im}\{\alpha_t\} \rightarrow 0$ and the wave function becomes a pure phase factor (except for some time-dependent norm coming from f_t), quantum motion is still present through both P_t and $\text{Re}\{\alpha_t\}$.

2.12.1 Free Gaussian Wave Packet

If the initial wave function is considered to be a Gaussian wave packet [102]

$$\Psi(x, 0) = \left(\frac{1}{2\pi\sigma_0^2} \right)^{1/4} e^{-(x-x_0)^2/4\sigma_0^2 + ip_0(x-x_0)/\hbar}, \quad (2.247)$$

then the initial conditions for the above Gaussian parameters and variables are $X_0 = x_0$, $P_0 = p_0$, $\alpha_0 = i\hbar/4\sigma_0^2$, and $f_0 = (i\hbar/4) \ln(2\pi\sigma_0^2)$. The corresponding initial probability distribution is given by

$$\rho(x, 0) = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-(x-x_0)^2/2\sigma_0^2}, \quad (2.248)$$

which provides us the spatial region for the initial conditions of the Bohmian trajectories.

After integration of the aforementioned equations of motion, we have that

$$x_t = x_0 + \frac{p_0}{m\gamma} (1 - e^{-\gamma t}), \quad (2.249)$$

$$p_t = p_0 e^{-\gamma t}, \quad (2.250)$$

$$\alpha_t = \frac{\alpha_0}{1 + (2\alpha_0/m\gamma)(1 - e^{-\gamma t})} \quad (2.251)$$

$$f_t = \frac{i\hbar}{4} \ln \left[\frac{\pi\hbar}{2\text{Im}\{\alpha_0\}} \right] + \frac{i\hbar}{2} \ln \left[1 + \frac{2\alpha_0}{m} \left(\frac{1 - e^{-\gamma t}}{\gamma} \right) \right] + S_{\text{cl},t}, \quad (2.252)$$

where

$$S_{\text{cl},t} = \int_0^t L_{t'} dt' \quad (2.253)$$

is the associated classical action. This term only adds a time-dependent phase factor, which does not play any role in the Bohmian dynamics (its gradient vanishes). Equation (2.251) can be alternatively expressed in terms of an effective time-dependent spreading

$$\tilde{\sigma}_t = \sigma_0 \left[1 + \frac{i\hbar}{2m\sigma_0^2} \left(\frac{1 - e^{-\gamma t}}{\gamma} \right) \right], \quad (2.254)$$

which is connected to α_t by the simple relationship $\alpha_t = i\hbar/4\sigma_0\tilde{\sigma}_t$. Accordingly, Eq. (2.252) can be recast in a simpler form,

$$f_t = \frac{i\hbar}{4} \ln(2\pi\tilde{\sigma}_t^2) + S_{\text{cl},t}. \quad (2.255)$$

It is worth mentioning that, in terms of the canonical variables, the functional form of this wave packet is the same as that displayed by a standard free wave packet if t is replaced by

$$\tau = \frac{1 - e^{-\gamma t}}{\gamma} \quad (2.256)$$

in the former; in other words, a time contraction coming from the dissipative process and associated with an eventual freezing displayed by the wave packet.

In the free dispersion limit, it is straightforward to show that (2.237) approaches the well-known solution for the free Gaussian wave packet

$$\Psi(x, t) = \left[\frac{1}{2\pi(\tilde{\sigma}_t^0)^2} \right]^{1/4} e^{-(x-x_t)^2/4\sigma_0\tilde{\sigma}_t^0 + ip_0(x-x_t)/\hbar + iEt/\hbar}, \quad (2.257)$$

where $x_t = x_0 + (p_0/m)t$ provides the instantaneous centroidal position, $E = p_0^2/2m$ is its total mechanical energy, and

$$\sigma_t^0 = |\tilde{\sigma}_t^0| = \sigma_0 \sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2} \right)^2} \quad (2.258)$$

is its spreading along time, with $\tilde{\sigma}_t^0 = \sigma_0 [1 + (i\hbar t/2m\sigma_0^2)]$. However, with friction, the wave packet undergoes asymptotically (i.e., for $t \rightarrow \infty$) a damping in its propagation (according to Eq. (2.249), stopping at the position $x_\infty = x_0 + (p_0/m\gamma)$) as well as in its spreading, described by

$$\sigma_t = |\tilde{\sigma}_t| = \sigma_0 \sqrt{1 + \left(\frac{\hbar}{2m\sigma_0^2} \right)^2 \left(\frac{1 - e^{-\gamma t}}{\gamma} \right)^2}. \quad (2.259)$$

Notice that asymptotically, $\sigma_\infty = \sigma_0 \sqrt{1 + (\hbar/2m\gamma\sigma_0^2)^2}$.

The corresponding Bohmian trajectories, which are obtained after integration of the equation of motion (2.246), are given by

$$x(t) = x_t + \frac{\sigma_t}{\sigma_0} [x(0) - x_0], \quad (2.260)$$

which is formally equivalent to the expression that one obtains for the free, frictionless case (see Chap. 1). In the case with friction, Eq. (2.260) reaches the asymptotic limit

$$x(t \rightarrow \infty) = x_0 + \frac{p_0}{m\gamma} + \sqrt{1 + \left(\frac{\hbar}{2m\gamma\sigma_0^2} \right)^2} [x(0) - x_0]. \quad (2.261)$$

Thus, the wave packet becomes localized: motionless and with the spreading being frozen. For strong friction, it becomes essentially parallel to the classical or centroidal trajectory, since the time-dependence vanishes very quickly and, therefore, σ_t becomes a constant value very rapidly. To some extent, this is a step towards the classicality of the quantum system without appealing to the more standard limiting procedure of $\hbar \rightarrow 0$.

In Fig. 2.7 a series of wave-packet properties and Bohmian trajectories are shown for different values of the friction coefficient: $\gamma = 0.025$ (black solid line), $\gamma = 0.1$ (blue dashed line), and $\gamma = 0.5$ (red dash-dotted line). The numerical simulations have been carried out with the following initial conditions: $\sigma_0 = 1$, $x_0 = 0$ and $p_0 = 2.5$ (atomic units). In the upper row, we show the average position (a), (spatial) dispersion (b), and energy (c) as a function of time. To compare with, we have also included the frictionless values, denoted with the gray dotted line. The energy

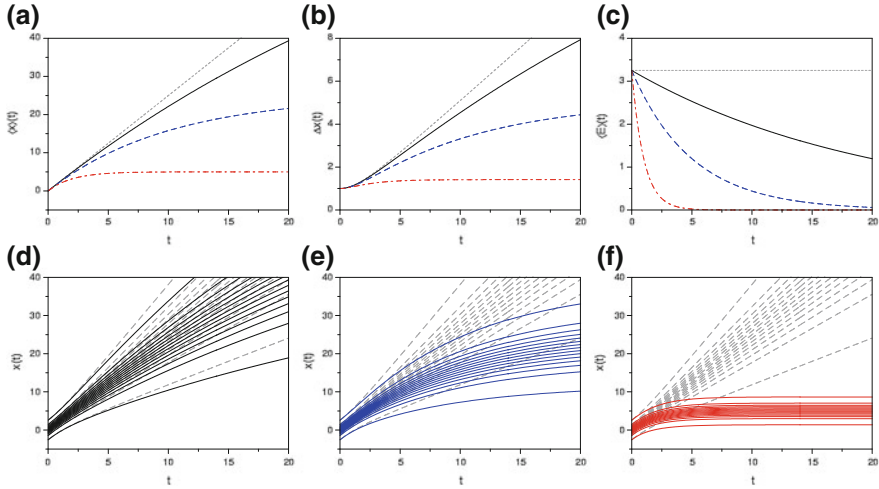


Fig. 2.7 *Top* Average position (a), dispersion (b), and energy (c) for a Gaussian wave packet in free space affected by friction. Different values for the friction coefficient have been considered: $\gamma = 0.025$ (black solid line), $\gamma = 0.1$ (blue dashed line), and $\gamma = 0.5$ (red dash-dotted line). To compare with, the frictionless case ($\gamma = 0$) has also been included and is denoted with the gray dotted line. The value of the other parameters considered in these simulations were: $x_0 = 0$, $p_0 = 2.5$ ($E_0 = 3.25$), $\sigma_0 = 1$, $m = 1$, and $\hbar = 1$. *Bottom* Bohmian trajectories associated with the three dissipative cases considered atop: **d** $\gamma = 0.025$, **e** $\gamma = 0.1$, and **f** $\gamma = 0.5$. Again, to compare with, the trajectories for the frictionless case (with the same initial conditions) have also been included in each panel (gray dashed lines). The initial positions have been distributed according to the initial Gaussian probability density

expectation value is given by

$$\bar{E} = \left(\frac{p_0^2}{2m} + \frac{\hbar^2}{8m\sigma_0^2} \right) e^{-2\gamma t}, \quad (2.262)$$

i.e., it is suppressed at twice the rate γ . Bohmian trajectories illustrating these dissipative cases are displayed in the three lower panels, from left to right: (d) $\gamma = 0.025$, (e) $\gamma = 0.1$, and (f) $\gamma = 0.5$. The trajectories for the frictionless case have also been included in each panel (gray dashed lines). To better appreciate the different effect of the wave-packet spreading and how it is suppressed as γ increases, 15 trajectories are chosen with initial positions distributed according the initial Gaussian probability density. Thus, for small frictions, it is observed that trajectories starting in the “wings” of the wave packet will increase faster their distance with respect to the centroid than those closer to the latter. Moreover, this distance will be faster for trajectories starting behind the centroid than in front of it due to the larger relative difference between their associated velocities. This effect is, however, damped as the friction coefficient increases, thus producing a smaller separation among trajectories and eventually a freezing of their position for times larger than γ^{-1} . These frozen positions are given by Eq. (2.261).

2.12.2 Interference of Two Gaussian Wave Packets

Let us consider now the interference problem of two free wave packets. As is known, a general solution to this problem can be expressed as a coherent superposition,

$$\Psi = \mathcal{N}(\Psi_1 + \Psi_2), \quad (2.263)$$

with $\mathcal{N}$ being the overall norm factor (it is assumed that each Gaussian wave packet, given by Eq. (2.257), is normalized). As it can be shown, the associated Bohmian equation of motion reads as [102]

$$\begin{aligned} \dot{x} &= \frac{\rho_1}{\rho} \dot{x}_1 + \frac{\rho_2}{\rho} \dot{x}_2 + \frac{\hbar}{2mi\rho} (\Psi_1^* \partial_x \Psi_2 - \Psi_2 \partial_x \Psi_1^*) e^{-\gamma t} \\ &\quad + \frac{\hbar e^{-\gamma t}}{2mi\rho} (\Psi_2^* \partial_x \Psi_1 - \Psi_1 \partial_x \Psi_2^*) e^{-\gamma t} \\ &= \frac{\rho_1}{\rho} \left[\frac{p_{t,1}}{m} + \frac{2\text{Re}\{\alpha_{t,1}\}}{m} (x - x_{t,1}) e^{-\gamma t} \right] \\ &\quad + \frac{\rho_2}{\rho} \left[\frac{p_{t,2}}{m} + \frac{2\text{Re}\{\alpha_{t,2}\}}{m} (x - x_{t,2}) e^{-\gamma t} \right] \\ &\quad + 2 \cos \xi_{12} \frac{\sqrt{\rho_1 \rho_2}}{\rho} \left[\frac{p_{t,1} + p_{t,2}}{2m} + \left[\frac{\text{Re}\{\alpha_{t,1}\}(x - x_{t,1}) + \text{Re}\{\alpha_{t,2}\}(x - x_{t,2})}{m} \right] e^{-\gamma t} \right] \\ &\quad - 2 \sin \xi_{12} \frac{\sqrt{\rho_1 \rho_2}}{\rho} \left[\frac{\text{Im}\{\alpha_{t,1}\}(x - x_{t,1}) - \text{Im}\{\alpha_{t,2}\}(x - x_{t,2})}{m} \right] e^{-\gamma t}, \end{aligned} \quad (2.264)$$

where $\dot{x}_i$ refers to the equation of motion for the i th wave packet and $\xi_{12} = (S_1 - S_2)/\hbar$, being ρ_i and S_i the probability density and real phase associated with the i th wave packet when it is expressed in polar form. As it can be seen, this expression simply reflects the sum of two separate fluxes, each one associated with one wave packet, plus another one coming from their interference.

Depending on the value given to the parameters of each wave packet, one can generate different dynamics. For example, if they have the same width ($\alpha_{t,1} = \alpha_{t,2} = \alpha_t$) and are located at symmetric positions with respect to $x = 0$ ($x_{t,1} = x_0 = -x_{t,2}$), then (2.264) simplifies to

$$\begin{aligned} \dot{x} &= \frac{\rho_1}{\rho} \left[\frac{p_{t,1}}{m} + \frac{2\text{Re}\{\alpha_t\}}{m} (x - x_0) e^{-\gamma t} \right] + \frac{\rho_2}{\rho} \left[\frac{p_{t,2}}{m} + \frac{2\text{Re}\{\alpha_t\}}{m} (x + x_0) e^{-\gamma t} \right] \\ &\quad + 2 \cos \xi_{12} \frac{\sqrt{\rho_1 \rho_2}}{\rho} \left[\frac{p_{t,1} + p_{t,2}}{2m} + \frac{2\text{Re}\{\alpha_t\}}{m} x e^{-\gamma t} \right] \\ &\quad + 2 \sin \xi_{12} \frac{\sqrt{\rho_1 \rho_2}}{\rho} \left[\frac{2\text{Im}\{\alpha_t\}}{m} x_0 e^{-\gamma t} \right]. \end{aligned} \quad (2.265)$$

This situation can simulate the two slit experiment when each wave packet is associated with one of the diffracted beams in a viscid medium. In such a case, if the

longitudinal propagation (parallel to the diffractive screen) is slower than the perpendicular one (in the direction of the diffracted beam), both motions can be decoupled and treated as two independent one-dimensional propagations, one longitudinal and the other translational, the latter being well accounted for by a plane wave. Now, if one assumes that $p_{0,1} = p_{0,2} = 0$, i.e., there is no translational motion along the longitudinal direction, but only spreading of the two wave packets [103], the above expression (2.265) will read as

$$\begin{aligned} \dot{x} = & \frac{\rho_1}{\rho} \left[\frac{2\text{Re}\{\alpha_t\}}{m} (x - x_0) e^{-\gamma t} \right] + \frac{\rho_2}{\rho} \left[\frac{2\text{Re}\{\alpha_t\}}{m} (x + x_0) e^{-\gamma t} \right] \\ & + 2 \cos \xi_{12} \frac{\sqrt{\rho_1 \rho_2}}{\rho} \left[\frac{2\text{Re}\{\alpha_t\}}{m} x e^{-\gamma t} \right] \\ & + 2 \sin \xi_{12} \frac{\sqrt{\rho_1 \rho_2}}{\rho} \left[\frac{2\text{Im}\{\alpha_t\}}{m} x_0 e^{-\gamma t} \right]. \end{aligned} \quad (2.266)$$

Results after integration of this equation of motion for different values of γ (the same values as in the case of the free wave packet treated above) can be seen in Fig. 2.8. As it can be seen through the sets of trajectories selected, the friction of the medium leads to the localization of the two wave packets by gradually “freezing” them rather than by annihilating the coherence between them due to the interaction with an environment. In other words, the reason why interference is not observed in a quantum viscid medium is because the wave packets cannot be seen each other, rather than because the destruction (over time) of their mutual coherence.

Several types of interference dynamics can be devised by changing the initial values of the parameters involved in this superposition problem [102].

2.12.3 Linear Potential

For a linear interaction potential like a gravitational or an electric field, the classical solutions are also readily obtained [102, 104]. Thus, if $V(x) = -max$ (a being a positive parameter), we have that

$$x_t = x_0 + \frac{p_0}{m} \left(\frac{1 - e^{-\gamma t}}{\gamma} \right) + a \left(\frac{\gamma t - 1 + e^{-\gamma t}}{\gamma^2} \right), \quad (2.267)$$

$$p_t = p_0 e^{-\gamma t} + ma \left(\frac{1 - e^{-\gamma t}}{\gamma} \right), \quad (2.268)$$

and α_t and γ_t keep the same functional form as in the free damped case (although L_t varies for the latter due to the presence of a nonzero potential function), because only second-order derivatives influence the evolution of those parameters (through V_t'' , as seen in Eq. (2.244)).

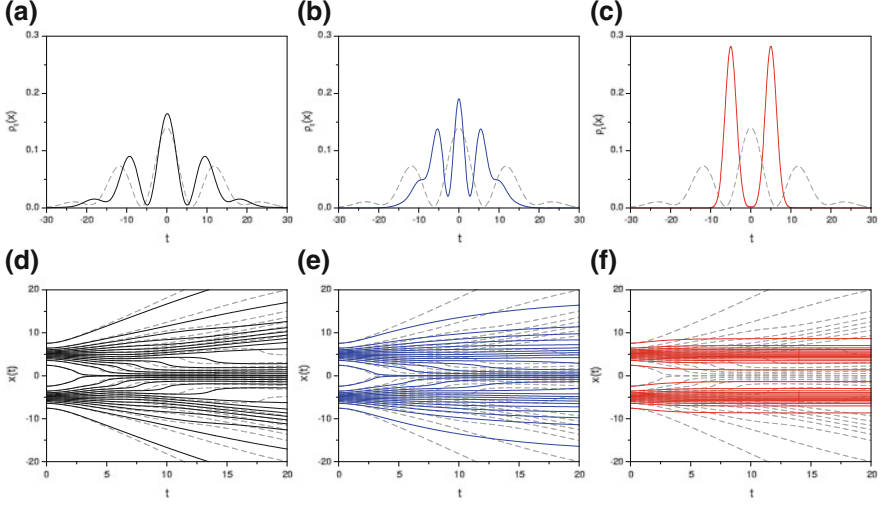


Fig. 2.8 *Top* Final probability density (at $t = 20$) for a coherent superposition of two Gaussian wave packets in free space affected by friction. The same friction values as in Fig. 2.7 have been considered: **a** $\gamma = 0.025$ (black solid line), **b** $\gamma = 0.1$ (blue solid line), and **c** $\gamma = 0.5$ (red solid line). To compare with, the frictionless case ($\gamma = 0$) has also been included in each panel (gray dashed line). The value of the other parameters considered in these simulations were: $x_{0,1} = 5 = -x_{0,2}$, $p_{0,1} = p_{0,2} = 0$ ($E_0 = 3.25$), $\sigma_{0,1} = \sigma_{0,2} = 1$, $m = 1$, and $\hbar = 1$. *Bottom* Bohmian trajectories associated with the three dissipative cases considered at top: **d** $\gamma = 0.025$, **e** $\gamma = 0.1$, and **f** $\gamma = 0.5$. Again, to compare with, the trajectories for the frictionless case (with the same initial conditions) have also been included in each panel (gray dashed lines). The initial positions have been distributed according to the initial Gaussian probability density

The frictionless limit $\gamma \rightarrow 0$ leads us to the well-known expressions for uniform accelerated motion, with $x_t = x_0 + (p_0/m)t + (a/2)t^2$ and $p_t = p_0 + mat$. The wave packet also approaches the expression corresponding to the solution to ramp-like potentials [104], equal to (2.257), except for the different functional form of E_t ($E_t = p_0^2/2m - max_0$) and an extra term coming from the classical action. Regarding the long-time limit for finite friction (i.e., for $t \gg \gamma^{-1}$), we find that while the wave packet freezes its spreading, as in the previous example, it still keeps moving due to the constant limit momentum, $p_\infty = ma/\gamma$. Accordingly, the centroid of the wave-packet displays a uniform motion described by

$$x_{t \rightarrow \infty} = x_0 + \frac{p_0}{m\gamma} - \frac{a}{\gamma^2} + \frac{a}{\gamma} t. \quad (2.269)$$

With γ , the transition from a uniformly accelerated motion, displayed by the wave-packet centroid, to a uniform rectilinear one, as a consequence of the damping, becomes more apparent. The expression for the average energy is given by

$$\begin{aligned}\bar{E} = & \frac{p_0^2}{2m} e^{-2\gamma t} - max_0 - p_0 a \gamma \left(\frac{1 - e^{-\gamma t}}{\gamma} \right)^2 \\ & + \frac{ma^2}{2} \left(\frac{3 - 2\gamma t - 4e^{-\gamma t} + e^{-2\gamma t}}{\gamma^2} \right) + \frac{\hbar^2}{8m\sigma_0^2} e^{-2\gamma t}.\end{aligned}\quad (2.270)$$

In the limit $\gamma t \gg 1$, this expression approaches

$$\bar{E} = -max_0 - \frac{p_0 a}{\gamma} + \frac{ma^2}{2\gamma^2} (3 - 2\gamma t). \quad (2.271)$$

Unlike the example of the free wave packet, here the energy does not approach zero asymptotically, but it continues decreasing below it as the wave packet slides downhill (unless some additional constraint is imposed in the dynamics to avoiding this situation). Nevertheless, although there is no suppression of the motion, spatial localization is still present.

On the other hand, due to the fact that α_t does not depend on the potential function, the functional form displayed by the Bohmian trajectories is exactly the same as in the free case, except for the fact that these trajectories contain information about the acceleration undergone by the centroid (this information is transmitted through x_t). Now, once the exponentials have vanished, all these trajectories evolve parallel one another, just like classical trajectories under similar circumstances.

2.12.4 Damped Harmonic Oscillator

In a frictionless situation, the wave functions for a harmonic potential given by $V(x) = m\omega_0^2 x^2/2$ are expressed as

$$\Phi_n(x, t) = N_n e^{-(m\omega_0/2\hbar)x^2 - i(n+1/2)\omega_0 t} H_n(\sqrt{m\omega_0/\hbar}x), \quad (2.272)$$

with energies $E_n = (n + 1/2)\hbar\omega_0$, and where H_n is the Hermite polynomial of degree n and $N_n = (1/\sqrt{2^n n!})(\pi\hbar/m\omega_0)^{-1/4}$ is the normalization constant. These energy values can be obtained by employing the same method used above to derive the analytical expression of the time-evolved wave packets [105]. Analogously, it can also be used to determine the dissipative counterpart of Eq. (2.272) [102],

$$\begin{aligned}\Phi_n(x, t) = & N_n e^{-(m\Omega/2\hbar)(1+i\gamma/2\Omega)e^{\gamma t}x^2 - i(n+1/2)\Omega t + \gamma t/4} H_n(\sqrt{m\Omega/\hbar}e^{\gamma t/2}x) \\ = & N_n e^{-(m\Omega/2\hbar)e^{\gamma t}x^2 - i(n+1/2)\Omega t - i(m\gamma/4\hbar)e^{\gamma t}x^2 + \gamma t/4} H_n(\sqrt{m\Omega/\hbar}e^{\gamma t/2}x).\end{aligned}\quad (2.273)$$

However, contrary to Eqs. (2.272), (2.273) describes a *quasi-stationary state*. As formerly shown by Vandyck [106], these states, at each time, are eigenstates of the

dissipative Schrödinger equation and eventually collapse to zero. Of course, these states are only defined for $\omega_0 > \gamma/2$.

Concerning the associated Bohmian trajectories, from Eq. (2.273), we have that

$$\dot{x} = -\frac{\gamma}{2} x, \quad (2.274)$$

which after integration renders

$$x(t) = x(0)e^{-\gamma t/2}. \quad (2.275)$$

That is, regardless of the eigenstate considered, any trajectory falls down to the bottom of the potential at the same rate, $\gamma/2$, and therefore merging asymptotically at $x = 0$. The reason for such a behavior is that the model is fully dissipative and there is no possibility for a feedback with an environment, as happens when a Brownian-like motion is assumed. In this latter case, the stochastic fluctuations accounting for the feedback with a surrounding medium would be enough to sustain a dynamical regime (even if stationary) and avoid its full collapse.

We are going to consider here the case of a coherent (or minimum uncertainty) Gaussian wave packet initially centered around the turning point $x = x_0$ ($p_0 = 0$). At any subsequent time, this wave packet is described by

$$\Psi(x, t) = \left(\frac{1}{2\pi\sigma_0^2} \right)^{1/4} e^{-(x-x_t)^2/4\sigma_0^2 + ip_t(x-x_t)/\hbar - i\omega_0 t/2 + ip_t x_t/\hbar}, \quad (2.276)$$

with $x_t = x_0 \cos \omega_0 t$ and $p_t = -m\omega_0 x_0 \sin \omega_0 t$. The corresponding probability density reads as

$$|\Psi(x, t)| = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-[x-x_0 \cos(\omega_0 t)]^2/2\sigma_0^2}, \quad (2.277)$$

where $\sigma_0^2 = \hbar/(2m\omega_0)$ for the wave packet (2.276) to be coherent (otherwise, the wave packet will keep its Gaussian shape and will display an oscillating variation of its width or “breathing” as it moves back and forth between the two turning points). The corresponding quantum action is

$$S(x, t) = -\frac{1}{2} \hbar\omega_0 t - \frac{m\omega_0}{4} [4xx_0 \sin(\omega_0 t) - x_0^2 \sin(2\omega_0 t)], \quad (2.278)$$

which leads to Bohmian trajectories oscillating with the same frequency as x_t , but around their initial position

$$x(t) = [x(0) - x_0] + x_0 \cos(\omega_0 t). \quad (2.279)$$

As also happens in classical mechanics, in order to proceed analytically in the dissipative case, it is important to distinguish three cases depending on whether ω_0 is larger than, equal to or smaller than $\gamma/2$, i.e., if we have underdamped oscillatory motion, critically damped motion, or overdamped motion, respectively. These situations lead to the following solutions for the centroidal trajectory:

$$\omega_0 > \gamma/2 \implies \begin{cases} x_t = \left(\frac{\omega_0}{\Omega}\right) x_0 e^{-\gamma t/2} \cos(\Omega t - \varphi) \\ p_t = -m \left(\frac{\omega_0^2}{\Omega}\right) x_0 e^{-\gamma t/2} \sin \Omega t \end{cases}, \quad (2.280)$$

$$\omega_0 = \gamma/2 \implies \begin{cases} x_t = x_0 \left(1 + \frac{\gamma}{2} t\right) e^{-\gamma t/2} \\ p_t = -m x_0 \left(\frac{\gamma}{2}\right)^2 e^{-\gamma t/2} \end{cases}, \quad (2.281)$$

$$\omega_0 < \gamma/2 \implies \begin{cases} x_t = \left(\frac{\omega_0}{\Gamma}\right) x_0 e^{-\gamma t/2} \cosh(\Gamma t + \phi) \\ p_t = -m \left(\frac{\omega_0^2}{\Gamma}\right) x_0 e^{-\gamma t/2} \sinh \Gamma t \end{cases}, \quad (2.282)$$

where $\Omega = \sqrt{\omega_0^2 - (\gamma/2)^2}$, $\varphi = (\tan)^{-1}(\gamma/2\Omega)$, $\Gamma = i\Omega$, and $\phi = (\tanh)^{-1}(\gamma/2\Gamma)$. The relationship between ω_0 and γ also influences the calculation of α_t and f_t . In the case of α_t , the equation of motion to be solved is

$$\dot{\alpha}_t = -\frac{2\alpha_t^2}{m} e^{-\gamma t} - \frac{1}{2} m \omega_0^2 e^{\gamma t}, \quad (2.283)$$

which can be conveniently rearranged by introducing the change $\alpha_t = g_t e^{\gamma t}$. This leads to the equation of motion

$$\dot{g}_t = -\frac{2}{m} \left[g_t^2 + \frac{m\gamma}{2} g_t + \left(\frac{m\omega_0}{2}\right)^2 \right] = -\frac{2}{m} (g_t - g_+)(g_t - g_-), \quad (2.284)$$

which does not contain exponential terms, and where

$$g_{\pm} = \frac{m}{2} \left[-\frac{\gamma}{2} \pm \sqrt{\left(\frac{\gamma}{2}\right)^2 - \omega_0^2} \right]. \quad (2.285)$$

From the latter expression, it is now clear how the three cases of damped motion also rule the behavior of α_t , although there are some physical subtleties to take into account. If $\omega_0 \neq \gamma/2$, the general solution for g_t reads as

$$g_t = \frac{g_+(g_0 - g_-)e^{\beta t} - g_-(g_0 - g_+)e^{-\beta t}}{(g_0 - g_-)e^{\beta t} - (g_0 - g_+)e^{-\beta t}}, \quad (2.286)$$

where $\beta = \sqrt{(\gamma/2)^2 - \omega_0^2}$ and g_0 is the initial condition. Otherwise, if $\omega_0 = \gamma/2$ (critically damped motion), we have $g_+ = g_-$ and Eq. (2.284) becomes

$$\dot{g}_t = -\frac{2}{m} (g_t - g_s)^2, \quad (2.287)$$

with $g_s = -m\gamma/4$. The integration over time of this equation of motion yields

$$g_t = g_s + \frac{g_0 - g_s}{1 + (g_0 - g_s)(2t/m)}. \quad (2.288)$$

If we now assume that our initial wave packet is (2.276) and consider the initial condition $g_0 = \alpha_0 = \alpha_t = im\omega_0/2$, then g_t becomes an oscillatory function of time for $\omega_0 > \gamma/2$, since $\beta = i\Omega$. Otherwise, it becomes a monotonically decreasing function of time, with the asymptotic limits $g_\infty = g_s$ if $\omega_0 = \gamma/2$, or $g_\infty = g_+$ (with $\beta = \Gamma$) if $\omega_0 < \gamma/2$.

Notice in Eq. (2.286) that g_t remains constant with time if we assume that g_0 is equal to either g_+ or g_- , which can be inferred either from Eq. (2.286) or also directly from Eq. (2.284) by setting $\dot{g}_t = 0$. This means $\alpha_t = g_+ e^{\gamma t}$, if $g_0 = g_+$, or $\alpha_t = g_- e^{\gamma t}$, if $g_0 = g_-$. In order to choose the appropriate solution, we consider the fact that in the limit $\gamma \rightarrow 0$ the chosen solution has to approach the non-dissipative value, i.e., $\alpha_t \rightarrow im\omega_0/2$, which only happens if $g_0 = g_+$. Therefore, we have that

$$\alpha_t = \frac{im\Omega}{2} \left(1 + \frac{i\gamma}{2\Omega}\right) e^{\gamma t}. \quad (2.289)$$

It should also be stressed that in the limit of vanishing friction, this value approaches the frictionless one mentioned above. More importantly, α_t has a real and an imaginary part, and therefore the wave function will be properly normalized. This can be readily seen by integrating the equation of motion for f_t , which leads to

$$f_t = \frac{i\hbar}{4} \ln \left(\frac{\pi\hbar}{m\Omega} \right) - \frac{\hbar\Omega}{2} \left(1 + \frac{i\gamma}{2\Omega} \right) t + S_{cl,t}. \quad (2.290)$$

Substituting all these parameters in the expression for the wave function, it reads as

$$\Psi(x, t) = \left(\frac{1}{2\pi\sigma_t^2} \right)^{1/4} e^{-(x-x_t)^2/4\sigma_t^2 + ip_t(x-x_t)/\hbar - i\Omega t/2 - (im\gamma/4\hbar)e^{\gamma t}(x-x_t)^2 + iS_{cl,t}/\hbar}, \quad (2.291)$$

with the width being $\sigma_t = e^{-\gamma t/2} \sqrt{\hbar/2m\Omega}$. As can be noticed, the first three arguments in the exponential of Eq. (2.291) are identical to those in Eq. (2.276), but replacing ω_0 by Ω . The wave function is properly normalized, but its width decreases exponentially with time according to

$$\Delta x = \sigma_t e^{-2\gamma t}. \quad (2.292)$$

Thus, it eventually collapses over the center of the harmonic well as the whole wave packet follows the motion of a damped harmonic oscillator. Along this transit, the system energy is also exponentially lost according to

$$\bar{E} = \frac{1}{2} m \omega_0^2 x_0^2 \left(\frac{\omega_0}{\Omega} \right)^2 \left[1 - \frac{\gamma}{2\omega_0} \sin(2\Omega t - \varphi) \right] e^{-\gamma t} + \frac{1}{2} \omega_0 \hbar \left(\frac{\omega_0}{\Omega} \right) e^{-\gamma t}. \quad (2.293)$$

It is worth stressing that under underdamped conditions, α_t , given by Eq. (2.289), is a complex function, which makes the wave function (2.291) to display a vanishing Gaussian shape plus a phase factor as the system oscillates, as seen in Eq. (2.291). Critically damped and overdamped conditions imply that the motion amplitude of the system exhibits a monotonic decrease to zero, with no oscillations. In the present context, where we are seeking for solutions such that $\dot{g}_t = 0$, this now translates into a rather puzzling quantum behavior. In order to analyze it, let us start from the overdamped condition, $\omega_0 < \gamma/2$. Equation (2.286) is still valid, although we have $g_{\pm} = \pm(m\Gamma/2)(1 \mp \gamma/2\Gamma)$. Between these two solutions, we choose g_+ , because it is consistent with Eq. (2.289) and also because it corresponds to the long-time limit of g_t in this case (i.e., for $\beta = \Gamma$). Accordingly, the spreading factor will read as

$$\alpha_t = \frac{m\Gamma}{2} \left(1 - \frac{\gamma}{2\Gamma} \right) e^{\gamma t}, \quad (2.294)$$

which is a pure real function. Thus,

$$f_t = f_0 + \frac{i\hbar\Gamma}{2} \left(1 - \frac{\gamma}{2\Gamma} \right) t + \mathcal{S}_{\text{cl},t}, \quad (2.295)$$

where f_0 is now left as a free parameter, although its imaginary part has to be such that the initial plane wave is still normalized. Notice that in this case the corresponding wave function is written now as

$$\Psi(x, t) = e^{-(im\Gamma/2\hbar)(1+\gamma/2\Gamma)e^{\gamma t}(x-x_t)^2 + ip_t(x-x_t)/\hbar + \Gamma t(1+\gamma/2\Gamma)/2 + if_0 + i\mathcal{S}_{\text{cl},t}/\hbar}, \quad (2.296)$$

which is a pure phase factor multiplied by a diverging time-dependent exponential. It is interesting to emphasize that, although the wave function itself diverges, the associated Bohmian trajectories are well-defined and approach asymptotically the classical overdamped centroid, x_t (see below).

Regarding the critically damped motion, if we consider here the initial value $g_0 = g_s$, the stationary solution is $g_t = g_s = -m\gamma/4$, and therefore

$$\alpha_t = -\frac{m\gamma}{4} e^{\gamma t}. \quad (2.297)$$

As it can be seen, this value of α_t allows us to connect smoothly those two previously obtained in underdamped and overdamped cases as the friction γ is gradually increased.

In spite of the type of motion displayed in each one of the regimes discussed above, the Bohmian equation of motion for the trajectories can be recast in the same form for all of them,

$$\frac{d(x - x_t)}{x - x_t} = -\frac{\bar{\gamma}}{2} dt, \quad (2.298)$$

where $\bar{\gamma} = \gamma$ for underdamped and critically damped motions, and $\bar{\gamma} = \gamma - 2\Gamma$ for overdamped motions. As it can be noticed, this equation looks exactly the same as Eq. (2.274) for the eigenstates, although replacing x by $x - x_t$. Thus, the solutions,

$$x(t) = x_t + [x(0) - x_0]e^{-\bar{\gamma}t/2}, \quad (2.299)$$

are also very similar. In the case of Eq. (2.275), since the associated wave function is a quasi-eigenstate, the trajectory approaches asymptotically the origin or, in other words, it falls down to the bottom of the well. In the case of Eq. (2.299), and differently to what we have seen before, any trajectory will eventually coalesce with the centroidal one. This is an interesting case where the Bohmian non-crossing rule seems to be violated. Actually, the evolution of the trajectories is in compliance with the shrinking undergone by the wave function in the damped oscillatory regime and its evanescent nature in the overdamped regime. These trajectories, described generically by Eq. (2.299), have the following analytical form

$$x(t) = \begin{cases} \left\{ [x(0) - x_0] + x_0 \left(\frac{\omega_0}{\Omega} \right) \cos(\Omega t - \varphi) \right\} e^{-\gamma t/2}, & \omega_0 > \gamma/2 \\ \left\{ [x(0) - x_0] + x_0 \left(1 + \frac{\gamma t}{2} \right) \right\} e^{-\gamma t/2}, & \omega_0 = \gamma/2 \\ \left\{ [x(0) - x_0]e^{\Gamma t} + x_0 \left(\frac{\omega_0}{\Gamma} \right) \cosh(\Gamma t + \phi) \right\} e^{-(\gamma - 2\Gamma)t/2}, & \omega_0 < \gamma/2 \end{cases} \quad (2.300)$$

where the first expression looks very similar to that for the unperturbed harmonic oscillator, with the exception of the overall exponentially decaying factor and the dephasing in the cosine function.

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