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Bohmian Mechanics, Open Quantum Systems and Continuous Measurements

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ISBN 978-3-319-53651-4 ISBN 978-3-319-53653-8 (eBook)
DOI 10.1007/978-3-319-53653-8

Library of Congress Control Number: 2017932636

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

To Isabela, Clarissa and Priscilla

Antonio B. Nassar

and

To Virginia, Jessica, David, my parents and brother†

Salvador Miret-Artés

Preface

In standard quantum mechanics, the collapse of the wave function resulting of the interaction of a given system with a measuring apparatus is a clear unsatisfactory assumption. As is well known, this assumption, due to von Neumann, was established around 1932 by means of the so-called reduction (or collapse or projection) postulate. A unitary Schrödinger evolution can never lead to such a collapse and, therefore, at some point, the time evolution of a quantum system undergoing a measurement has to be suspended and replaced by a discontinuous, noncausal, nonlineal, nonunitary (but norm-preserving) and stochastic one. The collapse is postulated to happen in accordance with the well-known Born probability rule, with no dynamical theory behind such a mechanism. It is also very well known that the absence of macroscopic superpositions is at the heart of the measurement problem in quantum mechanics. Another aspect worth mentioning is the emergence of the classical features from the quantum world; in other words, the conversion of a coherent superposition into a mixture. The resulting decoherence process leads to the selection of one of the components of this mixture. This selection of one out of many alternatives still remains obscure. Thus, we still do not understand why the measurement process destroys the linear superposition of the initial states and why macroscopic objects are not found in superposed states. Even more, as asked by Bell, where is the quantum-classical dividing line? Mesoscopic systems are also ideal to address this fundamental question. In brief, too many open questions are even today waiting for some sort of satisfactory response.

Many physicists believe that there is a *measurement problem* in quantum mechanics. Even more, measurement definitely and unavoidably affects the dynamics of the measured system. In the Copenhagen interpretation of quantum theory, the world is divided into *system* and *apparatus*. In the simplest case, the system, which is quantum mechanical, is characterized by a wave function. This interpretation implies that the apparatus that performs and records measurements on the system must be classical. In practice, experimenters are always on the classical side of the line. As pointed out by Bell, the lack of clarity in regard to where the transition between the classical and quantum worlds is located is one aspect of the measurement problem. This problem represents one of the most important

conceptual difficulties in quantum mechanics. The presence of a classical apparatus considerably affects the behavior of the observed quantum system and measurements typically fail to have outcomes of the sort the theory was created to explain. Another conceptual difficulty is that in a system under observation there are many degrees of freedom such that information can be lost in the couplings which may account for dissipation and decoherence. It appears that the measurement problem before alluded is becoming slowly a critical or singular quantum process (converted to a dynamical problem) rather than a conceptual issue. In other words, it is no longer considered as a conceptual or philosophical problem but a typical many-body problem (with all the computational issues involved in its resolution).

A measurement can be seen as a physical process by which the state of a quantum system influences somehow a classical variable of a macroscopic apparatus. This influence is usually described by an interaction between the system of interest (S) and the apparatus (A). Then, the combined quantum system SA has properties that S and A alone do not have and it is said that S and A are entangled by means of quantum correlations due to the quantum nonlocality. It is widely accepted that A can also be considered as an environment. In 1970, Zeh proposed to analyze the measuring process within the context of the theory of open quantum systems and see it as a typical many-body interaction problem. In 1984, Gisin carried out a theoretical connection between them. Furthermore, almost any interaction with an environment produces localization (or reduction) in position space. It is very often alluded that the system can not have a state on its own when interacting with its environment and, therefore, the only description in the standard quantum formalism is by means of the density matrix. The measurement process then implies the conversion of a coherent superposition into a mixture together with the selection of one of the components (or alternatives) of the mixture leading to a definite measurement readout. Thus, this decoherence process leads to the emergence of the classical world (classicality). Decoherence, which is ubiquitous in nature, is extremely effective and virtually impossible to escape (only irreversible when the environment is macroscopic). It is a pure quantum process and has no classical counterpart. Furthermore, entanglement is the key process underlying decoherence. This fundamental process has been and is still being studied from many, many points of view emphasizing its very different aspects and subtleties. The number of articles and books devoted to such an important and fundamental issue is extremely huge; to cite only some of them, we have the Ghirardi–Rimini–Weber model of continuous spontaneous collapse, the entropic-dynamic approach to quantum evolution and the Fisher information based derivation of the fundamental Lagrangians leading to relativistic wave equations. Several stochastic approaches are being used nowadays within the quantum theory which could be classified according to the following scheme: group or semigroup algebra, the influence functional, the restricted path integral, consistent histories, effective wave equations and quantum state diffusion equations. They are mathematically connected. Continuous quantum measurement theory is playing a fundamental role in this context since it provides new aspects and ingredients to the global quantum theory. For example, quantum transitions can be monitored as well as perturbed,

altering the dynamics of the measured system. However, very few studies within the Bohmian framework can be found in literature. This approach should also be considered in the measuring process since the outcome of an experiment is very often the position of a particle. In Bohmian mechanics, particles are assumed to have well-defined positions in configuration space. Moreover, the description provided by this mechanics to the measurement process is entirely compatible with Born's rule in standard quantum mechanics.

Bohmian mechanics, which is also called the de Broglie–Bohm theory, the pilot-wave model, and the causal interpretation of quantum mechanics, was originated in the 1920s by Louis de Broglie, re-discovered and developed in 1952 by David Bohm. Its roots are also in the pioneering works of Madelung's hydrodynamic formulation of quantum mechanics. No one more eloquently than John Bell has championed this theory in recent decades. It should be remembered that Bell's inequalities were inspired by his reaction to the work by Bohm. Bell and Bernstein also argued convincingly that the de Broglie–Bohm interpretation of quantum mechanics should be part of any college curriculum on the subject. Tegmark and Wheeler also considered this theory as one of the most significant elements in the history of quantum mechanics. Comprehensive discussions of Bohmian mechanics can be found everywhere in the literature. This mechanics mainly arose as a result of the unsatisfactory interpretation of standard quantum mechanics, which claimed that the wave function provides the most general and complete physical information about a quantum system. This led to a very exciting, never-ending debate focussed on the completeness of the wave function and the quantum theory of measurement. Within Bohmian mechanics, a quantum system has a well-defined (in space and time) trajectory, namely a quantum or Bohmian trajectory; the evolution of this trajectory is determined by the wave function associated with the system. Quite recently, a revival of the debate about the role played by this mechanics in quantum physics can be found in the specialized literature. There are several groups for whom this theory constitutes the natural framework of quantum mechanics, whereas other groups consider it as an alternative and exact formulation able to characterize, interpret and predict quantum processes, standing on equal footing with the standard theory. In fact, it can also be considered as a picture of quantum mechanics at the same level as those due to Schrödinger, Heisenberg, Dirac (Interaction) and Feynman. As Aharanov says, this theory provides the same experimental predictions than quantum mechanics and it contains additional hidden variables which are nonlocal in time that account for the results of every measurement. In this sense, there is no way to decide from experiment which picture is prevalent. This formulation has also received an important impulse over the last 20 years from different communities, which translates into an impressive and fruitful theoretical development. Furthermore, from our own longstanding experience in the field, Bohmian mechanics can tackle any quantum problem as standard quantum mechanics can do it. Obviously, the amount of time and effort invested by many researchers in standard quantum mechanics completely outweigh that invested in Bohmian mechanics. However, we think that this situation will be corrected in the near future owing to the fact that this theory appears in more and more modern

quantum mechanics books at the introductory level. We are going to deal with quantum or causal trajectories but they must not be confused with the same concept introduced by several authors in optics and quantum state diffusion which can be seen as the realizations of the wave function or state vector considered as an underlying stochastic process in Hilbert space. Unfortunately, the concept of quantum trajectory (stochastic or deterministic) is not unique and there is an important proliferation of quantum stochastic trajectories in different fields of research within the theory of open quantum systems as well as the Bohmian mechanics.

The scope of the book is to tackle such conceptual difficulties mentioned above. In particular, when certain conditions are met, an answer to the alluded challenge posed by Bell on the dividing line between the quantum and classical regimes in a measurement problem is also discussed and proposed. In Bell's opinion, the most important element in quantum theory was that the subjectivity of the orthodox version, the necessary reference to the observer, could be eliminated. The theoretical procedure followed here it is inspired from Mensky's theory about restricted path integrals, combined with the so-called Langevin–Schrödinger equation or Kostin equation (which can be seen as an effective wave equation) within the Bohmian framework. This new approach presents several advantages. First, it provides a causal aspect to the dynamics of the measuring process. Second, the proposed stochastic nonlinear approach is an alternative and complementary view of the continuous quantum measurement. Furthermore, in this context, it is put on equal footing the stochastic character coming from the presence of the environment and the phenomenological contribution coming from the measuring process. Third, the information due to the readout of the measurement is governing the equations of motion of Bohm through the quantum potential which is the nonlocal agent of this theory. Fourth, the correspondence principle, established in terms of the smallness of the quantum potential (that is, when it is approaching a zero value), provides a natural way to the emergence of the classical world. Fifth, the gradual decoherence process due to the interaction with the measuring device is introduced and described in terms of quantum stochastic trajectories; that is, in a continuos way with no collapse of the wave function. And sixth, following a dressing scheme, the quantum (stochastic) trajectory is always split into a classical trajectory plus a quantum or nonlocal term.

With this goal, and in order to be as self-contained as possible, although a minimal background on stochastic processes is assumed, this monograph is divided into four chapters. In Chap. 1, a brief historical description and short and updated account of Bohmian mechanics is provided for closed and open quantum systems; in particular, how open quantum systems and the measurement problem are typically considered in this formalism. This introductory chapter aims at providing the essential tools and background to better understand the rest of the monograph. It is clear that this mechanics is not the only one describing quantum mechanics in terms of trajectories but maybe it is becoming more and more known and widely used.

In Chap. 2, 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 is not carried out by means of a systematic exposition of conservative quantum processes but following some illustrations of solutions to some key quantum mechanical problems 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 ending with the well-known Caldirola–Kanai Hamiltonian for dissipative processes. 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.

In the last decades, many nonlinear extensions of the Schrödinger equation have been proposed in literature either to explore the fundamental aspects of quantum mechanics, with the usual linear theory representing only a limiting case, or to describe open quantum systems. In Chap. 3, one of those nonlinear quantum equations is introduced and widely developed. For the description of nonconservative quantum systems, Kostin formulated in an heuristic way the so-called Schrödinger–Langevin (SL) equation or Kostin equation for the Brownian motion. This equation has been subsequently rederived, improved and extended for its use in numerous applications, mainly without including the noise term. Numerous features of this SL equation can be better revealed within the framework of de Broglie–Bohm (quantum hydrodynamical trajectory formulation) of quantum mechanics resulting the Schrödinger–Langevin–Bohm (SLB) equation. Within this formalism, several dissipative problems are presented and discussed: the Ramsauer–Townsend effect, the tunneling dynamics through a barrier, the plasma fluid formulation and the Lorentz–Abraham (extended electron) equation for a point-charge electron. These two last examples are also discussed in order to see the correspondence between classical and quantum dynamics. Very few applications of this SL equation are devoted to stochastic problems in the literature where the noise term needs to be included. The so-called Bohmian–Brownian motion is introduced in the context of surface diffusion with single adsorbates. An extension to interacting adsorbates is discussed within a simple, phenomenological model. Interestingly enough, this study leads us to quantum anomalous diffusion. Finally, a generalization of the SL equation is proposed for nonlinear dissipation.

Chapter 4 is devoted to the study of continuous or repeated (prolonged in time) measurements on a quantum system. This is a very active field since it is directly connected to the foundations of quantum mechanics, the theory of quantum measurements being one of its main topics. Following a phenomenological approach, a general theory for decoherence in the framework of restricted path integrals (RPI) has been proposed by Mensky. The corresponding propagator is modified according to the information provided by the measurement through the so-called quantum corridors, which correspond to different readouts of the measurement. The

action uncertainty principle is then ruling the corresponding measurement process. The measured system is also considered in this theory as an open system since the back reaction of the environment, considered as a measuring apparatus, is taken into account implicitly. In this Chapter, the RPI formulation is briefly presented and discussed since our approach is inspired from Mensky's procedure. The linear time-dependent Schrödinger equation derived from this formulation is reached for a non-Hermitian (complex) effective Hamiltonian which takes into account the measurement readout. The RPI formulation is equivalent to a master equation, a special case of the Linblad equation, and to a stochastic Schrödinger equation. A nonlinear equation is proposed and discussed, within the Kostin framework, by extending Mensky's approach to be analyzed in terms of Bohmian trajectories, the so-called SLB equation for continuous measurement. When a time-dependent Gaussian shape is assumed for the probability density, soliton-like solutions are first analyzed in order to establish the dividing line between the quantum and classical trajectories, leading to the concept of Bohmian time. Afterwards, the solutions of the SLB equation for continuous measurement are analyzed in terms of mathematical stability for three simple cases, that is, the free particle and the linear and harmonic potentials. In particular, the continuous position measurement is seen that it is no longer governed by a standard continuity equation. The sign of the extra source/sink term appearing in this new equation is critical for the stability of the solutions. Two types of general solutions are found: (i) the stationary wave packet considered becomes unstable (that is, this solution is not a physically acceptable solution for that process since, as time evolves, the width of the corresponding wave packet becomes more delocalized) and (ii) the probability density becomes more and more localized at asymptotic times (the stationary wave packet is then an attractor of the corresponding width dynamics); in terms of trajectories, this analysis indicates that the Bohmian trajectories are not approaching the corresponding classical ones. These conclusions are also corroborated by carrying out an analysis of the entropy. Finally, it is also briefly discussed the question of coupling classical variables (apparatus) to quantum ones (system) in terms of Lyapunov exponents.

In the epilogue of this monograph some concluding remarks and future perspectives towards the establishment of a complete theory of continuous quantum measurement, within the Bohmian mechanics, are briefly presented and discussed.

This monograph is the result of more than 30 years working on trajectory-based formalisms; in particular, on Bohmian mechanics. Concerning citations, we have tried to furnish a historical development of the different topics presented here. However, to provide a selection of the very last references in a very active field is really difficult. We apologize to those who think they should be cited and are not. During this long but exciting time, we have benefitted from discussions with many colleagues from all over the world. In particular, we would like to acknowledge fruitful discussions and collaborations with P.T.S. Alencar, P. Bargueño, J.M.F. Bassalo, I. Besieris, M.S.D. Cattani, H. Peñate-Rodríguez, J. Margalef-Roig, R. Martínez-Casado, G. Rojas-Lorenzo, A.S. Sanz, E. Outerelo, E. Pollak and O. Roncero. ABN would like to thank all members of the Harvard-Westlake Science Department, the UCLA Extension Science Department

and the College of the Canyons for the constant support and encouragement throughout the process of writing this monograph. Analogously, SMA would also like to thank all members (past and present) of the *Departamento de Física Atómica, Molecular y de Agregados* of the *Instituto de Física Fundamental* belonging to the *Centro de Física Miguel A. Catalán* (Consejo Superior de Investigaciones Científicas, CSIC) in Madrid. This work has been partially supported by the project FIS2014-52172-C2-1-P from the *Ministerio de Economia y Competitividad* (Spain).

Finally, we thank our Editor A. Lahee for her interest when we proposed this monograph as well as her patience when extending several times the deadline for finishing this project.

Los Angeles, USA — Antonio B. Nassar
Madrid, Spain — Salvador Miret-Artés
December 2016

Contents

Chapter 1
Historical and Introductory Account of Bohmian Mechanics

Abstract Bohmian mechanics, which is also called the de Broglie-Bohm theory, the pilot-wave model, and the causal interpretation of quantum mechanics, was originated in the 1920s by Louis de Broglie, re-discovered and developed in 1952 by David Bohm. No one more eloquently than John Bell has championed this theory in recent decades. Bell and Bernstein also argue convincingly that the de Broglie-Bohm interpretation of quantum mechanics should be part of any college curriculum on the subject. Comprehensive discussions of Bohmian mechanics can be found everywhere in the literature. In this introductory chapter, a brief historical description and short and updated account of this mechanics is provided for closed and open quantum systems; in particular, how the measurement problem is typically considered in this formalism. This chapter aims at providing the essential tools and background to better understand the rest of the monograph. It is clear that this mechanics is not the only one describing quantum mechanics in terms of trajectories but maybe it is becoming more and more known.

1.1 Introduction

John Bell was a theoretical physicist famous for his results in the field of foundations of quantum mechanics [1]. The famous *Bell inequalities* and similar results provide strict constraints on any future theory of quantum phenomena. His work is as monumental as the work of Kurt Gödel [2] on the *Incompleteness Theorems* in mathematics. Bell was a highly cultured and thoughtful thinker. His writings are still sending shock waves in the field of quantum mechanics. Bell presented his theory with extraordinary lucidity coupled with a vividness of expression. Tegmark and Wheeler have written an excellent and basic review about the 100 years of quantum mechanics [3].

Bell championed the theory put forth by de Broglie in 1927 and advanced by David Bohm in 1952 [4, 5], the so-called de Broglie-Bohm quantum theory, the pilot-wave model, the causal interpretation of quantum mechanics and Bohmian mechanics [6–14]. In fact, due to initial criticism of his theory, de Broglie abandoned his *guiding waves* project and so it lay abandoned until Bohm revived it. The particle motion

A.B. Nassar and S. Miret-Artés, *Bohmian Mechanics, Open Quantum Systems and Continuous Measurements*, DOI 10.1007/978-3-319-53653-8_1

dependens thus on the wave evolution with time, giving rise to quantum or Bohmian trajectories. The uncertainty principle in Bohmian mechanics is then understood from the initial conditions determining the trajectory, which are subject to the usual quantum mechanical uncertainties. The motions of the particles on their trajectories are deterministic, but which trajectory the particle is on is subject to probability. Bell was convinced that the de Broglie-Bohm interpretation of quantum mechanics should be part of any college curriculum on the subject. Bohmian mechanics stands out by being both historically influential and highly developed. Its position is further strengthened not only by Bell's theorem, which showed that all such theories have to be nonlocal as well as the experimental confirmation in 1981 due to Aspect et al. [15–17] and by recent experiments [18–20].

In the simplest pilot-wave theory, Bohmian mechanics, paradoxes of quantum mechanics can be resolved in a simple way – while the particles have positions, they move according to Schrödinger's equation. For example, one of the most famous paradoxes (in the standard interpretation) at the heart of quantum mechanics is the double-slit experiment. By using the concept of weak-value measurements introduced originally by Aharanov et al. [21],[1] recent experiments with single photons in a double-slit interferometer have revealed that single-particle trajectories can be processed in a indirect way and plotted. Weak measurements have then shown that it is possible to operationally define a set of trajectories for an ensemble of quantum particles. In this fashion, these results have reproduced those *predicted* by Bohmian mechanics (non-crossing trajectories) [19, 20, 22] in spite of the fact that this mechanics is developed for particles with mass. However, what qualifies some physical systems to play the role of a "meter"? After all, there is no reference to a measuring process in Schrödinger's equation. Besides, quantum mechanics should explain some aspects of macroscopic measurements. Bohm's ideas were applied to different prototypical models of quantum mechanics [7] during the late 1970s and particularly the 1980s and early 1990s. However, in the last 20 years or so, Bohmian mechanics has passed from being a mere way to formulate a quantum mechanics "without observers" [8, 9] to become a well-known (and increasingly accepted) theoretical framework used as a source for new quantum computational methods as well as quantum interpretations [12, 23, 24]. These two aspects of Bohmian mechanics are what Wyatt [12] has termed the *synthetic* and *analytic* approaches of this theory. The first approach essentially starts with the former numerical schemes developed to obtain quantum information without solving Schrödinger's equation, but its equivalent Bohmian counterparts [12, 25–27]. Since then, this computational branch of Bohmian mechanics has diversified into a myriad of numerical approaches, which can be summarized by the type of answer they try to give. For example, for wave packet propagation, different Lagrangian, Eulerian and combined Eulerian-Lagrangian algorithms have been developed [12]. Semiclassical initial value representation schemes based on Bohmian mechanics have been implemented [28–32].

[1] Following these authors, in principle it would be possible to measure transition probabilities in such a way that they would allow us to determine "any physical variable to a certain (even forbidden) value", e.g., canonically conjugate variables.

The purpose of avoiding and, therefore, solving the so-called *nodal problem* has led to schemes such as, for example, the bipolar ansatz [33–36]. The starting point for the second approach, on the other hand, based on obtaining the quantum trajectories from the wave function as a tool to interpret and simulate realistic experiments, can be established in the former studies of rare gas atom diffraction by metal surfaces [13, 14].

Bohmian mechanics allows us to understand and explain quantum systems in terms of the motion displayed (in configuration space) by a swarm of quantum trajectories. Each one of these trajectories represents the evolution in time of a particular initial state specified by a point on the configuration space associated with the system. Thus, unlike standard quantum mechanics, where the wave function determines the state of the system on the *whole* available configuration space, in Bohmian mechanics it is possible to follow one particular point of such a space. The time-evolution of this point is given according to some prescribed quantum laws of motion. The evolution of the trajectory ensemble is equivalent to the evolution of a quantum flow —this is precisely the viewpoint of quantum hydrodynamics. The Bohmian view does not invalidate at all other ways of understanding quantum systems; it only allows us to think of them on similar grounds as classical ones, i.e., using a similar intuitive scheme, which differs from a purely classical one precisely in the types of motion one can observe. However, unlike any classical approach to quantum mechanics, Bohmian mechanics is not an approximated theory, but an exact one. Furthermore, by looking at one of those diffraction experiments carried out with electrons [37] or atoms [38], one notices that a single measurement or detection is meaningless, many of them being necessary in order to visualize the diffraction pattern and then obtain information either about the diffracted particle or the diffracting object. In other words, individual particles behave like individual point-like particles, though their distribution displays a wave-like behavior, in accordance with Schrödinger's equation. It is therefore clear that ensemble properties need of an ensemble description, i.e., a density distribution function, whose role is played in quantum mechanics by the probability density or, at a more elementary level, the wave function. This is in agreement with Born's statistical interpretation of quantum mechanics. However, if (individual) particles are regarded as moving along single trajectories, are these trajectories the ones obtained from the guiding condition? Bohmian trajectories reproduce all the features of quantum mechanics and, therefore, one would be tempted to think that this is so. However, Bohmian equations are regarded as hydrodynamic equations, the corresponding trajectories obtained from the guiding condition should not be regarded as the trajectories pursued by real electrons, but rather as streamlines associated with the corresponding quantum fluid or paths along which quantum probability flows. Very interesting work is being addressed to several problems in quantum optics and atom interferometry by Sanz and coworkers [39–41] under this approach. Electrons may move or not like that, basically depending on the laminar or turbulent regimen displayed by the fluid, but surely not exactly as Bohmian trajectories. This description allows us to infer dynamical properties of the quantum fluid, which are usually hidden when studied by means of the wave function formalism. Therefore, Bohmian particles can be seen as the quantum equivalent

of classical tracer particles in a fluid, so that they can help us to visualize its flow dynamics by moving along *streamlines*, i.e., lines along which the fluid current goes or energy is transported. For example, if the fluid is gaseous, one can use smoke; if it is a liquid, one can make use of tinny floating particles, e.g., pollen or charcoal dust, or another liquid, e.g., ink. In the case of the hydrodynamical approaches utilized to the universe dynamics in cosmology, the tracer particles can be stars, galaxies or clusters [13, 14].

The problem of many-body interactions —or, equivalently, many degrees of freedom— can be tackled from different points of view, since it appears in many different physical, chemical and biological contexts. For example, quantum chemistry constitutes nowadays one major field in importance and interest. In order to carry out the large-scale calculations and simulations, an increasing computational capacity of modern computers is critical. The corresponding theoretical analysis relies on considering the so-called *Born-Oppenheimer approximation*, which allows us to simplify the study of any molecular system (simple molecules, solid surfaces, polymeric chains, clusters, crystalline structures, etc.) by splitting it into its electronic and nuclear parts. By solving the Schrödinger equation associated with the electronic Hamiltonian, which is the ultimate goal of electronic structure methods, one determines electronic configuration of a (multi-electron) system, i.e., the way how electrons distribute throughout such a system. This knowledge will essentially determine its chemical properties, e.g., chemical bonding, intermolecular interactions, electronic charge distributions, dipole and multipole moments, or vibrational/rotational frequencies. Non–adiabatic problems have also been tackled within the Bohmian complex formalism [42, 43].

When the dimensionality of the problem considered increases, as happens with many systems of quantum chemistry and solid state physics, computational problems increase and start becoming unaffordable. To overcome this drawback, a series of approaches based on the density matrix theory [44] were also developed; for example, the independent electron approximation or Thomas-Fermi model [45, 46]. These models can be considered direct predecessors of the so-called *density functional theory* (DFT) [47], based on the principles established by Hohenberg, Kohn and Sham [48, 49]. Here we go from the Thomas-Fermi model [45, 46], where the electron kinetic energy of an atom is expressed as a functional of the atom electronic distribution, to the modern DFT [47], where the fundamental physical information about the molecular system is obtained from a single-particle density in a three-dimensional space, derived variationally either within a time-independent framework [47] (ground state) or a time-dependent one [50, 51] (excited states). The density functional theory is a very popular calculation method nowadays, not only in quantum chemistry, but also in solid state physics or condensed matter physics; in particular, due to its computational simplicity combined with its (numerical) accuracy. Accordingly, the relevant physical information about the ground state of a many-body system is obtained from single-particle densities in a three-dimensional space, which are determined variationally within a time-independent framework. Nonetheless, all practical applications of DFT rely on essentially uncontrolled approximations [52]

and therefore the validity of this approach is conditioned to its ability to provide results sufficiently close to the experimental data.

Standard DFT is commonly applied to determine ground states in time-independent problems. However, its time-dependent generalization, the so-called time-dependent DFT (TD-DFT), are needed when processes and phenomena are intrinsically time-dependent [51]. This is the case, for example, of reactive and non-reactive scattering processes, or of atoms and molecules in laser fields, where the calculation of excited states is important. This approach was formerly started by Bartolotti [53–55] and Deb and Ghosh [56, 57], although the proofs of the fundamental theorems involved were later on provided by Runge and Gross [58]. One of these theorems corresponds to a version of the Hohenberg–Kohn theorem for time-dependent Schrödinger equation. Thus, as happens with standard DFT, TD-DFT can be started directly from the many-body time-dependent Schrödinger equation, the density being then determined from solving a set of time-dependent Schrödinger equations for single, non-interacting particles. A slightly extended version is based on Madelung's quantum hydrodynamic picture of wave mechanics [59] which has been widely exploited in the chemical physics community, giving rise to the so-called quantum hydrodynamic or quantum fluid DFT. According to Hirschfelder [60–62], quantum hydrodynamics facilitates the study of problems involving external electric and magnetic fields in molecular systems, since it contains in a natural way the concept of *equation of change* for any arbitrary quantum properties in configuration space. For instance, these equations can be used to study the energy flow from one part of a molecule to another, the nature of molecular collisions, or the magnetic properties of molecules. We would also like to notice an interesting relationship between this formulation and the weak measurement or weak value [21], proposed about twelve years after Hirschfelder's work. As mentioned above, experiments carried out by Kocsis et al. [19, 20] are not only in accordance to Bohmian mechanics but also to Bayesianism proposed by Wiseman [63]. As pointed out by Hiley [64], these weak measurements are not other thing that standard transition probabilities within the Bohmian scenario, i.e., just a particular type of equation of change, according to Hirschfelder.

On the other hand, strictly speaking, real physical systems do not exist in complete isolation in nature. All physical systems are open systems in the sense that the interaction with their environments can never be totally neglected. From its inception, the motion of particles in quantum mechanics was thought to happen in the presence of an environment and could be understood in terms of a stochastic process. In fact, a formal analogy between the Brownian motion and the Schrödinger equation was noticed by Fürth [65] in 1933. Afterwards, Fényes [66] and Weizel [67–69] developed this approach with more mathematical detail. The search for a stochastic support for quantum mechanics has taken place since the early 1950s. In particular, the first attempt in the Bohmian mechanics due to Bohm and Vigier [70] was reported in 1954. These authors assumed that the electron is a particle suspended in a Madelung fluid [59] (the hydrodynamical model of quantum mechanics was lately developed by Takabayasi [71, 72]) whose general motion is determined by the resolution of the Schrödinger equation, providing the probability density from the amplitude of the

wave function and the deterministic contribution to the local velocity from its phase. The stochastic contribution to the local velocity is due to the random fluctuations arising from the presence of the fluid. In general, the aim was to show how close it is to classical theory of Brownian motion and Newtonan mechanics, and how the Schrödinger equation might have been discovered from this point of view. The theory was neatly established by Nelson [73] starting from a different point of view of those proposed by Fényes, Weizel, Kershaw [74], Comisar [75] and de la Peña [76]. After Nelson, every particle of a given mass, m, is subject to a Brownian motion with diffusion coefficient $\hbar/2m$ and no friction in order to preserve Galilean covariance. He explicitly wrote that his theory is not a causal theory and the physical interpretation is entirely classical. Olavo [77] also followed previous works but starting from a more axiomatic formulation. The main advantage of implementing this stochastic mechanics was to exploit the well developed mathematical methods of probability theory and stochastic processes. In a review written by Guerra [78] in 1981, one still can read "there is no stochastic interpretation of quantum mechanics different to the standard one... stochastic mechanics can be seen simply as a reformulation of it in terms of the language of stochastic processes". Grabert, Hänggi and Talkner analyzed the connection between both mechanics and concluded that quantum mechanics is not equivalent to a Markovian diffusion process [79]. Most of the work in this domain ignored Bohm's view of standard and stochastic quantum trajectories. In this respect, we can claim that the depart of Bohm and collaborators is again a breakthrough. Bohm and Hiley [10, 80] make clear that there is no way to avoid non-locality in the stochastic interpretation of quantum mechanics. After Vink [81], the causal and stochastic interpretations are two known examples of what is denominated beable interpretations as developed by Bell [1]. Lorenzen et al. [82] have recently extended Bell's beables to encompass dissipation, decoherence and the quantum-to-classical transition through quantum trajectories.

Concurrently, Nelson and de la Peña opened up an alternative route for deriving generalized nonlinear Schrödinger equations. Within the quantum hydrodynamical framework, Nassar [83, 84] proposed a generalized nonlinear equation containing some of the most well-known equations due to Kostin [85], Süssmann and Hasse [86], Bialynicki-Birula–Mycielski [87], Stocker-Albrecht [88] and Schuch–Chung–Hartmann [89, 90]. More recently, Olavo et al. [91] have provided an alternative way of combining Bohmian equations and the Langeving and Fokker–Planck equations and the Feynman propagator was analyzed for eight nonlinear Schrödinger equations [92] within this formalism. Garashchuk et al. [93] and Chou [94] applied the so-called Kostin equation to the symmetric and asymmetric double well potential for ground states. In the same framework, Nassar [95] also studied the linear Schrödinger equation within the Caldirola-Kanai model [96, 97]. A detailed analysis of quantum trajectories in the Caldirola-Kanai model has also been carried out by Sanz et al. [98].

The theory of open quantum systems has also been developed by different routes from the very beginning leading to different stochastic derivations of the Schrödinger equation. Traditionally, the so-called system-plus-reservoir methods are being largely used in this context, working either in the Schrödinger picture (density matrix

formalism) or the Heisenberg picture of quantum mechanics (quantum Langevin equation). The reader interested in these different alternatives can look at, for example, Refs. [13, 14, 99–105]. In this context, the terminology of quantum trajectory is also used but it should not be confused with the corresponding Bohmian trajectory. When dealing with open quantum systems within the Bohmian formalism in the following chapters, these trajectories will be handled with care.

Dealing with measurements, the physical system to be measured together with the apparatus can also be considered as an open system [106]. In classical physics, measurements on a physical system are carried out without appreciably disturbing it. Positions and momenta can be empirically determined with arbitrary precision at the same time. In classical ontology terms, one assumes the existence of particles and fields to be essentially independent of the human observer. Moreover, following Holland [7], two successive observations of an apple, in a tree and then on the ground are connected to one another. In fact, they are causally connected. Non-disturbing measurements which simply reveal a preexisting reality cannot be sustained when we approach the quantum realm [10]. After Bohr, one cannot separate the behavior of the quantum objects from their interaction with the instruments. However, the key concept in this mechanics is the concept of a quantum state along the lines initiated by Dirac and von Neumann. After Dirac, each physical quantity is represented by an Hermitian operator which is called an observable. When this property is measured by an apparatus, the system is left with a wave function corresponding to an eigenfunction of this observable. Afterwards, we can measure the same observable again and again with the same result that the wave function does not change significantly (except for a phase factor). After von Neumann, the wave function provides the most complete possible description of what he called quantum reality (no further concepts, e.g., involving hidden variable could be introduced that would make possible a more detailed description of the state of the system than is afforded by the wave function). In 1955, von Neumann proposed to divide the world into two parts: an observed system and a system that may "observe", say a meter or a pointer. In other words, he was led to make a distinction between the quantum and classical levels. Between them, he said there was a cut or *a dividing line*. The location of the cut is to a large extent arbitrary. The apparatus must combine quantum and classical properties. The Schrödinger equation can not map a pure state into a mixture, or better said, a proper mixture killing the interference terms. Von Neumann also proposed a different evolution, discontinuous, noncausal and nonunitary, the so-called *projection postulate* or the hypothesis of *wave function collapse or reduction* which is an irreversible process and takes place instantaneously. Thus, the many-body Schrödinger theory is no longer applicable in the measuring process and this implies a massive incompleteness in the quantum mechanical treatment. No one knows when the collapse is supposed to occur, how long it takes or what brings it about. This process of reduction or collapse of the wave function is the simplest example of decoherence or conversion of a superposition state into one of the eigenstates of the observable measured with probability given by the squared modulus of the corresponding coefficient. The emergence of the classical world implies the phenomenon of decoherence, that is, the conversion of a coherent superposition of states into a mixture since superposition

states are not observable. One of the components of the mixture has to be somehow selected to lead to a definite measurement readout. In other words, the measuring process is the selection of one out of many alternatives. Irreversibility is then settled.

Recently, Nassar [107] has proposed a different starting point within the Bohmian formalism when considering the measuring process as an open quantum dynamics. Following the phenomenological approach to continuous measurement by Mensky [108] which uses restricted path integrals, a new logarithmic nonlinear Schrödinger equation has been derived and analyzed in terms of quantum trajectories. A close connection between stochastic mechanics and the path integral formulation of quantum mechanics due to Feymann is noticeable. Furthermore, as an extension, the *stochastic weak measurement* is also introduced in this context following Hiley arguments [64]. As a further extension of this work, Nassar and Miret-Artés [109] and Bargueño and Miret-Artés [110] have derived new generalized Schrödinger-Langevin equations by considering continuous measurement for a dissipative and stochastic dynamics, respectively. Furthermore, Zander, Plastino and Díaz-Alonso [111] have investigated time-dependent solutions for the nonlinear equation proposed by Nassar and Miret-Artés.

This chapter is organized as follows. In Sect. 1.2, the main concepts and developments derived for closed or isolated quantum systems are briefly reviewed. In Sect. 1.3, the same is done but now for open quantum systems. Finally, in Sect. 1.4 some dynamical aspects of the measuring process are presented. This introductory chapter aims at providing the essential tools and background to better understand the rest of the monograph.

1.2 Closed Quantum Systems. Quantum Trajectories

1.2.1 Quantum Hydrodynamics Framework

In 1926, Madelung [59] provided an alternative interpretation to quantum mechanics which is known nowadays as *quantum hydrodynamics*. This interpretation is, for example, directly connected to some relevant phenomena in quantum mechanics, such as superconductivity [112] or Bose–Einstein condensation [113]. Furthermore, in chemical physics, it provides an ideal framework to understand and interpret quantum processes, going from chemical reactivity in collinear reactions [62, 114] to the understanding of molecular magnetic properties within a framework encompassing both electronic structure and topology [115–117].

In this framework, one starts by considering the wave function of a particle in the configuration space and in polar form such as

$$\Psi(\mathbf{r},t) = \phi(\mathbf{r},t)e^{iS(\mathbf{r},t)/\hbar} \tag{1.1a}$$

$$\rho(\mathbf{r},t) = \phi(\mathbf{r},t)^2 = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t), \tag{1.1b}$$

$$\mathbf{J}(\mathbf{r},t) = \rho(\mathbf{r},t)\mathbf{v}(\mathbf{r},t) = \phi^2(\mathbf{r},t)\,\frac{\nabla_{\mathbf{r}}S(\mathbf{r},t)}{m}, \tag{1.1c}$$

where $\rho(\mathbf{r},t)$ is the probability density, $\mathbf{J}(\mathbf{r},t)$ is the quantum probability density current and $\mathbf{v}(\mathbf{r},t)$ is the velocity field, which describes the flow of the latter. In order to simplify the notation of equations, the arguments of the fields will be very often omitted and $\nabla_{\mathbf{r}}$ will be replaced simply by ∇ (for one or N particles). By substituting Eq. (1.1a) in the time dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = H\Psi(\mathbf{r},t) \tag{1.2}$$

where H is the Hamiltonian operator of a particle expressed as

$$H = K + V = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \tag{1.3}$$

K being the kinetic energy operator and V the interaction potential, the following two coupled equations are easily obtained

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J} = 0, \tag{1.4a}$$

$$\frac{d\mathbf{v}}{dt} = \frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = -\frac{1}{m}\,\nabla(V+Q). \tag{1.4b}$$

The first equation is the so-called *continuity equation* and the second one is a Newtonian like equation in the quantum domain, or quantum Newton equation (or quantum Euler equation). In this last equation, the effective interaction potential consists of V and the so-called quantum potential Q expressed in terms of ρ as

$$Q = -\frac{\hbar^2}{2m}\,\frac{\nabla^2\rho^{1/2}}{\rho^{1/2}}. \tag{1.5}$$

Equations (1.4a) and (1.4b) constitute the formal basis of quantum hydrodynamics and have a direct correspondence with those of classical fluid mechanics, when m is identified with the mass of a piece of fluid separated from the rest by a closed surface, $m\rho$ is the fluid density and $\mathbf{v}$ is the velocity field of the flow (ideal classical fluid, that is, incomprenssible and nonviscous and thermal effects are not taken into account) [118]. The streamlines of the flow are lines along which the fluid current goes or energy is transported. Typically, some tracer particles are usually deposited on the

fluid in order to visualize such streamlines. The tangents to the streamlines give the directions of the velocities of fluid particles at various points in space at a given instant and are perpendicular to the constant phase (or $S(\mathbf{r}, t) = constant$) lines. These streamlines are defined by the solution of the coupled differential equations

$$\frac{dx}{v_x(\mathbf{r}, t)} = \frac{dy}{v_y(\mathbf{r}, t)} = \frac{dz}{v_z(\mathbf{r}, t)}. \tag{1.6}$$

However, unlike classical fluids, quantum fluids correspond to probability flows with no material structure [119]. That is, they only characterize statistical events at each point in space and time, in spite of the fact that the time evolution of these events can be better understood when compared with the motion of ordinary fluids. Moreover, whereas the classical concept of fluid can be applied to describe the statistical behavior of a macroscopic ensemble of particles, in quantum mechanics it is applied to single particles.

When this formal similarity with the evolution of classical hydrodynamical flows is established, one is faced to two types of theoretical schemes: the *Eulerian* and *Lagrangian* schemes [120]. In the first scheme, the importance relies on the full quantum fluid rather than in the particular trajectory dynamics. Equations (1.4a) and (1.4b) are then integrated directly with the aid of the velocity field, $\nabla S/m$, but with no need to obtain any particular trajectory. Alternatively, one can also work following a *Lagrangian scheme*, i.e., considering a framework co-moving with the quantum fluid along trajectories. This is the typical scheme considered in order to benefit from the computational advantages of quantum trajectories. Thus, the first step is to pass from the Eulerian scheme to the Lagrangian one by means of the well-known time derivative or Lagrangian operator,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla. \tag{1.7}$$

On the other hand, the classical Euler equation for the component v_i of $\mathbf{v}$ [121]

$$\rho\Big[\frac{\partial v_i}{\partial t} + (\mathbf{v} \cdot \nabla)v_i\Big] = \rho f_i + \frac{\partial}{\partial x_j}(-p\delta_{ij}), \tag{1.8}$$

where f_i is the external force acting on the fluid along the i–direction and p the fluid pressure, shows how the flow dynamics is determined by the influence of both, an external force and other internal one, given by $\rho^{-1}\partial(-p\delta_{ij})/\partial x_j$ and that depends on the fluid properties. Equation (1.4b) can then be rewritten in the form of Eq. (1.8) as

$$\rho\Big[\frac{\partial v_i}{\partial t} + (\mathbf{v} \cdot \nabla)v_i\Big] = \rho f_i + \frac{\partial T_{ij}}{\partial x_j}, \tag{1.9}$$

by defining the *quantum stress tensor* as

$$T_{ij} = \frac{\hbar^2}{4m^2}\,\rho\,\frac{\partial \ln \rho}{\partial x_{ij}}, \tag{1.10}$$

which is the quantum counterpart of the classical stress tensor $-p\delta_{ij}$, and whose explicit dependence on ρ can be easily obtained by expressing Q as

$$Q = -\frac{\hbar^2}{2m}\left[\frac{1}{2}\,(\nabla \ln \rho)^2 + \nabla^2 \ln \rho\right]. \tag{1.11}$$

In classical fluid dynamics, the Navier–Stokes equation [118] expresses the rate of change in the momentum density, which is defined as the linear momentum times the fluid density. In the quantum version, apart from the classical contributions, quantum contributions are clearly identified and are related to quantum stress and pressure.

As also happens with classical fluids, in quantum hydrodynamics one can also observe the presence of vortices and the corresponding associated (vortical) dynamics. The first theory on quantum vortices was first formulated by Dirac [122] in connection with the existence of magnetic monopoles. This theory has been described in detail in the literature [61, 123], finding some interesting applications [124]. More recent and explicit developments of the quantum theory of magnetic monopoles had led to a generalization of the concept of quantum vortex [125], the well-known Aharonov–Bohm effect [126] (see Chap. 2) being related to this generalization.

The conditions leading to the formation of quantum vortices can be obtained from the fact that the complex character of the wave function implies the multivaluedness of its phase

$$S'(\mathbf{r}, t) = S(\mathbf{r}, t) + 2\pi n\hbar\,, \qquad n = 0,\ \pm 1,\ \pm 2,\ \ldots \tag{1.12}$$

This multivaluedness can only take place at those points where $\rho = 0$ (nodal points or nodes, $\Psi = 0$), where the smoothness of the wave function disappears and the value of S may undergo discrete jumps. According to Eq. (1.12), under these conditions, $\mathbf{J}$ vanishes but not the velocity field $\mathbf{v}$. By inspecting the circulation of $\mathbf{v}$ along a closed path, $\mathcal{C}$, one finds that this magnitude is quantized,

$$\oint_{\mathcal{C}} d\mathbf{l}\cdot\mathbf{v} = \oint_{\mathcal{C}} d\mathbf{l}\cdot\frac{\nabla S}{m} = \frac{1}{m}\oint_{\mathcal{C}} dS = \frac{2\pi n\hbar}{m}, \tag{1.13}$$

n being an integer number. Applying Stoke's theorem to this result, it can be alternatively expressed as

$$\int_{\Sigma} d\mathbf{r}\cdot(\nabla\times\mathbf{v}) = \frac{2\pi n\hbar}{m}, \tag{1.14}$$

where Σ is the region enclosed by $\mathcal{C}$. This result indicates the appearance of vortices when $n \neq 0$, which happens only at those points where the wave function presents nodes. At these points, the streamlines will be closed paths around the nodes, which is consistent with the fact that the quantum density current vanishes at those points

and the impossibility of passing through the regions where $\rho = 0$. Conversely, the velocity field $\mathbf{v}$ will be irrotational in those regions free of quantum vortices.

1.2.2 The Equations of Motion for One Particle

In 1952, Bohm [4, 5] proposed a different interpretation of quantum mechanics in terms of "hidden" (trajectories) variables and based on the quantum hydrodynamics of Madelung and de Broglie's ideas of a pilot wave. In configuration space, the fundamental Bohmian equations of motion for a particle are usually derived from the standard version of quantum mechanics through the transformation $(\Psi, \Psi^*) \rightarrow (\rho, S)$, where Ψ and Ψ^* are generally complex-valued functions or fields of the position $(\mathbf{r})$ and time (t), and ρ and S are also real-valued functions or fields of the same variables. More explicitly, in analogy to previous section, the same transformation relation between both types of fields for a particle of mass m is given by Eqs. (1.1a) and (1.1b) After introducing Eq. (1.1a) into the time-dependent Schrödinger equation (1.2), two real, coupled partial differential equations are obtained,

$$\frac{\partial \rho}{\partial t} + \frac{1}{m} \nabla(\rho \nabla S) = 0, \tag{1.15a}$$

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V_{\text{eff}} = 0, \tag{1.15b}$$

which come from the imaginary and real parts, respectively, of the resulting equation. The former is again the *continuity equation*, which accounts for the probability conservation, while the latter is the so-called *quantum Hamilton–Jacobi equation*, with

$$V_{\text{eff}}(\mathbf{r}, t) = V(\mathbf{r}) + Q(\mathbf{r}, t) \tag{1.16}$$

being an *effective* potential (notice the different way of expressing the same equations previously, Eqs. (1.4a) and (1.4b)). The last term in the right–hand side of Eq. (1.16) is again the *quantum potential* explicitly written now as

$$Q = \frac{\hbar^2}{4m} \left[\frac{1}{2} \left(\frac{\nabla \rho}{\rho} \right)^2 - \frac{\nabla^2 \rho}{\rho} \right], \tag{1.17}$$

which, as well as ρ, depends on both $\mathbf{r}$ and t. This term is regarded as a potential because, like V, also rules the quantum particle dynamics. However, unlike V, it is not a preassigned function. Moreover, its nature is fully quantum-mechanical due

to its dependence on the quantum state via the evolution of ρ (state dependence). The quantum potential is not changed when the wave function is multiplied by an arbitrary constant, only its form (related to the curvature of the wave function) is important in the dynamics. Even more, again unlike V, this interaction does not necessarily fall off with the distance. Due to the fact that ρ describes statistically the evolution of a swarm of identical, non interacting particles, the dependence of Q on ρ means that the dynamics of a single particle from the swarm is going to be influenced by the behavior of the others. In other words, the quantum particle dynamics is *nonlocal*. Rather than being a particular feature of Bohmian mechanics, this property is inherent to quantum mechanics in general, which manifests through the kinetic energy operator, $K = -(\hbar^2/2m)\nabla^2$. Note that Q also arises from the action of this operator on Ψ after considering Eq. (1.1a)

$$K\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi = \frac{(\nabla S)^2}{2m} - \frac{\hbar^2}{2m}\frac{\nabla^2\rho^{1/2}}{\rho^{1/2}}, \tag{1.18}$$

and, therefore, it could also be associated with a sort of nonlocal kinetic energy [7].

Under the presence of an external potential, the de Broglie wavelength of the particle has to be modified due to the presence of the quantum potential. Thus, this variable is also state dependent,

$$\lambda_Q(\mathbf{r}, t) = \frac{h}{|\nabla S(\mathbf{r}, t)|} = \frac{h}{[2m(-\frac{\partial S(\mathbf{r},t)}{\partial t} - Q - V)]^{1/2}}. \tag{1.19}$$

In particular, when one is interested in calculating the turning points of a given problem, the quantum potential plays a very important role. In a certain sense, we have to differentiate the "classical" turning points (which are obtained from V) from the "quantum" turning points [127] (obtained from $V + Q$).

Paths along which quantum particles travel may be defined according to the so-called *guidance condition*

$$\mathbf{v} = \frac{\nabla S}{m} = \frac{\mathbf{J}}{\rho} = \frac{\hbar}{2im}\left[\frac{\nabla\Psi}{\Psi} - \frac{\nabla\Psi^*}{\Psi^*}\right], \tag{1.20}$$

with $\mathbf{v}(\mathbf{r}, t) = \dot{\mathbf{r}}$ being the local velocity field. The initial velocity of the particle is then determined by the initial field $\Psi(\mathbf{r}, 0)$. However, the resulting trajectories are of quantum nature and termed *quantum or Bohmian trajectories* This expression reminds us the so-called method of characteristics in the partial differential equations [128]. The integration of the guiding condition generates the corresponding characteristics perpendicular to the S-surface of constant phase (streamlines). Note that in standard quantum mechanics the system dynamics is only described by Ψ. However, in Bohmian mechanics, one focusses on the particular evolution in time of

a given initial system configuration (initial condition), which gives rise to the corresponding Bohmian trajectories. This evolution is strongly determined by the wave function which acts like a field, apart from any other external field described by the potential V. The particle is then always accompanied by its quantum field or wave function, this combined system being causally determined. However, the converse is not always true. Imagine the wave is split up into a set of parts with no appreciable spatial overlap (nodal regions in-between). The particle can only follow one of them, the remaining waves being called *empty waves* [7].

After the quantum Newton equation given by Eq. (1.4b), one can find asymptotic regions where the external potential V is zero or negligible but the quantum potential is still active. In other words, the quantum force or the acceleration of the particle can still be important in a classical free particle regime. Furthermore, we can also imagine a situation where the classical force cancels out the quantum force. This only occurs in a stationary state (the wave function can be taken to be real) and, therefore, the particle is at rest (zero momentum) in a fixed position. Similarly, the tunneling effect can also be easily explained in terms of the quantum potential since it lowers the barrier height given by V, thus permitting particles to enter it.

Due to the linearity of the Schrödinger equation, the superposition principle holds. Thus, if ψ_1 and ψ_2 are solutions of that equation, its superposition

$$\Psi(\mathbf{r},t) = c_1\psi_1(\mathbf{r},t) + c_2\psi_2(\mathbf{r},t) = c_1\left[\psi_1(\mathbf{r},t) + \sqrt{\alpha}\psi_2(\mathbf{r},t)\right] \tag{1.21}$$

is also a solution, with $\alpha = (c_2/c_1)^2$. There should also be an additional phase factor $e^{i\delta}$ multiplying ψ_2, but we will consider $\delta = 0$ here, for simplicity; the consideration of this phase is, on the contrary, important for some problems; in particular, as will be discussed in the next chapter, for the so-called Aharonov-Bohm effect. The particular interest in solutions like (1.21) relies on the fact that they express rather well the character of quantum interference [129], more apparent through the associated probability density,

$$\rho = |\Psi|^2 = c_1^2\left[\rho_1 + \alpha\rho_2 + 2\sqrt{\alpha}\sqrt{\rho_1\rho_2}\cos\varphi\right], \tag{1.22}$$

where both ψ_1 and ψ_2 are expressed in polar form ($\psi_j = \rho_j^{1/2}e^{iS_j/\hbar}$, $j = 1, 2$) and $\varphi = (S_2 - S_1)/\hbar$ with $\Psi = \rho^{1/2}e^{iS/\hbar}$. The presence of the oscillatory term in (1.22) constitutes an observable evidence of interference, since ψ_1 and ψ_2 form a *coherent superposition*. As can be noticed, ρ does not satisfy the superposition principle, as also happens with the associated probability density current,

$$\mathbf{J} = \frac{1}{m}\mathrm{Re}\left[\Psi^*\mathbf{p}\Psi\right] = -\frac{i\hbar}{2m}\left[\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right], \tag{1.23}$$

where $\mathbf{p} = -i\hbar\nabla$ is the momentum (vector) operator. Substituting Eq. (1.21) into (1.23), with again ψ_1 and ψ_2 expressed in polar form, yields

$$\mathbf{J} = \frac{c_1^2}{m}\Big[\rho_1 \nabla S_1 + \alpha\rho_2 \nabla S_2 + \sqrt{\alpha}\sqrt{\rho_1\rho_2}\nabla(S_1 + S_2)\cos\varphi + \hbar\sqrt{\alpha}(\rho_1^{1/2}\nabla\rho_2^{1/2} - \rho_2^{1/2}\nabla\rho_1^{1/2})\sin\varphi\Big]. \tag{1.24}$$

One can further proceed and determine probability streamlines (lines along which the probability flows), as in classical hydrodynamics. Now, from the guiding condition (1.20), well-defined (in space and time) quantum trajectories are obtained by integrating the equation of motion

$$\dot{\mathbf{r}} = \frac{\mathbf{J}}{\rho} = \frac{\nabla S}{m} = -\frac{i\hbar}{2m}\frac{\Psi^*\nabla\Psi - \Psi\nabla\Psi^*}{\Psi^*\Psi} = \frac{1}{m}\frac{\rho_1\nabla S_1 + \alpha\rho_2\nabla S_2 + \sqrt{\alpha}\sqrt{\rho_1\rho_2}\nabla(S_1 + S_2)\cos\varphi}{\rho_1 + \alpha\rho_2 + 2\sqrt{\alpha}\sqrt{\rho_1\rho_2}\cos\varphi} + \sqrt{\alpha}\frac{\hbar}{m}\frac{(\rho_1^{1/2}\nabla\rho_2^{1/2} - \rho_2^{1/2}\nabla\rho_1^{1/2})\sin\varphi}{\rho_1 + \alpha\rho_2 + 2\sqrt{\alpha}\sqrt{\rho_1\rho_2}\cos\varphi}, \tag{1.25}$$

and where the initial momentum of particles is predetermined by the choice of the initial wave function and, therefore, by $\rho_0(\mathbf{r})$.

Gaussian wave packets are very helpful and easy to manipulate in theoretical treatments. Let us consider a free one-dimensional, spinless quantum system of mass m with its initial state being described (in configuration space) by

$$\Psi_0(x) = \left(\frac{1}{2\pi\sigma_0^2}\right)^{1/4} e^{-(x-x_0)^2/4\sigma_0^2 + ip_0(x-x_0)/\hbar}, \tag{1.26}$$

where x_0 and p_0 are the position and (translational or propagation) momentum of its center (in brief, the centroidal position and momentum), respectively, and σ_0 its initial spatial spreading. The exact time-dependent form of this wave function in free space $[V(x) = 0]$ can be readily obtained

$$\Psi_t(x) = \left(\frac{1}{2\pi\tilde{\sigma}_t^2}\right)^{1/4} e^{-(x-x_t)^2/4\sigma_0\tilde{\sigma}_t + i\,p_0(x-x_t)/\hbar + iE_0t/\hbar}, \tag{1.27}$$

where the centroidal position and momentum are given by $x_t = x_0 + (p_0/m)t$ and $p_t = p_0$, respectively, and correspond to a classical trajectory describing a rectilinear uniform motion. This means that the wave packet travels with a speed or *group velocity* $v_0 = p_0/m$ and has a total mechanical energy $E_0 = p_0^2/2m$. On the other hand, taking into account that

$$\tilde{\sigma}_t = \sigma_0 \left(1 + \frac{i\hbar t}{2m\sigma_0^2}\right), \tag{1.28}$$

the spreading of the wave packet at a time t is given by

$$\sigma_t = |\tilde{\sigma}_t| = \sigma_0 \sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2}. \tag{1.29}$$

Therefore, the evolution of a wave packet is characterized by two types of motion: translational or extrinsic, and spreading or intrinsic [14].

By considering the wave packet as a whole rather than a superposition of plane waves, one can associate its spreading along time with a type of internal or intrinsic kinetic energy [129]. This can be seen when computing the expectation or average value of the total energy,

$$\bar{E} = \langle \hat{H} \rangle = \frac{p_0^2}{2m} + \frac{p_s^2}{2m}. \tag{1.30}$$

Here we observe a second contribution to the energy, which comes from averaging the quantum potential [129] and is directly connected with the spreading of the wave packet. Hence, we can we can define an effective *spreading momentum*,

$$p_s = \frac{\hbar}{2\sigma_0}. \tag{1.31}$$

It is interesting that this momentum also appears when one computes the wave-packet energy dispersion (variance),

$$\Delta E \equiv \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2} = \sqrt{\frac{2p_s^2}{m}} \sqrt{\frac{p_0^2}{2m} + \frac{p_s^2}{4m}}. \tag{1.32}$$

The relationship between p_s and the wave-packet spreading becomes more apparent when (1.31) is analyzed in the light of Heisenberg's uncertainty principle: a spreading of the size of σ_0 gives rise to a spreading in momenta of the order of p_s. Actually, one could be tempted to think that classical-like regimes correspond to conditions where spreading momenta vanish.

Given these two types of motions governing the time-evolution of a wave packet, it is clear that the ratio between the corresponding velocities, v_t ($= p_t/m$) and v_s ($= \hbar/2m\sigma_0$), will play an important role in many physical processes such as, for example, interference and tunneling. From Eq. (1.29), one can always define the following time scale

$$\tau = \frac{2m\sigma_0^2}{\hbar} = \frac{\sigma_0}{v_s}, \tag{1.33}$$

which is associated with the relative spreading of the wave packet. Depending on the relationship between t and τ, we can identify three dynamical regimes [130]:

1. The very-short-time or *Ehrenfest-Huygens regime*, $t \lll \tau$, where the wave packet remains almost spreadless: $\sigma_t \approx \sigma_0$.
2. The short-time or *Fresnel regime*, $t \ll \tau$, where the spreading increases nearly quadratically with time: $\sigma_t \approx \sigma_0 + (\hbar^2/8m^2\sigma_0^3)t^2$.
3. The long-time or *Fraunhofer regime*, $t \gg \tau$, where the Gaussian wave packet spreads linearly with time: $\sigma_t \approx (\hbar/2m\sigma_0)t$.

This scheme results very useful in order to determine a way to elucidate which process, translational motion or spreading, is going to dominate the future evolution of the wave packet. Let us recast (1.29) in terms of v_s and consider that t is the time required for the centroidal position to cover a distance $d = v_0 t \approx \sigma_0$. Substituting the latter expression into (1.29), we have that

$$\sigma_t = \sigma_0 \sqrt{1 + \left(\frac{v_s}{v_0}\right)^2}. \tag{1.34}$$

Accordingly, using only information about the initial preparation of the wave packet, some information can be extracted about its subsequent dynamical behavior. More specifically, if $v_s \ll v_0$, the wave-packet spreading will be relatively slow, this being equivalent to the condition in time $t \ll \tau$. Furthermore, if $v_s \gg v_0$, the wave packet will spread very rapidly compared to its propagation along x, which corresponds to the time condition $t \gg \tau$.

From this brief wave packet analysis, and within the Bohmian formalism, the superposition principle in one dimension can be easily analyzed. Let us consider the interference between two identical Gaussian wave packets propagating in opposite directions at the same speed (by assuming $\alpha = 1$) [129]. In Fig. 1.1, the corresponding dynamics is illustrated showing quantum or Bohmian trajectories ((a) panel) for the coherent superposition of the two counter-propagating Gaussian wave packets with an initial velocity $v_0 = 10$ (in arbitrary units) and spreading motion with velocity $v_s = 1$ (also in arbitrary units). The (b)–(f) panels and transversal dashed lines correspond to different times in this coherent evolution. For simplicity in the discussion, we will refer to the two non-overlapping regions where ψ_1 and ψ_2 are initially placed as I (red plot) and II (black plot), respectively. If $t_{\max}^{\text{int}}$ denotes the time at which interference is maximum (see Fig. 1.1d), then for $t \gg t_{\max}^{\text{int}}$ ψ_1 will continue its evolution in II. Now, the wave packets (or, to be more precise, their probability densities) can be interpreted statistically as describing a swarm of identical, noninteracting quantum particles distributed accordingly. As also seen in Fig. 1.1a, Bohmian trajectories avoid crossing the line $x = 0$ at any time, this leading us to interpret the superposition principle in a different way. Quantum statistics retains the essence of (quantum) coherence and transmits it to the corresponding dynamics, leading to a zero velocity field at $x = 0$. Thus, a net flux of probability (or particles) crossing between regions I and II is not possible. In other words, trajectories starting in

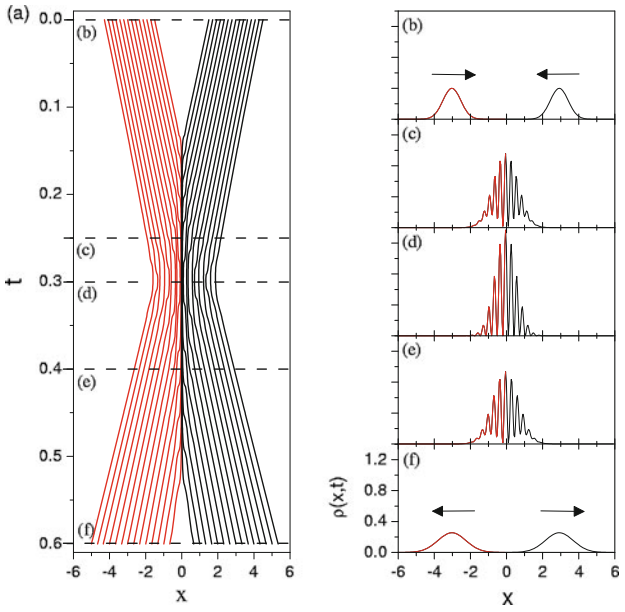

Fig. 1.1 **a** Bohmian trajectories associated with the coherent superposition of two counter-propagating Gaussian wave packets with $v_0 = 10$ and $v_s = 1$. Panels **b–f** represent snapshots illustrating the time-evolution of the superposition at the times indicated by the transversal dashed lines in panel (**a**)

region I, for example, will always keep moving inside this region. Correspondingly, the outgoing wave packet in region I (see Fig. 1.1f) accounts for the same swarm of trajectories associated with ψ_1 in Fig. 1.1b. This whole process can then be understood as a sort of bouncing motion of the wave packets once they have reached the intermediate position between them.

In spite of the fact that the two swarms of trajectories do not cross each other, the swarm associated initially with one of the wave packets behaves asymptotically as associated with the other one. Thus, from the standard picture provided by quantum mechanics for the superposition principle, the wave packets cross each other. However, from the Bohmian picture, the process should be understood as a transfer or interchange of probabilities from region I to region II, and vice versa, with the velocity field also changing its sign. Similarly to a particle-particle elastic scattering process, where particles exchange their momenta, here the swarms of particles exchange their probability distributions elastically.

On the other hand, nonlocality only disappears when $Q \equiv 0$, that is, when the particle dynamics becomes fully classical. In this case, the classical Hamilton–Jacobi equation is recovered and one has then to replace S by S_c. According to the *correspondence principle* stated by Bohr, quantum systems may behave classical-like under certain conditions, thus being describable by means of the classical mechanical laws. This is usually regarded as the *classical limit* of quantum mechanics. Usually,

this limit relies on assuming that the value of a certain magnitude of interest becomes meaningless (e.g., $\hbar$) or, on the contrary, very large (e.g., the principal quantum number) —though not always different classicality criteria lead to the same limit [131, 132]. This limit can also be satisfied in Bohmian mechanics, for example, by increasing the mass m of the particles under consideration. However, though this may seem the correct way to operate, what one really observes is that this condition does not ensure the appearance of classical trajectories, as reported in atom–surface scattering [133]. Similarly, the quantum trajectories do not behave at all as their classical counterparts, for they still contain some nonlocal information (i.e., *coherence*) through ρ. Remember that regarding dynamical effects the "shape" of ρ is more relevant than its intensity. Thus, very small variations and tinny values of ρ may lead to very dramatic dynamical effects. This is in sharp contrast with other limits in physics, like the passage from relativistic to Newtonian mechanics, where a gradual, smooth transition is observed as particle velocities become much smaller than the speed of light. Ehrenfest's theorem helps us to establish certain criteria of classicality, e.g., obtaining the conditions for the center of a wave packet to move like a classical particle [134]. Such a wave packet can be interpreted as a swarm of non-interacting particles moving according to the motion given by

$$\frac{d\langle \mathbf{r}\rangle}{dt} = \frac{\langle \mathbf{p}\rangle}{m}, \tag{1.35a}$$

$$\frac{d\langle \mathbf{p}\rangle}{dt} = -\langle \nabla V_{\text{eff}}\rangle = -\langle \nabla V\rangle. \tag{1.35b}$$

where $\langle Q\rangle = 0$ at any time. This does not mean necessarily that Bohmian particles move like classical ones, but only on average (i.e., their distribution). A good example illustrating this fact is the one mentioned above on atom–surface scattering, where the mass of the incident particles is gradually increased [133]: the average distributions reproduce classical-like results, but quantum trajectories behave very differently with respect to their classical counterparts.

It is interesting to show very briefly that quantum trajectories can be interpreted as classical trajectories but "dressed" with a series of terms coming from quantum interference [135]. Ehrenfest's theorem may constitute a first step when trying to render some light on the transition to the classical limit. However, the WKB approximation results more insightful when dealing with Bohmian mechanics. Due to the expansion in series in terms of $\hbar$ —though not always this is a good criterion— of the wave function, it yields a more direct correspondence between Bohmian and classical mechanics, i.e., to establish a closer connection between two trajectory-based formulations. Thus, as in optics [136], here one also proceeds with the ansatz

$$\Psi(\mathbf{r}, t) = e^{\mathrm{i}\bar{S}(\mathbf{r},t)/\hbar}, \tag{1.36}$$

with $\bar{S}$ being a complex function that varies slowly in space. When (1.36) is substituted into the time-dependent Schrödinger equation, one obtains

$$\frac{\partial \bar{S}}{\partial t} + \frac{\left(\nabla \bar{S}\right)^2}{2m} + V + \frac{\hbar}{2mi} \nabla^2 \bar{S} = 0. \tag{1.37}$$

In the classical limit $\hbar \to 0$, it can be assumed that $\bar{S}$ can be expanded as a series of $\hbar/i$,

$$\bar{S} = \sum_{n=0}^{\infty} \left(\frac{\hbar}{\mathrm{i}}\right)^n \bar{S}^{(n)}, \tag{1.38}$$

where the functions $\bar{S}^{(n)}$ are real. Inserting this series into (1.37), the following equation is reached

$$\sum_{n=0}^{\infty} \left(\frac{\hbar}{\mathrm{i}}\right)^n \frac{\partial \bar{S}^{(n)}}{\partial t} + \frac{1}{2m} \sum_{n=0}^{\infty} \left(\frac{\hbar}{i}\right)^n \sum_{k=0}^{n} \nabla \bar{S}^{(k)} \cdot \nabla \bar{S}^{(n-k)} + V + \frac{1}{2m} \sum_{n=0}^{\infty} \left(\frac{\hbar}{i}\right)^{n+1} \nabla^2 \bar{S}^{(n)} = 0. \tag{1.39}$$

The WKB approximation consists of solving order by order, in powers of $\hbar/i$, the coupled equations involved in (1.39). Thus, at zero order,

$$\frac{\partial \bar{S}^{(0)}}{\partial t} + \frac{\left(\nabla \bar{S}^{(0)}\right)^2}{2m} + V = 0, \tag{1.40}$$

which is the classical Hamilton–Jacobi equation, with $\bar{S}^{(0)}(\mathbf{r}, t)$ being the classical action, S_{cl}. Note that although $\bar{S}$ is not a real function in general, $\bar{S}^{(0)}$ is real because (1.40) is real.

Regarding the remaining terms of Eq. (1.39), they lead us to a hierarchy of equations which couple the different higher orders of $\bar{S}$. These equations can be expressed in a general form as

$$\frac{\partial \bar{S}^{(n)}}{\partial t} + \frac{1}{2m} \sum_{k=0}^{n} \nabla \bar{S}^{(k)} \cdot \nabla \bar{S}^{(n-k)} + \frac{1}{2m} \nabla^2 \bar{S}^{(n-1)} = 0, \tag{1.41}$$

which couple the nth order with the remaining lower ones. Here, it is interesting to note that, since (1.41) is real as well as $\bar{S}^{(0)}$, all the remaining n orders will also be real.

If the wave function (1.36) is expressed in polar form, taking (1.38) into account,

$$\phi = \exp\left[\sum_{n=0}^{\infty}(-1)^n \hbar^{2n} \bar{S}^{(2n+1)}\right], \tag{1.42a}$$

$$S = \sum_{n=0}^{\infty}(-1)^n \hbar^{2n} \bar{S}^{(2n)}. \tag{1.42b}$$

Substituting Eq. (1.42b) into the guiding condition (1.20), one obtains the expression of the quantum trajectories within the WKB approach, i.e., in terms of $\hbar$,

$$\dot{\mathbf{r}} = \frac{1}{m}\sum_{n=0}^{\infty}(-1)^n \hbar^{2n} \nabla \bar{S}^{(2n)} = \dot{\mathbf{r}}_{\mathrm{cl}} + \frac{1}{m}\sum_{n=1}^{\infty}(-1)^n \hbar^{2n} \nabla \bar{S}^{(2n)}, \tag{1.43}$$

where $\dot{\mathbf{r}}_{\mathrm{cl}} = \nabla \bar{S}_t^{(0)}/m$ is the classical law of motion. Therefore, from (1.43) one can interpret quantum trajectories as classical trajectories "dressed" with a series of terms coming from quantum interference, showing the capital difference between both types of trajectories. This type of dressing scheme is going to be recurrent along this monograph. Moreover, also from (1.43) it is very apparent how classical mechanics underlies quantum mechanics and, therefore, how quantum phenomena will keep a reminiscence of a classical-like feature —which will be stronger as the classical limit is approached.

As we have previously mentioned, the phase function or field $S(\mathbf{r}, t)$ is multivalued. However, its gradient is a single-valued function of position; in other words, at each point in configuration space and at each instant of time, there is a unique tangent vector associated with the corresponding gradient. Thus, quantum trajectories can not cross each other or even touch (*noncrossing property*). A given space point may have more than one trajectory pass through it at different times. A single-valued trajectory field is called a *congruence* [7]. In classical mechanics, something similar can be found when dealing with the phase space although the evolution of the system is only determined by external fields or preassigned functions.

On the other hand, particles can not pass at all through nodal regions (nodes or points where $\Psi = 0$). This fact is closely related to the emergence of vortices or vortical dynamics. For example, within the field of surface physics, the presence of this vortical motion has been theoretically observed in the atom–surface scattering process with presence of impurities, where atoms may undergo a series of loops before they scape from the surface [137, 138].

Equations (1.15) form a closed set of coupled partial differential equations. Different numerical techniques have been suggested to solve this set of equations [12], which is analogous to those describing the evolution of classical hydrodynamical flows (see Sect. 1.2.1). Within the Lagrangian scheme, the trajectories are calculated one by one, obtaining ρ and S and, therefore, Ψ can be synthesized. Hence, from a computational point of view, this can be regarded as a "local" calculation. However, it is important to stress that this locality has nothing to do with the nonlocal dynamical behavior mentioned above. Note that the information related to the whole ensemble (though evaluated along one particular path) appears in a very precise and

unambiguous manner in V_{eff}, as seen in Eq. (1.16), and influences the field S. Thus, it is always very important to distinguish between the locality of the calculations and the nonlocality inherent to the dynamical behavior of quantum particles [135].

By using the Lagrangian operator, Eq. (1.15b) becomes

$$\frac{dS}{dt} = \frac{1}{2}\, m\mathbf{v}^2 - V_{\text{eff}}, \tag{1.44}$$

where, as in classical mechanics, the time–derivative of the quantum action S is equal to a generalized quantum Lagrangian,

$$S[\mathbf{r}(t)] - S[\mathbf{r}(0)] = \int_0^t \mathcal{L}_Q[\mathbf{r}(t')]dt', \tag{1.45}$$

with $\mathcal{L}_Q \equiv m\mathbf{v}^2/2 - V_{\text{eff}}$. As is known, the wave formulation of quantum mechanics can also be derived from the (quantum) Lagrangian density [7, 139],

$$\mathcal{L}_q = \frac{i\hbar}{2}\left(\Psi^* \frac{\partial \Psi}{\partial t} - \frac{\partial \Psi^*}{\partial t}\,\Psi\right) - \frac{\hbar^2}{2}\,\nabla\Psi \cdot \nabla\Psi^* - V|\Psi|^2, \tag{1.46}$$

when the corresponding integral is required to be stationary with respect to variations in the complex-valued field variables Ψ and Ψ^*. Then, when variations are taken with respect to Ψ^*, the Euler–Lagrange equations yield the time-dependent Schrödinger equation (as well as its complex conjugate when variations are considered with respect to Ψ). Similarly, one can also proceed taking into account the polar form, Eq. (1.1a), which gives rise to the Lagrangian density [71, 72]

$$\begin{aligned}\mathcal{L}_q &= -\left[\frac{\partial S}{\partial t} + \frac{1}{2}\,(\nabla S)^2 + V\right]\rho - \frac{\hbar^2}{8}\left(\frac{\nabla\rho}{\rho}\right)^2\rho \\ &= -\left[\frac{\partial S}{\partial t} + \frac{1}{2}\,(\nabla S)^2 + \frac{1}{2}\,(\nabla \mathcal{K})^2 + V\right]\rho,\end{aligned} \tag{1.47}$$

where

$$\mathcal{K} \equiv \frac{\hbar}{2}\,\ln\rho \tag{1.48}$$

is a term, as we know, from which the quantum potential emerges. In this regard, note that it would be more appropriate to associate this term (and therefore the quantum potential) with a sort of inner kinetic energy, since Q does not appear explicitly in the Lagrangian density as the external potential V does. This is in correspondence with the previous analysis on the evolution of a wave packet which is ruled by two types of motions, one associated with its translation (and, therefore, with ∇S) and another one with its spreading (i.e., with $\nabla\mathcal{K}$). Furthermore, it is the presence of this term what makes quantum motion so different from the classical one, as can be readily seen when Eq. (1.47) is compared with its classical counterpart.

Finally, it is worth mentioning the so-called the wave equation of classical mechanics [140–144]. From the Lagrangian given by Eq. (1.46) and varying with respect to the complex fields Ψ^* and Ψ, the following nonlinear, time-dependent wave equation is reached

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi + \frac{\hbar^2}{2m}\frac{\nabla^2|\Psi|}{|\Psi|}\Psi. \tag{1.49}$$

The term which is responsible for the nonlinearity is proportional to the quantum potential (the last term on the right hand side of Eq. (1.49)); as mentioned by Holland [7], a nonlinear differential equation may be a limiting case of a linear equation, the time-dependent Schrödinger equation). Furthermore, a nonlinear quantum-classical transition equation has been proposed by introducing a degree of quantumness by Richardson et al. [145] which is governed by a simple parameter ϵ with $\epsilon \in [0, 1]$. The corresponding transition equation can then be written as

$$i\hbar\frac{\partial\Psi_\epsilon}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi_\epsilon + V\Psi_\epsilon + (1-\epsilon)\frac{\hbar^2}{2m}\frac{\nabla^2|\Psi_\epsilon|}{|\Psi_\epsilon|}\Psi_\epsilon. \tag{1.50}$$

This transition is thus seen as a gradual process starting from $\epsilon = 0$ (classical regime) and going up to $\epsilon = 1$ (quantum regime). Several interesting applications with Gaussian wave packets dealing with this transition equation can be found in the literature [146–149]. However, no decoherence dynamics is established since we are dealing with closed quantum systems. The decoherence process emerges when interaction with an environment or an apparatus (open quantum systems) is present. This is the subject of the last two chapters of this monograph.

1.2.3 Restricted Probability and Tubes

As it can be inferred from Eq. (1.44), in the Lagrangian scheme it is also necessary the evaluation of the quantum potential along the trajectory. However, instead of integrating the continuity equation to obtain $\rho(t)$, one can alternatively proceed as in semiclassical mechanics [150] assuming that the solution of Eq. (1.15a) along the Bohmian trajectory $\mathbf{r}(t)$ is given by

$$\rho[\mathbf{r}(t)] = \left|\frac{\partial\mathbf{r}(0)}{\partial\mathbf{r}(t)}\right| \rho[\mathbf{r}(0)]. \tag{1.51}$$

This procedure has been used with practical computational purposes in the literature (see, for example, Refs. [28–31]), with the idea of applying Bohmian mechanics as a sort of quantum initial value representation numerical approach. Substituting Eq. (1.51) into (1.17), one finds

$$Q[\mathbf{r}(t)] = \frac{\hbar^2}{4m}\left[\frac{\partial \mathbf{r}(0)}{\partial \mathbf{r}(t)}\right]^2 \left\{\frac{1}{2}\left[\frac{\nabla_{\mathbf{r}(0)}\rho[\mathbf{r}(0)]}{\rho[\mathbf{r}(0)]}\right]^2 - \frac{\nabla^2_{\mathbf{r}(0)}\rho[\mathbf{r}(0)]}{\rho[\mathbf{r}(0)]}\right\}, \tag{1.52}$$

where $\nabla_{\mathbf{r}(0)} \equiv \partial/\partial\mathbf{r}(0)$ is the action of the ∇–operator evaluated at $\mathbf{r}(0)$. In this way, $\rho[\mathbf{r}(t)]$ and $Q[\mathbf{r}(0)]$ can be both determined from $\rho[\mathbf{r}(0)]$. On the other hand, $\rho(\mathbf{r}, t)$ can be obtained by sampling the initial probability density with a sufficient number of initial conditions (trajectories). Of course, the numerical evaluation of the derivatives of ρ within this Lagrangian framework can lead to instabilities, as also happens in classical hydrodynamics, due to the approaching of the particle to nodal regions. Some alternative methods have been proposed in the literature to solve these drawbacks [151, 152].

When dealing with trajectories, a causal connection between the initial and the final states is readily established. Making use of the noncrossing property in configuration space, a kind of *probability tubes* can be defined [153]. The interest of these particular tubes arises from the fact that Bohmian mechanics is the only formulation of quantum mechanics that allows to specify such a connection in a unique and unambiguous way. Once the initial region Ω_0 is defined, one has also a clear and unambiguous prescription to follow its causal evolution throughout configuration space and a mapping $\Omega_t = \Phi_Q(\Omega_0)$ ('Q' here for 'quantum map') can also be established. Thus, trajectories distributed along the boundary $\partial\Sigma_0$ of Ω_0 will subsequently form the boundary $\partial\Sigma_t$ of Ω_t. These are called *separatrix trajectories* [10]. Furthermore, the deformation of the tubes with time is not completely arbitrary since the noncrossing rule of trajectories has to be always preserved.

A direct consequence of dealing with quantum probability tubes is the following: if we define a *partial* or *restricted probability* [154–156] as the fraction of the total probability that has ended up inside a region or domain $\mathcal{D}$ of the system configuration space,

$$\mathcal{P}_{\mathcal{D}}(\infty) \equiv \lim_{t\to\infty} \mathcal{P}_{\mathcal{D}}(t) = \lim_{t\to\infty} \int_{\mathcal{D}} \rho(\mathbf{r}, t) d\mathbf{r}, \tag{1.53}$$

it will remain constant in time whenever $\mathcal{D}$ corresponds to a probability tube. This means that, in principle, asymptotic probabilities like (1.53) can be specified from the initial state without any further calculation if we know: (i) the analytical form for the separatrix defining the initial boundary $\partial\Sigma_0$, and (ii) any *bifurcation* or *branching process* undergone by the probability tubes between t_0 and $t \to \infty$. The presence of branchings is actually a very important issue: any region Ω_t (including Ω_0) may consist of more than one separate subregions, which emerge or disappear along time.

Let $\mathcal{P}_{\Omega_t}(t)$ be a quantity describing the time-evolution of a certain probability of interest (e.g., a reaction probability, a transmittance, a cross-section, etc.) inside a

region Ω_t of the corresponding configuration space. This quantity can be expressed in terms of the restricted probability as

$$\mathcal{P}_{\Omega_t}(t) \equiv \int_{\Omega_t} \rho(\mathbf{r}, t) d\mathbf{r}. \tag{1.54}$$

The variation of $\mathcal{P}_{\Omega_t}(t)$ with time inside Ω_t is

$$\frac{d\mathcal{P}_{\Omega_t}}{dt} = \int_{\Omega_t} \frac{\partial \rho}{\partial t}\, d\mathbf{r}, \tag{1.55}$$

although it can also be written as

$$\frac{d\mathcal{P}_{\Omega_t}}{dt} = -\int_{\Omega_t} (\nabla \cdot \mathbf{J})\, d\mathbf{r} = -\int_{\partial \Sigma_t} \mathbf{J} \cdot d\mathbf{S}. \tag{1.56}$$

In the second equality of Eq. (1.56), which is a straightforward application of the divergence or Gauss-Ostrogradsky theorem, $d\mathbf{S}$ denotes a vector normal to a surface element $d(\partial \Sigma_t)$ of Ω_t and pointing outwards. By combining Eqs. (1.55) and (1.56), we find that the losses or gains of $\mathcal{P}_{\Omega_t}(t)$ inside Ω_t are described, respectively, by the outgoing or ingoing probability flux $\mathbf{J}$ through $\partial \Sigma_t$. This is a well-known result, which translates into the continuity equation when generalizing to the whole configuration space and making the flux to be independent of Ω_t. However, an additional interesting result which is worth mentioning is when the time-evolution of this region follows some particular rule, then one could keep the value of $\mathcal{P}_{\Omega_t}(t)$ constant all the way through.

From the above statements, an interesting consequence is easily deduced: any restricted probability can be determined directly from the initial state if the end points of the associated separatrix trajectories as well as any intermediate branching process are known. That is, in principle, one could determine or estimate final probabilities without carrying out the full calculation, only from the particular region covered by the initial wave function causally connected with the feature of interest [157]. Let us consider that in the restricted probability (1.53), the domain $\mathcal{D}$ corresponds to the region Ω_∞ which is the asymptotic extreme of a probability tube starting in Ω_0 at $t = 0$. By integrating back in time (i.e., considering the inverse mapping transformation $\Omega_0 = \Phi_Q^{-1}(\Omega_\infty)$), we find that

$$\mathcal{P}_{\Omega_\infty} = \int_{\Omega_\infty} \rho(\mathbf{r}, \infty) d\mathbf{r} = \lim_{t\to\infty} \int_{\Omega_t} \rho(\mathbf{r}, t) d\mathbf{r} = \lim_{t\to\infty} \mathcal{P}_{\Omega_t}(t). \tag{1.57}$$

The difference of this expression with respect to the guiding condition is that now we can keep track of the amount of probability going into $\mathcal{D} = \Omega_\infty$ by means of an unambiguous time-dependent relationship. But, since the probability inside the corresponding tube remains constant, we can just write down (1.57) as

$$\mathcal{P}_{\Omega_\infty} = \int_{\Omega_0} \rho(\mathbf{r}, 0) d\mathbf{r} = \mathcal{P}_{\Omega_0}(0). \tag{1.58}$$

The initial restricted probability $\mathcal{P}_{\Omega_0}$ can be computed from an appropriate sampling of (Bohmian) initial conditions (according to $\rho(\mathbf{r}, 0)$ inside Ω_0), as in classical mechanics. By proceeding in this way, the physical meaning of Eq. (1.58) becomes more apparent (and almost trivial): given a certain set of initial conditions enclosed in some region of the configuration space, their total number is conserved regardless of how the ensemble evolves. This is a result of *general* validity, which goes again beyond standard quantum mechanics, for it states that the probability within a certain region of the configuration space can be conveyed to another one causally connected, i.e., in an unambiguous way when following probability tubes.

The previous results lead us straightforwardly to establish a connection with the so-called Born rule [158–163]. This is readily seen as follows. If two arbitrary times, t and t' (we will assume $t' > t$), are considered, it follows from Eq. (1.58) that

$$\int_{\mathbf{r}(t')} \rho[\mathbf{r}(t')] d\mathbf{r}(t') = \int_{\mathbf{r}(t)} \rho[\mathbf{r}(t)] d\mathbf{r}(t). \tag{1.59}$$

On the other hand, because of the causal connection or mapping between $\mathbf{r}(t)$ and $\mathbf{r}(t')$ in Bohmian mechanics, one can also define a Jacobian

$$\mathcal{J}[\mathbf{r}(t)] = \frac{\partial \mathbf{r}(t')}{\partial \mathbf{r}(t)}. \tag{1.60}$$

This relation is equivalent to the one found in classical mechanics when solving the (classical) continuity equation [150, 164, 165], although in that case it includes the corresponding momenta, since it is defined in phase space. Thus, taking into account Eq. (1.59) and the connection between the layers defined by $d\mathbf{r}(t)$ and $d\mathbf{r}(t')$ enabled by the Jacobian

$$d\mathbf{r}(t') = |\mathcal{J}[\mathbf{r}(t)]| d\mathbf{r}(t), \tag{1.61}$$

the probability density evaluated along a quantum trajectory at a time t' is related through the inverse Jacobian transformation with its value at an earlier time t, as

$$\rho[\mathbf{r}(t')] = |\mathcal{J}[\mathbf{r}(t')]| \rho[\mathbf{r}(t)], \tag{1.62}$$

with $|\mathcal{J}[\mathbf{r}(t')]| = |\mathcal{J}[\mathbf{r}(t)]|^{-1}$. That is, Born's rule is preserved along time whenever the evolution of the probability $\rho[\mathbf{r}(t)]$ is monitored within the probability tube defined by the swarms of quantum trajectories $\mathbf{r}(t)$ and $\mathbf{r}'(t) = [\mathbf{r} + d\mathbf{r}](t)$,

$$\rho[\mathbf{r}(t')] d\mathbf{r}(t') = \rho[\mathbf{r}(t)] d\mathbf{r}(t). \tag{1.63}$$

In order to illustrate the notion of tubes, the scattering of a wave function off a rectangular barrier is a convenient example [153]. Let the initial wave function be

an arbitrary coherent superposition of three Gaussian wave packets,

$$\Psi_0(x) = A_0 \sum_{i=1}^{3} c_i \psi_i(x), \tag{1.64}$$

where each ψ_i is described by

$$\psi_0(x) = \left(\frac{1}{2\pi\sigma_0^2}\right)^{-1/4} e^{-(x-x_0)^2/4\sigma_0^2 + ip_0(x-x_0)/\hbar}, \tag{1.65}$$

with x_0 and p_0 being respectively the (initial) position and momentum of the wave-packet centroid (i.e., $\langle\hat{x}\rangle = x_0$ and $\langle\hat{p}\rangle = p_0$), and σ_0 its initial spreading. Without loss of generality, the parameters chosen are: $(c_1, c_2, c_3) = (1.0, 0.75, 0.5)$, $(x_{0,1}, x_{0,2}, x_{0,3})=(-10, -12, -9)$, $(p_{0,1}, p_{0,2}, p_{0,3}) = (10, 20, 15)$, $(\sigma_{0,1}, \sigma_{0,2}, \sigma_{0,3}) = (0.2, 1.6, 0.8)$, and $m = \hbar = 1$. The initial wave function Ψ_0 is hence normalized, this being denoted by the constant prefactor A_0 in Eq. (1.64). The square barrier is assumed to consist of a sum of two hyperbolic tangents,

$$V(x) = \frac{V_0}{2}\left\{\tanh\left[\alpha(x - x_-)\right] - \tanh\left[\alpha(x - x_+)\right]\right\}, \tag{1.66}$$

with $V_0 = 150$, $\alpha = 10$, and $x_\pm = \pm 2$. The quantum dynamics is carried out by means of a standard wave-packet propagation method, while the associated Bohmian trajectories are computed "on-the-fly", substituting the wave function resulting at each iteration into the guiding condition (1.20) and then integrating this equation of motion.

The initial and final probability densities are displayed in Fig. 1.2a (black and red solid lines, respectively); the barrier being plotted in the blue shadowed region. The system wave function is evolved until the probability within the intra-barrier region is negligible (our asymptotic time). In panel (b), the transmission (green dashed line), reflection (blue dash-dotted line) and intra-barrier (red dotted line) probabilities are displayed along time. In the calculation of these restricted probabilities, it is assumed that: $\mathcal{D}_\mathrm{T}$ is the region beyond the right-most barrier edge, $\mathcal{D}_\mathrm{I}$ is the region confined between the two barrier edges, and $\mathcal{D}_\mathrm{R}$ is the region to the left-most edge. As seen in the figure, after $t \approx 1.15$, we find that $\mathcal{P}_\mathrm{R} \approx 0$ and $\mathcal{P}_\mathrm{T}$ reaches its maximum (asymptotic) value, which already remains constant with time.

The initial wave function is then splitted up into reflected and transmitted, with Ω_0 encompassing the portion associated with the latter. The upper bound for this region can be the initial position, $x(0)$, of any trajectory on the right-most border of the initial probability density, for which $\rho(x(0)) \approx 0$. For the lower boundary, a search has to be done [157], so that it is ensured that the chosen trajectory is the last (or nearly the last) one in crossing the right-most barrier edge and not exhibiting a backwards motion. Determining this trajectory constitutes a major drawback, since Bohmian trajectories are not analytical in general, neither there is a simple, general

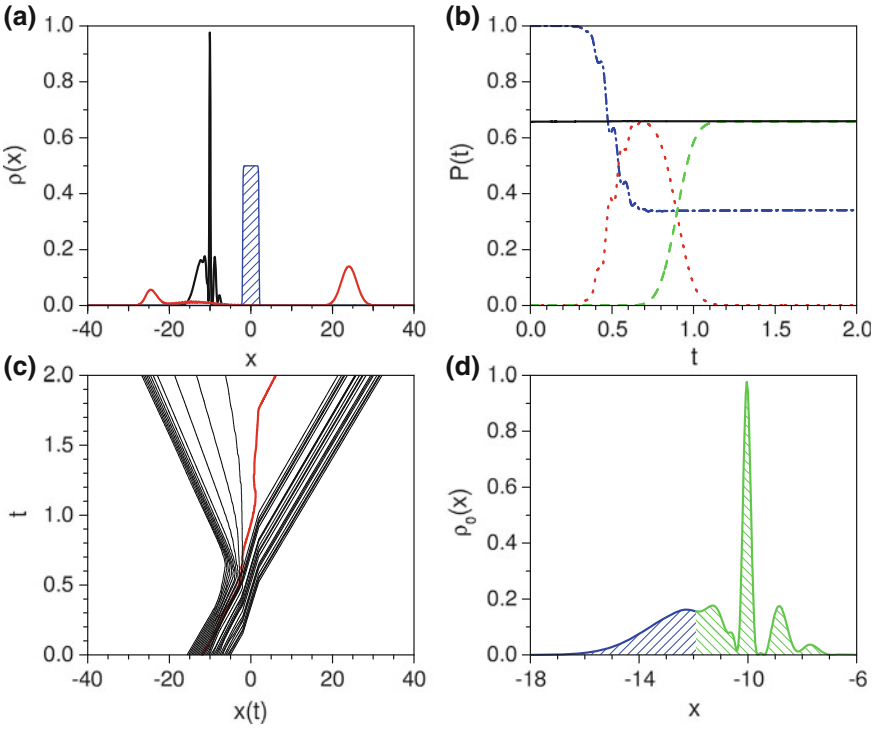

Fig. 1.2 **a** Initial (*black line*) and final (*red line*) probability densities in the problem of scattering off a nearly square barrier (*blue* shadowed region). *b* Time-dependence of the transmission (*green dashed line*), reflection (*blue dash-dotted line*) and intra-barrier (*red dotted line*) probabilities. The probability enclosed in Ω_t and obtained with the aid of the Bohmian calculation is displayed with *black solid line*. **c** Bohmian trajectories illustrating the process dynamics; the separatrix is denoted with *red thicker line*. **d** Splitting of the initial probability density according to the separatrix initial position. Only the *green* shadowed region (Ω_0) contributes to transmission

way to make an estimate [157]. This initial condition has to be then determined either from a series of sampling runs or just fixing the asymptotic value of the trajectory and running backwards in time the dynamics until $t = 0$.

A sampling set of Bohmian trajectories is shown in Fig. 1.2c, with their initial positions evenly distributed along the extension covered by the initial probability density. The red thicker line denotes the separatrix splitting the initial swarm into two groups of trajectories: those that will surmount the barrier (transmitted) and those that will bounce backwards (reflected). Accordingly, at any time t, the region Ω_t (i.e., the time-evolved of Ω_0) always confines trajectories that eventually become transmitted; $\partial\Sigma_t$ is determined by the positions at t of two trajectories, namely the separatrix and the rightmost one considered. The evolution of these two trajectories defines the corresponding transmission probability tube, along which all the transmitted probability density flows. Bearing this scheme in mind, it is now rather

simple and straightforward to determine which part of the initial probability density contributes to tunneling transmission, denoted by the green shadowed area in panel (d). The integral over this area readily provides the value otherwise found from the asymptotic $\mathcal{P}_{\mathrm{T}}$ (see panel (b)). Actually, the evaluation of $\mathcal{P}_{\Omega_t}(t)$ at each time renders a constant value (see black solid line in panel (b)), thus proving the conservation of the probability inside Ω_t. Furthermore, this also proves our previous assertion that final probabilities can be, in principle, directly and unambiguously obtained from the initial state by means of Bohmian trajectories.

1.2.4 Local and Expectation Values

Though Bohmian mechanics allows us to describe the evolution of quantum processes and phenomena in terms of individual trajectories, it is clear that any observable will be extracted from a statistical treatment of the corresponding quantum trajectories. In other words, any observable will arise as a consequence of the counting of trajectory arrivals at a certain region, which is much connected with the way how experiments occur. For example, in a typical diffraction experiment, the diffraction pattern arises by counting (detecting) individual arrivals [37, 38, 166–168]. Similarly, when using Bohmian mechanics one can reproduce the experiment by counting the arrivals of quantum trajectories [121, 127]. Thus, taking this into account, the statistical nature of quantum mechanics arises in a very natural way, where expectation values are directly associated with average (ensemble) values.

In order to understand the relationship between the expectation value of a quantum operator and the statistical Bohmian description, suppose A is a Hermitian operator, which can be a function of the position and momentum operators, $\mathbf{r}$ and $\mathbf{p} = -\mathrm{i}\hbar\nabla$, i.e., $A = A(\mathbf{r}, -\mathrm{i}\hbar\nabla)$. The expectation value of this operator is defined as

$$\langle A\rangle = \langle\Psi|A|\Psi\rangle = \frac{\int \Psi^*(A\Psi)d\mathbf{r}}{\int \Psi^*\Psi\, d\mathbf{r}}, \tag{1.67}$$

where $\Psi(\mathbf{r}, t) = \langle\mathbf{r}|\Psi(t)\rangle$ is the wave function in the system configuration space and

$$A\Psi(\mathbf{r}, t) \equiv \langle\mathbf{r}|A\left(\int |\mathbf{r}'\rangle\langle\mathbf{r}'|d\mathbf{r}'\right)|\Psi(t)\rangle = \int A(\mathbf{r}, \mathbf{r}')\Psi(\mathbf{r}', t)d\mathbf{r}', \tag{1.68}$$

with $A(\mathbf{r}, \mathbf{r}') \equiv \langle\mathbf{r}|A|\mathbf{r}'\rangle$. Moreover, one can also consider the quantity

$$\mathcal{A} \equiv \frac{\mathrm{Re}\,\{\Psi^* A\Psi\}}{\Psi^*\Psi} \tag{1.69}$$

to represent the *local* value of the operator A, given in terms of the associated field function $A(\mathbf{r}, t)$ [7]. For example, the local field functions

$$\mathbf{r}(\mathbf{r},t) = \frac{\mathrm{Re}\,\{\Psi^*\mathbf{r}\Psi\}}{\Psi^*\Psi} = \mathbf{r}(t), \tag{1.70a}$$

$$\mathbf{p}(\mathbf{r},t) = \frac{\mathrm{Re}\,\{\Psi^*(-\mathrm{i}\hbar\nabla)\Psi\}}{\Psi^*\Psi} = \nabla S \tag{1.70b}$$

$$E(\mathbf{r},t) = \frac{\mathrm{Re}\left\{\Psi^*\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi\right\}}{\Psi^*\Psi} = \frac{(\nabla S)^2}{2m} + V_{\mathrm{eff}}, \tag{1.70c}$$

provide us the position, momentum and energy of a Bohmian particle when they are evaluated along its trajectory.

If instead of a particle there is a statistical ensemble of them (or, equivalently, some set of initial conditions has to be sampled) distributed according to $\rho(\mathbf{r},t)$, the average value of A can be computed as

$$\bar{A}(t) = \int \rho(\mathbf{r},t)\; A(\mathbf{r},t)\; d\mathbf{r}. \tag{1.71}$$

In particular, we have

$$\bar{\mathbf{r}} = \int \rho\mathbf{r}d\mathbf{r} = \int \Psi^*\mathbf{r}\Psi d\mathbf{r} = \langle\mathbf{r}\rangle, \tag{1.72a}$$

$$\bar{\mathbf{p}} = \int \rho\nabla S d\mathbf{r} = \int \Psi^*(-\mathrm{i}\hbar\nabla)\Psi d\mathbf{r} = \langle\mathbf{p}\rangle, \tag{1.72b}$$

$$\bar{E} = \int \rho\left[\frac{(\nabla S)^2}{2m} + V_{\mathrm{eff}}\right]d\mathbf{r} = \int \Psi^*\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\Psi d\mathbf{r} = \langle H\rangle, \tag{1.72c}$$

which coincide with the corresponding expectation values obtained from standard quantum mechanics, this showing the equivalence at a predictive level of both approaches. Obviously, from a trajectory viewpoint, i.e., when the associated local field functions are evaluated along trajectories, Eqs. (1.72) read as

$$\bar{\mathbf{r}}_B = \frac{1}{N}\sum_{i=1}^{N} w_i\mathbf{r}_i(t), \tag{1.73a}$$

$$\bar{\mathbf{p}}_B = \frac{1}{N}\sum_{i=1}^{N} w_i\nabla S(\mathbf{r}_i(t)), \tag{1.73b}$$

$$\bar{E}_B = \frac{1}{N}\sum_{i=1}^{N} w_i\left\{\frac{[\nabla S(\mathbf{r}_i(t))]^2}{2m} + V_{\mathrm{eff}}(\mathbf{r}_i(t))\right\}, \tag{1.73c}$$

where N is the total number of trajectories considered, w_i is the associated weight —if the trajectories are initially sampled according to ρ_0, then $w_i = 1$ for all trajectories, otherwise $w_i \approx \rho(\mathbf{r}(t_0))$— and the subscript B means that these average values are computed from a sampling of Bohmian trajectories. As in classical statistical treatments, provided the sampling of initial conditions is properly carried out according to some initial distribution function (this role is played here by $\rho(0)$), in the limit $N \to \infty$, the quantities issued from Eqs. (1.73) will correspond with their quantum homologous equations (1.72), respectively. One readily notes that the uncertainty principle can be directly related to a statistical result instead of to an inherent impossibility to measure positions or momenta —the source for this impossibility would be rather associated with the way how things happen (interact) at quantum scales. In this sense, the inequality

$$\Delta r_i \Delta p_i \geq \frac{\hbar}{2} \tag{1.74}$$

expresses the relationship between two statistical quantities (in this case, position and momentum) in quantum mechanics, where

$$(\Delta r_i)^2 = \overline{r_i^2} - \overline{r_i}^2 \approx \overline{r_{B,i}^2} - \overline{r_{B,i}}^2, \tag{1.75a}$$

$$(\Delta p_i)^2 = \overline{p_i^2} - \overline{p_i}^2 \approx \overline{p_{B,i}^2} - \overline{p_{B,i}}^2, \tag{1.75b}$$

and $i = 1, 2, 3$.

It is clear from the above discussion that the role played by time in Bohmian mechanics and in quantum mechanics differs. Time in the quantum theory is not an observable, but a parameter, i.e., there is no time operator such that its eigenvalues provide us with some information (for example, about the time a particle needs to cross a barrier by tunnel effect, the time of a scattering process or the lifetime of a resonance phenomenon). Actually, when the time calculated through a given expression is compared to some experimental data value, things become more troublesome. This important issue has been considered in length in the literature [169–171], where several definitions of time can be found, such as dwell time, tunneling time, interaction time, arrival time, etc. This situation changes within the context of Bohmian mechanics, where the concept of arrival time is unambiguously defined because it is based on the concept of well-defined trajectories. Indeed, from the guidance condition or the trajectory, just by integration or by inspecting a graph [7], information about arrival times can be readily obtained with no need for a time operator.

1.2.5 Complex Quantum Trajectories

Bohmian mechanics arises when a transformation from the complex fields (Ψ, Ψ^*) to the real fields (ρ, S) is carried out. Alternatively, the wave function can be expressed

in terms of a complex phase as in Eq. (1.36) and therefore there will be a one–to–one correspondence between Ψ and $\bar{S}$ —except for a constant $2\pi n\hbar$, as in Eq. (1.12). Of course, in the particular case

$$\bar{S}(\mathbf{r},t) = S(\mathbf{r},t) - i\hbar \ln \phi(\mathbf{r},t) = S(\mathbf{r},t) - \frac{i\hbar}{2} \ln \rho(\mathbf{r},t), \tag{1.76}$$

standard Bohmian mechanics is recovered. After substitution of Eq. (1.36) into the time-dependent Schrödinger equation, one obtains

$$\frac{\partial \bar{S}}{\partial t} + \frac{(\nabla \bar{S})^2}{2m} + \bar{V}_{\text{eff}} = 0, \tag{1.77}$$

which is a complex quantum Hamilton–Jacobi equation that can be regarded as the time-dependent Schrödinger equation associated with a logarithmic wave function. In this equation,

$$\bar{V}_{\text{eff}} \equiv V - \frac{i\hbar}{2m} \nabla^2 \bar{S} \tag{1.78}$$

is now an effective complex potential, whose second component is a *complex quantum potential*,

$$\bar{Q} = -\frac{i\hbar}{2m} \nabla^2 \bar{S} = \frac{i\hbar}{2} \left[\left(\frac{\nabla \Psi}{\Psi} \right)^2 - \frac{\nabla^2 \Psi}{\Psi} \right]. \tag{1.79}$$

This (complex) quantum potential can also be referred to a sort of (complex) quantum kinetic energy, since

$$K\Psi = \frac{(\nabla \bar{S})^2}{2m} - \frac{i\hbar}{2m} \nabla^2 \bar{S}. \tag{1.80}$$

Actually, if Eq. (1.76) is substituted into the right–hand side of (1.80),

$$\begin{aligned} K\Psi &= \frac{1}{2m} \left\{ \left[(\nabla S)^2 - \frac{\hbar^2}{4} \left(\frac{\nabla \rho}{\rho} \right)^2 - \frac{i\hbar}{\rho} \nabla \rho \nabla S \right] \right. \\ &\quad \left. - i\hbar \left[\nabla^2 S - \frac{i\hbar}{2} \frac{\nabla^2 \rho}{\rho} + \frac{i\hbar}{2} \left(\frac{\nabla \rho}{\rho} \right)^2 \right] \right\} \\ &= \frac{(\nabla S)^2}{2m} + Q - \frac{i\hbar}{2m\rho} \nabla(\rho \nabla S). \end{aligned} \tag{1.81}$$

From the second equality it is very apparent that the real part of the complex kinetic energy contains the real quantum potential. Furthermore, its imaginary part provides

us with information about the quantum flux conservation (in terms of the rate of change $\partial\rho/\partial t$).

In analogy to standard Bohmian mechanics, complex quantum trajectories can also be defined by analytic continuation of Eq. (1.77) to the complex plane, which is necessary for the corresponding equation of motion

$$\bar{\mathbf{v}} = \frac{\bar{\nabla}\bar{S}}{m} = \frac{\hbar}{im}\frac{\bar{\nabla}\bar{\Psi}}{\bar{\Psi}}, \tag{1.82}$$

to be self-consistent. If $\bar{S}$ is complex, $\bar{\mathbf{v}}$ has also to be complex-valued and, therefore, the integrated trajectory. This also implies that $\bar{S}$ (and eventually Ψ) will be evaluated along a complex trajectory $\mathbf{z}(t)$ rather than along a real coordinate $\mathbf{r}$ (this is the reason why $\bar{\Psi}$ and $\bar{\nabla}$ are used in Eq. (1.82), instead of Ψ and ∇), though its value will be (physically) meaningful only along the real axis. The relationship between the real Bohmian velocity and its complex counterpart,

$$\bar{\mathbf{v}} = \mathbf{v} - \frac{i\hbar}{2m}\frac{\nabla\rho}{\rho}, \tag{1.83}$$

can be followed from Eq. (1.76). Formerly, Rosen [143, 144, 172] considered this expression a sort of total quantum mechanical momentum (or velocity) field which explains why it is possible to observe non vanishing momenta in cases where the momentum ∇S vanishes. This effect would arise from the second term on the right–hand side of Eq. (1.83), which is assumed to be a "local" momentum assigned to the quantum mechanical field with which the particle interacts. In this way, Eq. (1.83) becomes the momentum that matches the momentum distributions provided by standard quantum mechanics, rather than the momentum ∇S from Bohmian mechanics, which is quite different [173–175]. This is consistent with the fact that Bohmian trajectories only carry information about the dynamics of the quantum flow, while complex quantum trajectories will also include information about the probability (as inferred from the analytic continuation of $\bar{S}$ from Eq. (1.76)). The dynamics in the complex configuration space thus explains in a natural way how to obtain the correct momentum distribution. This also explains why algorithms based on complex trajectories are quite stable and accurate.

In one dimension, it is clear that if $\bar{\mathbf{v}}$ is assumed to be complex, depending on the z–variable, while $\mathbf{v}$ and ρ depend on the real variable x, then (1.83) becomes an inequality. In the literature [176–179], (1.83) has been considered as an identity, particularly within the so-called *stochastic Bohmian mechanics* (see Sect. 1.3.1),[2] where the second term on the right–hand side is interpreted as a stochastic diffusive term. However, not only this is not mathematical consistent, but the inequality forbids to associate the real part of the complex quantum trajectories with the (real, standard) Bohmian trajectories, as assumed in the literature [176–181]. That is, assuming

[2]This terminology is again somehow confusing when alluding to open quantum systems within the Bohmian framework in the rest of this monograph.

$z(t) = z_r(t) + iz_i(t)$ describes the complex trajectory, with z_r and z_i being its real and imaginary parts, respectively, both being real functions, the equality $z_r(t) = x(t)$, where $x(t)$ would represent the standard Bohmian trajectory, does not hold as t goes on even if $z_0 = x_0$ at $t = 0$. Note that, from a strict Bohmian viewpoint, the equality $z_r(t) = x(t)$ means that the same (projected) z_r may present different (quantum) velocities, something contrary to what happens in standard Bohmian mechanics, where only one velocity can be associated with a space coordinate. Of course, only when one moves to the complex plane realizes that, effectively, that univaluedness still continues, except in those cases where a node of the wave function appears.

Once it is assumed that both terms in Eq. (1.83) depend on the complex **z**–variable, and then **v** and ρ are some generalized complex Bohmian functions ($\tilde{\mathbf{v}}$ and $\tilde{\rho}$, respectively) depending on this variable instead of **r**, it is instructive to apply $\bar{\nabla}$ on both sides, which yields

$$\bar{\nabla}\bar{\mathbf{v}} = \bar{\nabla}\tilde{\mathbf{v}} + \frac{i\hbar}{2m}\left[\left(\frac{\bar{\nabla}\tilde{\rho}}{\tilde{\rho}}\right)^2 - \frac{\bar{\nabla}^2\tilde{\rho}}{\tilde{\rho}}\right]. \tag{1.84}$$

As seen, the second term in the right–hand side reminds the functional dependence of Q on ρ in Eq. (1.17), except for a 1/2 factor inside the square bracket. In this sense, the effects of the (real) quantum potential (i.e., the nonlocality) are still present in the complex dynamics although the corresponding complex quantum potential, which is proportional to $\bar{\nabla}\bar{\mathbf{v}}$, might be relatively small (or even zero).

Equation (1.77) was formerly derived by Pauli during his studies on the quantum WKB approximation [182, 183]. However, the formalism based on the complex version of Bohmian mechanics is relatively recent, receiving much attention in these last years. The work developed here can also be placed within the framework of the analytic versus synthetic approaches previously mentioned. From the analytic viewpoint, with interpretative purposes, one of the trends followed is the one aimed at studying stationary states. As can be easily shown, the velocity field **v** vanishes when the wave function is described by energy eigenfunctions associated with zero angular momentum states (i.e., s–waves) and, therefore, the corresponding Bohmian particles will remain standing at their initial positions at any time. In order to overcome this problem, different time-independent quantum Hamilton–Jacobi formulations have been formulated in the literature. For example, Floyd [184–187] and Faraggi and Matone [188, 189] developed time-independent quantum Hamilton–Jacobi-like formulations starting from real bipolar ansatz, though not fully equivalence to standard quantum mechanics at a predictive level. However, later on, John [180, 181] proposed a time-dependent complex quantum trajectory formalism, namely the "modified de Broglie–Bohm approach to quantum mechanics", which has also been used and further developed by other authors [176–179, 190] to understand the problem of Bohmian stationarity in other kind of problems. On the other hand, also with interpretative purposes, Eq. (1.77) was found [121, 135, 150] when trying to discriminate the amount of "quantumness" implicit in Bohmian trajectories (i.e., how different they are with respect to their classical counterparts) within the framework of the semiclassical WKB approximation. Finally, a series of fundamental works can also

be found in the literature dealing with the dynamics of problems in the continuum, such as interference [191–193], entanglement [177] or stochastic complex Bohmian mechanics [176, 179].

On the other hand, from the analytic viewpoint, Leacock and Padgett used [194, 195] the connection formula (1.36) —the same considered later by John— as an alternative way to tackle the problem of the calculation of stationary or bound states. This is formally equivalent to the more recent "Bohmian mechanics with complex action" developed by Tannor and coworkers [196–201] and the methodology developed by Wyatt and coworkers [202–205] for computational purposes without the need to solve the time-dependent Schrödinger equation. In principle, using analytical continuation it is possible to implement numerical codes that benefit from working in a complex configuration space —these advantages are similar to those that in electromagnetism, for example, lead to consider complex fields instead of real ones. More specifically, the main idea behind the development of computational tools based on the complex trajectory methodology is that the wave function on the whole real axis can be synthesized using the information transported by those particles crossing the real axis simultaneously. This allows us to define a curve, namely the *isochrone* [198, 205], which joins the specific initial positions of trajectories such that their crossing with the real axis occurs at the same time. Computationally, the main problem in dealing with the complex dynamics is locating isochrones, which is a problem similar to the root search problem in semiclassical mechanics [165]. In this regard, methods introduced in the latter may prove useful for the isochrone problem [205]. Actually, within this picture, three points are worth stressing. First, all the complex trajectories associated with an isochrone will reach the real axis simultaneously [204]. Second, the uniqueness in complex Bohmian mechanics arises from the bonds established by the initial real wave function, which is in the end the observable magnitude (through ρ). Therefore, though there might be many initial conditions leading to the same point on the real axis, only the isochrones connect the complex problem with the real one, thus establishing the same uniqueness observed in standard Bohmian mechanics. Third, a Bohmian trajectory does not correspond to a given complex trajectory or to the family of complex trajectories associated with a given isochrone, but to a family of complex trajectories such that their crossings with the real axes take place consecutively, one after the other. In other words, a Bohmian trajectory itself defines a family or set of complex quantum trajectories [191].

1.2.6 Many Particle Systems

Let us consider now two isolated quantum systems regardless of their size or properties where the total wave function describing them is a product state (factorizable) of the wave functions associated with each system. As already mentioned by Schrödinger [206, 207], as soon as these objects interact, the total wave function becomes non longer factorizable and they cannot be described as independent entities. The new quantum state becomes *entangled*, with the property that any quantum

operation performed on one of the objects will have important implications on the other one independently of how far apart they are [15–17, 208]. This property has led to the well-known quantum information theory [209] as well as mechanisms, such as decoherence, which are used to explain the emergence of the classical world from quantum mechanics [104, 210, 211].

Before going to the implications of entanglement, we focus on a set of N independent particles of mass m, each one represented at a given time by a solution of the corresponding separated Schrödinger equation. The total N–body wave function in the configuration space can be expressed as a product of N single wave functions,

$$\begin{aligned}\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) &= \psi_1(\mathbf{r}_1, t)\psi_2(\mathbf{r}_2, t)\cdots\psi_N(\mathbf{r}_N, t) \\ &= \Pi_{i=1}^{N}\rho_i^{1/2}(\mathbf{r}_i, t)\, e^{iS_i(\mathbf{r}_i,t)/\hbar}.\end{aligned} \tag{1.85}$$

In this case, it is easy to show that from this total wave function, individual solutions of the Bohmian equations of motion are obtained according to

$$\mathbf{v}_i = \dot{\mathbf{r}}_i = \frac{\nabla_{\mathbf{r}_i} S_i(\mathbf{r}_i, t)}{m}, \tag{1.86}$$

since the quantum potential is also separable as a sum of partial quantum potentials,

$$Q = \sum_{i=1}^{N} Q_i = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\nabla^2\rho_i^{1/2}}{\rho_i^{1/2}}. \tag{1.87}$$

This implies that the Bohmian trajectories described by the different particles are independent and no information is transmitted among them. Of course, this also happens if instead of N different particles, N different degrees of freedom are considered. Typically, factorizability is closely connected to *distinguishability*. For example, this is the case of particles describable by means of a Maxwell–Boltzmann statistics. For two particles, their total wave function can be expressed as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \Phi_A(\mathbf{r}_1, t)\Phi_B(\mathbf{r}_2, t). \tag{1.88}$$

Usually, the particles constituting this kind of ensembles are non-interacting and they can be accounted for by only taking into account how they distribute. When the particles forming an ensemble do interact among themselves and become indistinguishable (i.e., truly quantum-mechanical), apart from their distribution it is also very important to know how they interact. In this case, even if they are very far apart, their quantum state cannot be described in a simple manner since it is an entangled state. This is the case of the Fermi–Dirac or Bose–Einstein statistics, which describe fermions or bosons, respectively. That is, if two of these particles are considered, their total wave function will be

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = N_{\pm}\left[\Phi_A(\mathbf{r}_1, t)\Phi_B(\mathbf{r}_2, t) \pm \Phi_A(\mathbf{r}_2, t)\Phi_B(\mathbf{r}_1, t)\right], \tag{1.89}$$

where $N_{\pm}$ is the normalization factor and the minus sign stands for fermions (wave function with odd parity under exchange of the positions of the particles) and the plus sign for bosons (even parity).

As is known in quantum statistical physics, spatial correlation exist even if the particles are supposedly noninteracting. This is due to the symmetry properties of the corresponding wave function. This correlation is significant if the interparticle distances in the whole system are comparable with the so-called mean thermal wavelength of the particles [212]

$$\lambda_T = \frac{h}{(2\pi m k_B T)^{1/2}}, \tag{1.90}$$

where k_B and T are the Boltzmann constant and the temperature, respectively. A positive and negative spatial correlations are displayed by bosons and fermions, respectively. Many times, an alternative way to express such correlations is by means of the so-called statistical potential which is defined as

$$V_s(r) = -k_B T \ln[1 \pm exp(-2\pi r^2/\lambda_T^2] \tag{1.91}$$

where r is the interparticle distance. For bosons (plus sign), the statistical potential is attractive whereas for fermions (minus sign), the corresponding potential is repulsive; decaying in both cases rapidly to zero when r becomes larger than λ_T.

In general, given an entangled state described by the global wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) = \phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)\, e^{iS(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)/\hbar}, \tag{1.92}$$

the corresponding quantum trajectories will be obtained by integrating the equations of motion

$$\mathbf{v}_i = \frac{\nabla_i S}{m}. \tag{1.93}$$

This scheme gives rise to a set of N equations coupled through the total phase S, where the evolution of a particle will be strongly nonlocally influenced by the other (apart from other classical like interactions through V). This entanglement [206, 207] becomes more apparent through the quantum potential,

$$Q = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\nabla_i^2\phi}{\phi}, \tag{1.94}$$

where $Q = Q(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)$, which is nonseparable and, therefore, strongly nonlocal. In other words, the usual hydrodynamical magnitudes described above become now many-body functions. Thus, for example, in order to calculate any trajectory of a given particle, the initial positions of all particles have to be specified. Instantaneous

motion of any particle depends on the coordinates of all other particles at the same time. Disturbing a part of the system in a localized region, the configuration space of the whole system will respond instantaneously. The quantum force defined by the gradient of the quantum potential does not, in general, fall off with distance and interaction among particles can be rather strong even though the wave function amplitude is small. Different works in the literature have analyzed the trajectory correlation among entangled particles [213–217]. As Holland [7] mentioned, in this mechanics, the whole system is prior to its constituent particles displaying a radical, different behavior to the classical dynamics where the whole is the sum of the parts and their interacions. Furthermore, the symmetry properties of the wave function associated with a set of particles (bosons or fermions) implies clearly the introduction of forces between the particles making up the system. The correlations in their motions lead to quantum potentials distinct for each set of particles. Although identical particles are not distinguishable, they are distinguished by the continuity of their trajectories. In this sense, the separation or distance between two particles following two different trajectories has a precise meaning, at any instant of time. Furthermore, depending if we are dealing with a set of fermions or bosons the corresponding distance behaves with time differently.

Recently, the Bohmian formalism has been used to derive the ro-vibrational spectrum of diatomic molecules [218]. The same formalism was also used to devise some hybrid methods when systems of many degrees of freedom are considered [219, 220].

1.3 Open Quantum Systems. Quantum Stochastic Trajectories

1.3.1 The Causal Stochastic Approach

As has been already mentioned in the first section, Bohm and Vigier [10, 70] assumed that a particle could be thought to be suspended in a Madelung fluid. Their basic assumption was to express the velocity of a given particle in configuration space as

$$d\mathbf{v} = -\nabla(V + Q)dt + d\mathbf{W}(t) \tag{1.95}$$

where $d\mathbf{W}(t)$ is the increment vector (along the three directions) of the so-called Wiener stochastic process at time t which gives the random fluctuations (noise) of the velocity due to the presence of the environment.

This equation can provide us some sort of *quantum (Bohmian) stochastic trajectories*. In this approach, we are dealing with a statistical ensemble of particles with a probability distribution given by $P(\mathbf{r}, t)$. It is usually assumed that this probability

distribution has nothing to do with the wave function. Only after the evolution in a long interval of time of the corresponding dynamics, $P(\mathbf{r},t) \to \rho(\mathbf{r},t) = |\Psi(\mathbf{r},t)|^2$. One could suppose that the stochastic process could be come from some sort of vacuum fluctuations represented by a simple diffusion process [80]. The analysis of a Brownian particle in a gravitational field is simple and illustrative of some new concepts which should be introduced. If P is the probability density of particles, the probability current or flux and the conservation equation are given by

$$\begin{aligned} \mathbf{J} &= -D\nabla P \\ \frac{\partial P}{\partial t} &= -D\nabla\left(\frac{mg}{k_B T} z P + \nabla P\right), \end{aligned} \tag{1.96}$$

respectively, where D is the diffusion coefficient and k_B is the Boltzmann constant. The so-called osmotic velocity which gives us the drift component (due to the gravitational field) is written as

$$u = D\frac{mg}{k_B T} \tag{1.97}$$

and was introduced by Einstein. At equilibrium, $\partial P/\partial t = 0$, the well-known Boltzman factor is obtained,

$$P = Ae^{-mgz/k_B T} \tag{1.98}$$

where A is a constant. In other words, the particle is drifting downward in the gravitational field and the net upward diffusive movement is balanced to produce equilibrium.

In the quantum domain, we would like to have that the equilibrium state of the diffusion process corresponds to a probability density $P = |\psi|^2 = \rho$ and to a mean current $j = \rho\bar{v} = \rho\nabla S/m$. Such a state is a consistent possibility if the wave function of the particle, written in polar form as $\psi = \sqrt{\rho}\exp(iS/\hbar)$, satisfies the Schrödinger equation because this implies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla.\mathbf{j} = 0. \tag{1.99}$$

This could be accomplished with a suitable choice of the osmotic velocity. The origin of this osmotic velocity is not coming from a force field but from different causes. It could be postulated a field such as

$$\mathbf{u} = D\frac{\nabla\rho}{\rho}. \tag{1.100}$$

The total current is thus written as

$$\mathbf{j} = \frac{P}{m}\nabla S + DP\frac{\nabla\rho}{\rho} - D\nabla P \tag{1.101}$$

and the continuity equation as

$$\frac{\partial P}{\partial t} + \nabla . \left(P \frac{\nabla S}{m} + D P \frac{\nabla \rho}{\rho} - D \nabla P \right) = 0. \tag{1.102}$$

Then, the systematic velocity is given by

$$\mathbf{v} = \frac{\nabla S}{m} + D \frac{\nabla \rho}{\rho} \tag{1.103}$$

where the mean velocity arises from the guidance condition and the osmotic velocity is derivable from the potential

$$V_o = D \, ln \rho \tag{1.104}$$

ρ being a solution of

$$\frac{\partial \rho}{\partial t} + \nabla . \left(\rho \frac{\nabla S}{m} \right) = 0. \tag{1.105}$$

The equilibrium position implies that $P = \rho$, that is, it means that the osmotic velocity is balanced by the diffusion current so that the mean velocity is $\nabla S/m$. The next important question is, any arbitrary probability distribution P will always approach ρ? Bohm and Vigier [70] have shown that for the general case P approaches ρ. The osmotic velocity is then constantly pushing the particle to the regions of highest $|\psi|^2$ and this explains why most particles are found near the maxima of the wave function. Moreover, as previously stated, for stationary states, $S = const$ and therefore $\mathbf{p} = \nabla S = 0$. When considering the stochastic contribution, the sistematic velocity is no longer zero.

As a last remark, notice that Eq. (1.83) issued from the complex Bohmian mechanics is reminiscent of Eq. (1.103) when speaking about stochastic Bohmian mechanics with an imaginary diffusion coefficient D.

1.3.2 Diffusion. Quantum Brownian Motion

One of the simplest integrable dissipative quantum systems that we may devise is the diffusion of a wave packet on a flat surface. This is also a very instructive problem regarding the effects of stochastic dynamics on wave packets as well as an alternative way to also introduce quantum stochastic trajectories in this framework [13, 14]. Obviously, some of the results derived in this Section go beyond this particular context. In particular, the decoherence process which will be widely analyzed in Chap. 4.

The quantum Langevin equations for the Heisenberg position operators (for convenience in the notation, the operators will not be denoted with the usual 'hat') read for Ohmic friction, γ, or linear spectral density as [13, 14, 100, 221, 222]

$$\begin{aligned} \ddot{x}(t) &= -\gamma \dot{x}(t) + \delta F_x(t), \\ \ddot{y}(t) &= -\gamma \dot{y}(t) + \delta F_y(t). \end{aligned} \tag{1.106}$$

Here, x and y denote the position operators accounting for the motion of a single adsorbate across a flat surface, $V(x, y) = 0$. Lattice vibrational effects due to the surface temperature are assumed to be well described by a Gaussian white noise (per mass unit), which interacts and affects importantly the wave packet dynamics representing the adsorbate. Accordingly, the noise fluctuations acting on each degree of freedom are given by $\delta F_i(t) = F_i(t) - \langle F_i \rangle$, where $i = x, y$. At high (surface) temperatures, we have $\beta^{-1} \gg \hbar\gamma$ or, equivalently, $\gamma^{-1} \gg t_c \sim \hbar\beta$, where $\beta = (k_B T)^{-1}$ and the coherence time, t_c, is commonly known as *thermal time* and gives us an idea of the time scales at which thermal effects start playing a role. Under these conditions, the noise can be assumed to be classical and, hence, its autocorrelation function at two different times is well described by a Dirac δ-function.

Consider an adparticle of mass m initially placed at a given position on the flat surface. This particle is represented initially by a Gaussian wave packet,

$$\psi(x, y, 0) = \frac{1}{\sqrt{2\pi\sigma_0^2}}\, e^{-x^2/4\sigma_0^2 - y^2/4\sigma_0^2}, \tag{1.107}$$

with initial width, σ_0, along both directions. The adparticle is assumed to be initially in equilibrium with the reservoir or heat bath (surface) at a temperature T, but weakly coupled to the environment, so that dissipation can be neglected. The role of the initial conditions has been very often discussed in the literature (see, for example, Refs. [223, 224]). After a time t, the probability distribution to find the particle at a given position (x, y) is given by

$$P(x, y, t) = |\langle \psi(x, y, t) \rangle|^2 = \frac{1}{2\pi w_x(t) w_y(t)}\, e^{-x^2/2w_x^2(t) - y^2/2w_y^2(t)}, \tag{1.108}$$

which arises after averaging the survival probability over a thermal (Maxwell-Boltzmann) distribution [225] and ψ is solution of the free particle time dependent Schrödinger equation (see previous Section). Note here that the interaction with the environment makes the quantum state describing the system to pass from pure to a statistical mixture. According to Ford et al. [226–228], this normal distribution is also associated with two measurements at two different times. For each degree of freedom, the overall time-dependent spreading of the distribution (1.108) can be recast as

$$w_i^2(t) = \sigma_0^2 + \sigma_i^2(t) + s_i(t), \tag{1.109}$$

with $i = x, y$. The quantum contribution to this spreading is given by

$$\begin{aligned}\sigma_x^2(t) &= -\frac{[x(0), x(t)]^2}{4\sigma_0^2},\\ \sigma_y^2(t) &= -\frac{[y(0), y(t)]^2}{4\sigma_0^2},\end{aligned} \tag{1.110}$$

while $s_i(t)$ is the mean-squared displacement (MSD) along the i-th direction, i.e.,

$$\begin{aligned}s_x(t) &= \langle\{x(t) - x(0)\}^2\rangle,\\ s_y(t) &= \langle\{y(t) - y(0)\}^2\rangle.\end{aligned} \tag{1.111}$$

The quantum spreading depends on the commutator of the position operators at two different times, from which

$$\sigma_i^2(t) = \frac{\hbar^2}{4m^2\sigma_0^2\gamma^2}\,\Phi^2(\gamma t), \tag{1.112}$$

with $\Phi(\gamma t) = 1 - \exp(-\gamma t)$. For each degree of freedom, one obtains the same spreading because the initial width and the noise fluctuations are assumed to be the same in both directions (isotropic surface). The same happens with the MSD along each direction, which acquires the form

$$s_i(t) = \frac{2\hbar\gamma}{\pi m}\,t^2 G(\gamma t; T), \tag{1.113}$$

with

$$G(\gamma t; T) = \int_0^\infty \frac{1 - \cos z}{z(z^2 + \gamma^2 t^2)}\,\coth\left(\frac{\hbar z}{2tk_BT}\right) dz. \tag{1.114}$$

In our particular case, this G-function has an analytical solution, allowing us to express (1.113) as

$$s_i(t) = \frac{2k_BT}{m\gamma}\left[t - \frac{1}{\gamma}\Phi(\gamma t)\right]. \tag{1.115}$$

In the long-time or diffusion regime, $\gamma t \gg 1$, the quantum spreading becomes time-independent,

$$\sigma^2(t \to \infty) \approx \frac{\hbar^2}{4m^2\sigma_0^2\gamma^2}, \tag{1.116}$$

while the MSD is linear with time,

$$s(t) \approx \frac{2k_BT}{m\gamma}\,t. \tag{1.117}$$

Thus, Einstein's diffusion law is satisfied, with the diffusion constant given by

$$D = \frac{k_B T}{m\gamma} \tag{1.118}$$

in both directions. Accordingly, the overall time-dependent spreading can be expressed as

$$w^2(t) \approx \sigma_0^2 + \frac{\hbar^2}{4m^2\sigma_0^2\gamma^2} + \frac{2k_B T}{m\gamma}\, t. \tag{1.119}$$

In the short-time regime, $\gamma t \ll 1$, the quantum spreading (1.112) goes like t^2, according to

$$\sigma^2(t) \approx \frac{\hbar^2}{4m^2\sigma_0^2}\, t^2, \tag{1.120}$$

which corresponds to the wave packet spreading in the absence of dissipation. Analogously, the MSD also goes like t^2 according to

$$s(t) \approx \frac{k_B T}{m}\, t^2, \tag{1.121}$$

where the prefactor is the thermal velocity in two dimensions. Thus, the overall time-dependent spreading can be expressed in a more compact form as

$$w^2(t) \approx \sigma_0^2 + \langle v^2\rangle t^2, \tag{1.122}$$

with

$$\langle v^2\rangle = \frac{k_B T}{m} + \frac{\hbar^2}{4m^2\sigma_0^2}. \tag{1.123}$$

In this short-time regime (friction-free motion or ballistic regime), we have usually that $\langle v^2\rangle t^2 \ll \sigma_0^2$, that is, the wave packet has not spread too much compared to its initial spreading which can be assumed to be arbitrary large.

At low surface temperatures, we have $\gamma^{-1} \ll t_c \sim \hbar\beta$. In this case, the noise autocorrelation function is complex [229] and depends on the ratio between the interval of the two times and t_c (colored noise). In general, this noise function will act like a driving force and the surface dynamics is better described within the generalized Langevin framework as

$$\begin{aligned} \ddot{x}(t) + \int_{-\infty}^{t} dt' \gamma_x(t-t')\dot{x}(t') &= \delta F_x(t), \\ \ddot{y}(t) + \int_{-\infty}^{t} dt' \gamma_y(t-t')\dot{y}(t) &= \delta F_y(t), \end{aligned} \tag{1.124}$$

where $\gamma_x(t)$ and $\gamma_y(t)$ now represent the time-dependent frictions or memory functions along each direction —a one-dimensional expression for the noise function can be found in the literature [222, 230]. If we assume again an isotropic surface

and Ohmic friction, Eq. (1.124) reduce to (1.106). Thus, the corresponding quantum mechanical process is not a Markovian process in the customary sense of the term [222, 230]. The quantum spreading is then the same as before, i.e., given by (1.112), since it is independent of the surface temperature. However, the MSD along each direction, given by (1.113), now reads as

$$s_i(t) = \frac{2k_BT}{m\gamma}\left[t - \frac{1}{\gamma}\Phi(\gamma t)\right] + \frac{4}{\beta m}\sum_{n=1}^{\infty}\frac{\gamma - \nu_n - \gamma e^{-\nu_n t} + \nu_n e^{-\gamma t}}{\nu_n(\gamma^2 - \nu_n^2)}, \tag{1.125}$$

with

$$\nu_n = \frac{2\pi n}{\hbar\beta} \tag{1.126}$$

being the so-called *Matsubara frequencies*, which come from the Taylor series expansion of the coth-function in the integrand of (1.114). At high surface temperatures, Eq. (1.125) reduces to (1.115), while the sum over n plays an important role only at very low, but non-vanishing surface temperatures. Notice that in the limit of zero surface temperature, the sum vanishes —in this limit, the coth-function in (1.114) becomes unity and $G(\gamma t; 0)$ displays a different time-dependence. In this case ($T = 0$), the corresponding MSD expression reads as

$$s_i(t) = \frac{2\hbar}{\pi m\gamma}\left\{\gamma_E + \ln\gamma t - \frac{1}{2}\left[e^{\gamma t}\bar{E}i(-\gamma t) + e^{-\gamma t}Ei(\gamma t)\right]\right\}, \tag{1.127}$$

where $\gamma_E = 0.577$ is Euler's constant, and $\bar{E}i(-\gamma t)$ and $Ei(\gamma t)$ are the exponential integrals [231]. The environment no longer transfers energy to the adparticle due to the zero-point motion of the surface oscillators.

A similar dynamical analysis can also be carried out in terms of the short- and long-time regimes. The quantum spreading in both dimensions remains the same and is given by (1.112). However, the MSD is different due to its temperature dependence. Thus, in the short-time regime, $\gamma t \ll 1$, we find

$$s(t) \approx \frac{k_BT}{m}\,t^2 + \frac{\hbar\gamma}{\pi m}\,t^2, \tag{1.128}$$

which depends linearly on γ. Analogously, at zero surface temperature, we have

$$s(t) \approx \frac{\hbar\gamma}{\pi m}\,t^2\left(\frac{3}{2} - \gamma_E - \ln\gamma t\right), \tag{1.129}$$

where we observe essentially the same friction and time dependence, since the presence of the friction in the log-function is much weaker. On the other hand, in the long-time regime, it can be shown that

$$s(t) \approx \frac{2k_B T}{m\gamma}\, t + \frac{2\hbar}{\pi m}\frac{1}{\gamma + \nu_1}, \tag{1.130}$$

which becomes

$$s(t) \approx \frac{2\hbar}{\pi m\gamma}\,(\gamma_E + \ln \gamma t) \tag{1.131}$$

at zero surface temperature.

From this behavior, at equilibrium or diffusive regime [80], it is possible to determine the corresponding quantum potential and then to derive the corresponding quantum stochastic trajectories issued from the quantum Newton-like equation of motion

$$m\mathbf{a} = -\nabla(V + Q), \tag{1.132}$$

where **a** is the acceleration, V is the interaction potential between the adsorbate and the surface (in the free wave-packet problem, $V = 0$), and the quantum potential is given by Eq. (1.17). According to Eq. (1.108), $P(x, y, t)$ is identified with the probability density $\rho(x, y, t)$ displaying the total spreading of the wave packet with time. Only the spreading due to MSD depends explicitly on the surface temperature. However, the friction coefficient describing the interaction with the environment or bath is present in both the quantum and MSD spreadings. At very short times, in the ballistic regime, the stochastic dynamics is frictionless, but temperature dependent, as previously shown. On the contrary, in the diffusion regime, the corresponding dynamics depends on both, friction and temperature. Direct time integration of Newton's equation of motion gives the corresponding quantum stochastic trajectories. Very important implications such as the decoherence process and the violation of the

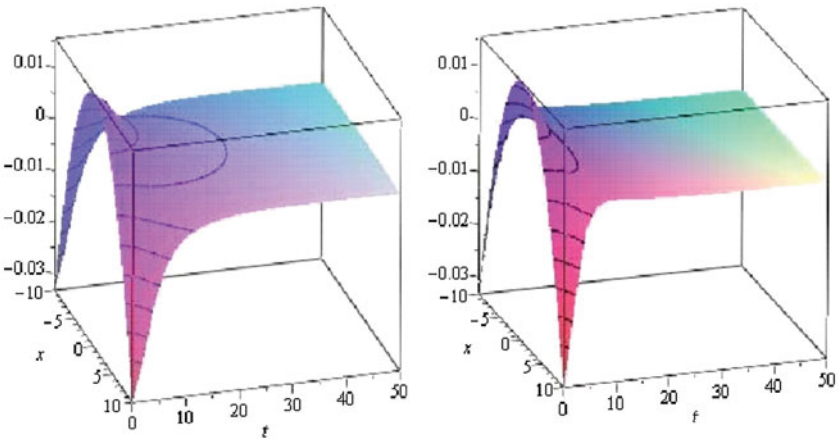

Fig. 1.3 Quantum potential for a friction $\gamma = 0.2$ and two surface temperatures: $T = 50$ K (*left*) and $T = 300$ K (*right*). The associated Gaussian wave packet describes a particle characterized by $m = 1$ and $\sigma_0 = 2$ ($\hbar = 1$)

noncrossing rule are worth mentioning. These points will be analyzed and discussed under a different perspective in the following chapters.

As an illustration, in Fig. 1.3 the quantum potential associated with a Gaussian wave packet with $m = 1$ and $\sigma_0 = 2$ ($\hbar = 1$) is displayed for a friction $\gamma = 0.2$ and two surface temperatures: $T = 50$ K (left) and $T = 300$ K (right). For simplicity, only the x-direction is plotted. The stronger variations of the quantum potential takes place at short times and large distances. The MSD is linear with the temperature as well as the total spreading of the Gaussian distribution.

This simple analysis can be extended to a many particle system. The non-local effects are now not only due to the quantum potential but also due to the osmotic velocity. This point is crucial to the stochastic methods derived from Nelson's approach.

It should be taken into account that when speaking about quantum stochastic trajectories in the Bohmian framework, there are several routes as the one followed in this Section. After Bohm and Vigier, the more formal approach is when one is starting with a Langevin-like equation such as Eq. (1.95). In any case, the osmotic and systematic velocities, given by Eqs. (1.100) and (1.103) respectively, can straightforwardly be obtained for the Brownian motion in the diffusive regime. In Chap. 3, a different approach is proposed and developed.

1.3.3 Stochastic Weak Values

As pointed out by Aharonov [232] the initial state of a closed system does not determine its final state, complete initial and final boundary conditions must be imposed. Thus, for an initial boundary condition (before the measurement) we are pre-selecting an incident wave function while for a final boundary condition we are post-selecting a final wave function. Both boundary conditions define what is called a pre- and post-selected ensemble, both wave functions being non-orthogonal. In this sense, the weak value of an operator A, is defined as

$$\langle A\rangle_w = \frac{\langle\psi_{final}|A|\psi_{initial}\rangle}{\langle\psi_{final}|\psi_{initial}\rangle}. \tag{1.133}$$

Thus, weak values reduce to expectation values when both wave functions coincide. A measurement of the observable A yielding $\langle A\rangle_w$ is a *weak* measurement.

Weak measurements are playing a very important role in measuring very tiny, but important effects [19, 233]. Most people think that this type of measurements will be important to shed some light to fundamental problems in quantum mechanics. As shown by Hiley [64], weak values which can be seen as complex, transition probability amplitudes are related to Bohm momentum, the Bohm energy, and the quantum potential. In one dimension, for example, the expectation value of the momentum

operator is given by

$$\langle\psi(t)|p|\psi(t)\rangle = \int \rho(x,t)\frac{\langle x|p|\psi(t)\rangle}{\langle x|\psi(t)\rangle}dx \tag{1.134}$$

where in atomic units

$$\langle x|p|\psi(t)\rangle = \int \langle x|p|x'\rangle\langle x'|\psi(t)\rangle dx' = -i\nabla_x\psi(x,t). \tag{1.135}$$

By writting as usual the wave function in polar form, the weak value obtained from measuring the position (post-selection) after the momentum is pre-selected leads to

$$\frac{< x|p|\psi(t) >}{< x|\psi(t) >} = \nabla_x S(x,t) - i\frac{\nabla_x\rho(x,t)}{2\rho(x,t)} \tag{1.136}$$

where it is a complex quantity where the real part is the Bohm momentum and the imaginary part is identical to the so-called osmotic velocity.

As we have also seen in open quantum systems, the osmotic velocity comes directly from an underlying diffusion motion (as introduced by Nelson in his stochastic theory [73]). This osmotic velocity is related to the probability density. Thus, when we are dealing with quantum stochastic trajectories, the weak values are also depending on the friction coefficient and the surface temperature. Further investigation along these lines are crucial to better understand future experiments.

1.3.4 The Density Matrix

When one has an ensemble of particles at different positions but the same state or wave function, we talk about a pure state, or better said a pure ensemble. On the contrary, if the states or wave function are different, a mixed state or ensemble is often used.

Concerning statistical properties of the quantum systems, two types of averaging is usually considered [10]. The first one is over the particle positions and the second one, over the distribution of wave functions. If the wave function is represented in terms of an orthonormal basis set, for example, eigenfunctions of the energy, we can always write

$$\Psi(\mathbf{r}) = \sum_{E,j} c_{Ej}\psi_{E,j}(\mathbf{r}) \tag{1.137}$$

where E runs over the energy eigenvalues and the index j over all the remaining quantum numbers. The complex coefficients c can also be expressed in polar form, $c_{Ej} = R_{Ej}exp[i\phi_{Ej}]$. Considering an ensemble of wave functions also means to have a probability distribution of amplitudes and phases. Thus, a given point in the

space of wave functions is given by all c_{Ej}'s or all R_{Ej}s and ϕ_{Ej}'s. The element of volume of this space can then be written as

$$d\Omega = \prod_{E,j} dp_{Ej} d\phi_{Ej} \tag{1.138}$$

where $p_{Ej} = R_{Ej}^2$. The mean number, dZ, of systems in this element of volume is given by

$$dZ = P(...R_{Ej}...; ...\phi_{Ej}...)d\Omega \tag{1.139}$$

P being the probability density of systems in this wave function space. The first averaging is then, for a given wave function ψ and physical operator O,

$$\langle O \rangle = \int \sum_{E,j} \sum_{E',j'} c_{Ej}^* c_{E'j'} \psi_{E,j}^*(\mathbf{r}) O \psi_{E'j'}(\mathbf{r}) d\mathbf{r} \tag{1.140}$$

and the second averaging can be expressed as

$$\begin{aligned} \langle\langle O \rangle\rangle = & \int \int \sum_{E,j} \sum_{E',j'} P(...R_{Ej}...R_{E'j'}...; ...\phi_{Ej}...\phi_{E'j'}...) \\ & . \; R_{Ej} R_{E'j'} e^{-i\phi_{Ej}} e^{i\phi_{E'j'}} \psi_{E,j}^*(\mathbf{r}) O \psi_{E'j'}(\mathbf{r}) d\mathbf{r} d\Omega \\ & = Tr(\rho O) \end{aligned} \tag{1.141}$$

where the usual density matrix is defined as

$$\begin{aligned} \rho_{EjE'j'} = & \int P(...R_{Ej}...R_{E'j'}...; ...\phi_{Ej}...\phi_{E'j'}...) \\ & . \; R_{Ej} R_{E'j'} e^{-i\phi_{Ej}} e^{i\phi_{E'j'}} d\Omega. \end{aligned} \tag{1.142}$$

It is clear that the density matrix determines the statistical results of all measurements in standard quantum mechanics [104, 105].

The density matrix does not determine the probability distribution P unambiguously. In other words, physical averages are extremely insensitive to the detail of the P-distribution. In fact, for a given density matrix, a very wide range of P-distributions is possible. A good illustration of this fact is the following. Let us consider a general wave function expressed as

$$\Psi(\mathbf{r}) = \sum_j R_j e^{i\phi_j} \psi_j(\mathbf{r}) \tag{1.143}$$

then the density matrix in the configuration space is given by

$$\rho(\mathbf{r},\mathbf{r}') = \int \sum_{j,j'} P(...R_j...R_{j'}...;\, ...\phi_j...\phi_{j'}...) \cdot\ R_j R_{j'} e^{i(\phi_j-\phi_{j'})} \psi_j^*(\mathbf{r})\psi_{j'}(\mathbf{r}')d\Omega. \tag{1.144}$$

Now, if we assume that the P-distribution is independent on the phases and these are random (random phase approximation),

$$\begin{aligned}\rho(\mathbf{r},\mathbf{r}') &= \int \sum_{j} P(...R_j...R_{j'}...) R_j^2 \psi_j^*(\mathbf{r})\psi_j(\mathbf{r}')d\Omega \\ &= \sum_j \langle R_j^2\rangle \psi_j^*(\mathbf{r})\psi_j(\mathbf{r}').\end{aligned} \tag{1.145}$$

If we further assume that the P-distribution is a symmetric function of the R_j's, $\langle R_j^2\rangle = \langle R^2\rangle$ and then

$$\rho(\mathbf{r},\mathbf{r}') = \sum_j \langle R^2\rangle \psi_j^*(\mathbf{r})\psi_j(\mathbf{r}') \tag{1.146}$$

where a very wide range of P-functions can lead to the above density matrix.

Finally, in order to also extract some useful information about the system of interest, one usually computes its associated reduced density matrix by tracing out over the total density matrix, $\hat{\rho}_t$, over the environment degrees of freedom. In the configuration representation and for an environment constituted by N particles, the system reduced density matrix is obtained after integrating $\hat{\rho}_t \equiv |\Psi\rangle_{t\,t}\langle\Psi|$ over the $3N$ environment degrees of freedom, $\{\mathbf{r}_i\}_{i=1}^N$,

$$\tilde{\rho}(\mathbf{r},\mathbf{r}',t) = \int \langle \mathbf{r},\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_n|\Psi(t)\rangle\langle\Psi(t)|\mathbf{r}',\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_n\rangle\, \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2\cdots\mathrm{d}\mathbf{r}_n. \tag{1.147}$$

The system (reduced) quantum density current can be derived from the following expression

$$\tilde{\mathbf{J}}(\mathbf{r},t) \equiv \frac{\hbar}{m}\,\mathrm{Im}[\nabla_{\mathbf{r}}\tilde{\rho}(\mathbf{r},\mathbf{r}',t)]\Big|_{\mathbf{r}'=\mathbf{r}}, \tag{1.148}$$

which satisfies the continuity equation

$$\dot{\tilde{\rho}} + \nabla\tilde{\mathbf{J}} = 0. \tag{1.149}$$

In (1.149), $\tilde{\rho}$ is the diagonal element (i.e., $\tilde{\rho} \equiv \tilde{\rho}(\mathbf{r},\mathbf{r},t)$) of the reduced density matrix and gives the measured intensity [234].

Taking into account (1.148) and (1.149), it is possible to define the velocity field, $\dot{\mathbf{r}}$, associated with the (reduced) system dynamics as

$$\tilde{\mathbf{J}} = \tilde{\rho}\dot{\mathbf{r}}, \tag{1.150}$$

which is analogous to the Bohmian velocity field. Now, from (1.150), a new class of quantum trajectories is define, which are the solutions to the equation of motion

$$\dot{\mathbf{r}} \equiv \frac{\hbar}{m} \frac{\mathrm{Im}[\nabla_{\mathbf{r}} \tilde{\rho}(\mathbf{r}, \mathbf{r}', t)]}{\mathrm{Re}[\tilde{\rho}(\mathbf{r}, \mathbf{r}', t)]} \Bigg|_{\mathbf{r}'=\mathbf{r}}. \tag{1.151}$$

These new trajectories are the so-called *reduced quantum trajectories* [235, 236], which are only related to the system reduced density matrix. As shown in [235], the dynamics described by (1.151) leads to the correct intensity (whose time-evolution is described by (1.149)) when the statistics of a large number of particles is considered. Moreover, it is also straightforward to show that (1.151) reduces to the well-known expression for the velocity field in Bohmian mechanics when there is no interaction with the environment.

The formalism of the density matrix (or reduced density matrix) is widely used in open quantum systems dynamics through master equations or, in general, when the decoherence process is also taken into account due to the presence of an apparatus [104, 105].

1.4 Dynamical Aspects of the Measuring Process

The idea behind the measuring process is to deal with devices to be considered as quantum systems. This view entails an arbitrary division of the world into classical and quantum parts. As mentioned at the beginning of this chapter, the issue of a dividing line is critical in this context. The equation of motion of Heisenberg is very advantageous because both the classical and quantum equations of motion for a given observable coincide, leading to a better understanding due to the analogy with the classical evolution in time [232]. Here, on the contrary, we are going to briefly discuss the measuring process from a dynamical perspective in the Schrödinger picture of quantum mechanics, more adequate for the Bohmian formalism. In any case, quantum measurements preserve the Heisenberg uncertainty relations (see Chap. 4).

Following von Neumann, let A be the Hermitian operator that is going to be measured and A_n and $\psi_n(\mathbf{x})$ its eigenvalues and eigenfunctions in the configuration space, respectively (for simplicity, a discrete and non-degenerate spectrum is assumed). The wave function of the pointer or apparatus with a large number of coordinates, represented globally by $\mathbf{y}$, is assumed to be described by a wave packet $\chi(\mathbf{y})$. The initial wave function of the composite system is then written as (the state preparation) [7, 10]

$$\Psi_i(\mathbf{x}, \mathbf{y}) = \chi(\mathbf{y}) \sum_n c_n \psi_n(\mathbf{x}). \tag{1.152}$$

If the interaction between the observed system and the pointer is very short, say T (impulsive measurement), and so strong that throughout that time the total Hamiltonian is only governed by the interaction term, the time-dependent Schrödinger equation can be written as

$$i\hbar\frac{\partial\Psi(\mathbf{x},\mathbf{y},t)}{\partial t} = H_I\Psi(\mathbf{x},\mathbf{y},t) = i\hbar\kappa A\frac{\partial\Psi(\mathbf{x},\mathbf{y},t)}{\partial\mathbf{y}} \tag{1.153}$$

which can be easily solved for the period of the interaction to give

$$\Psi(\mathbf{x},\mathbf{y},t) = \sum_n c_n\psi_n(\mathbf{x})\chi(\mathbf{y}-\kappa t A_n) \tag{1.154}$$

where κ is the strength of the coupling. During this period of time, the various components of the total wave function will overlap and interfere being non-factorizable. The total wave function at the end of the impulse is written as

$$\Psi_f(\mathbf{x},\mathbf{y},T) = \sum_n c_n\psi_n(\mathbf{x})\chi(\mathbf{y}-\kappa T A_n) \tag{1.155}$$

consisting of wave packets with centers given by $\kappa T A_n$. Under the condition

$$\kappa T\Delta A_n \gg 1 \tag{1.156}$$

where ΔA_n is the change of A_n for the different values of n, which means that the interaction is strong enough, the wave packets multiplying the different eigenstates of A will be distinct and non-overlapping (in order to prevent any influence on the observed system and extract unambiguous information) and evolve freely lately. In other words, to each wave packet of the pointer there will correspond an eigenfunction and eigenvalue of the system since both are correlated; the corresponding widths being much less than the separation between eigenvalues (complete measurement). Thus, when the wave packets cease to overlap, the interference terms are negligible and

$$|\Psi_f(\mathbf{x},\mathbf{y},T)|^2 \approx \sum_n |c_n|^2|\psi_n(\mathbf{x})|^2|\chi(\mathbf{y}-\kappa T A_n)|^2 \tag{1.157}$$

If the apparatus registers the value $\mathbf{y}$ (the registration step), according to Born's postulate, the total wave function will collapse to one of the many components or products $\psi_n(\mathbf{x})\chi(\mathbf{y}-\kappa T A_n)$, $|c_n|^2$ being the probability of the measurement A_n. A typical example of this type of measurements is given by the well-known Stern–Gerlach experiment where hydrogen atoms pass through an inhomogeneous magnetic field in the z-direction. The interaction Hamiltonian is then given by the gradient of the magnetic field times the z-component of the angular momentum operator. After the interaction, the three wave packets will eventually separate allowing their detection in a screen.

From a Bohmian perspective [7, 10], during the interaction time, the different wave packets strongly interfere and the quantum potential develops a quite complicated and rapidly varying space-time structure. When the interaction is over, the different wave packets or channels start to be well defined and the system will enter one of them, remaining from then on, since the probability of being between wave packets is zero. The rest of the wave packets will not contribute to the quantum potential (or to the guiding condition) acting on the the system and can therefore be ignored. They can be regarded as constituting inactive or physically ineffective information (the so-called empty waves). This fact is behind the possibility of a set of clearly distinct results of a quantum measurement and no mention to the collapse of the wave function is needed. The measuring process can be also considered as a quantum transition, from Ψ_i to one of the final states (or channels) explicitly written in Ψ_f with probability $|c_n|^2$. Therefore, in principle, there is no need to place any arbitrary cut between the quantum and classical worlds. In Chap. 4, this dividing line in the Bohmian formalism will be widely developed.

In Bohmian mechanics, the position of the system plays a key role since it is an intrinsic property. It is intrinsic in a double sense. First, it is defined in a way that is conceptually independent on the wave function or, in other words, it is not inherently dependent on the overall context, unlike the actual momentum of the sytem which depends on the total wave function (in particular, on the gradient of the wave function phase). And second, the position can be measured without being altered. Let us analyze the particular case of $A \equiv x$ when the interaction Hamiltonian is given by

$$H_I = \kappa x p_y. \tag{1.158}$$

Due to the fact that x is a continuous variable, the initial wave function can be written as

$$\Psi_i(x, y) = \int dx' c(x') \delta(x - x') \chi_0(y) \tag{1.159}$$

and the final wave function as

$$\Psi_f(x, y, T) = \int dx' c(x') \delta(x - x') \chi_0(y - \kappa x' T). \tag{1.160}$$

If δy is the width of the wave packet χ_0, the corresponding impulsive measurement will make possible an observable distinction between values of x' differing by $\delta x = \delta y / \kappa T$, the only change being the shifting of the argument of χ_0 (the x position is not altered and the corresponding momentum is also unchanged if χ_0 is assumed to be real). However, other properties are changed due to the fact that the total wave function has been modified.

On the other hand, for measuring properties other than position, the situation is quite different. Let us assume that we want to measure the momentum, that is, $A \equiv p_x$. Following the same procedure as before, the interaction Hamiltonian is written as

$$H_I = \kappa p_x p_y, \tag{1.161}$$

the initial wave function can be written as

$$\Psi_i(x, y) = \int dp_x c(p_x) e^{ip_x x} \chi_0(y), \tag{1.162}$$

and the final wave function as

$$\Psi_f(x, y, T) = \int dp_x c(p_x) e^{ip_x x} \chi_0(y - \kappa pT). \tag{1.163}$$

Again, the corresponding measurement will make possible an observable distinction between values of p_x differing by $\delta p_x = \delta y/\kappa T$ in momentum space and, in position space, $\delta x = 1/\delta p_x$. The wave packets do not interfere because they correspond to non-overlapping states of the apparatus variable. The initial and final true momenta may have different values. The final value depends not only of the total wave function but also on the details of the initial conditions of both the particle and the apparatus. After the standard interpretation of quantum mechanics, this fact can be considered contradictory because $[H_I, p_x] = 0$, so that one would have expected it to be a constant of motion. In Bohmin mechanics, the momentum operator is related to the particle momentum only when the wave function is an eigenfunction (a plane wave) of this operator. As mentioned before, this also means that the momentum is not an intrinsic property unlike the position. It is inherently context dependent so that it involves the participation of the measuring apparatus and the quantum system as a whole. This fact implies that the mean value of p^2, for example, has an extra term with respect to the standard result of quantum mechanics [7, 10]. The same is true for higher moments of the momentum.

The next straightforward question is what happens when trying to measure position and momentum together. The interaction Hamiltonian is now written as

$$H_I = \kappa(xp_y + p_x p_z), \tag{1.164}$$

where y and z are the coordinates of two independent meters corresponding to commuting operators. After the impulsive interaction, the three interacting systems become evidently correlated. As may be expected, the outcome of the joint measurement does not allow one to infer values for the particle position or momentum [7].

This theoretical treatment should be changed when noncanonical physical observables are considered such as velocity and other time derivatives of canonical observables [232].

In Chap. 4, the measurement problem is studied under a different and new point of view. The so-called continuous quantum measurement on a given system surrounded by an environment is tackled from a nonlinear wave equation.

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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.

A.B. Nassar and S. Miret-Artés, *Bohmian Mechanics, Open Quantum Systems and Continuous Measurements*, DOI 10.1007/978-3-319-53653-8_2

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

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

there exists a time-dependent invariant

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

provided that

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

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

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

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

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

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

$$i\hbar\left[\frac{\partial\phi}{\partial t} + \frac{i}{\hbar}\frac{\partial S}{\partial t}\phi\right] =$$

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

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

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

and

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

with the following definitions for the quantum hydrodynamical density

$$\rho(x,t) = \phi^2(x,t), \tag{2.8}$$

the velocity

$$v = \frac{1}{m}\frac{\partial S}{\partial x}, \tag{2.9}$$

the quantum potential

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

and the interaction potential

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

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, $\rho(x, 0) = \left[2\pi\delta^2(0)\right]^{-1/2} \exp\left[-x^2/2\delta^2(0)\right]$ then ρ vanishes for $|x| \to \infty$ at any time and we may rewrite

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

$\delta(t)$ 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

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

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

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

and

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

which implies that

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

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

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

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 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

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

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

where

$$U = \rho\left(\frac{1}{2}mv^2 + V + Q\right), \tag{2.20}$$

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

$$J = \rho v \tag{2.22}$$

and

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

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]

$$\delta(0) = \delta_0\ ,\ \dot{\delta}(0) = \mathrm{d}_0, \tag{2.24}$$

and

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

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

$$\delta(t) = r(\theta)\ \alpha(t) \tag{2.26}$$

where we define [13]

$$d\theta = dt/\alpha^2(t) \tag{2.27}$$

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

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

provided that

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

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

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

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,

$$\alpha_1(t) \equiv \alpha(t) \tag{2.31}$$

and

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

If initial conditions are imposed as follows

$$\alpha(0) = 1 \; and \; \dot{\alpha}(0) = 0 \tag{2.33}$$

we are led to

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

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

$$I_1 = d_0^2 + (\delta_0^2/\tau^2), \tag{2.35}$$

and

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

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

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

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

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

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

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

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 *ith* particle of the ensemble with an initial position x_{oi} can be calculated via Eq. (2.16)

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

or

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

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

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

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]

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

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

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

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

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

and

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

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

$$\psi_2(x,t) = \sqrt{\rho_2}\exp(iS_2/\hbar) \tag{2.50}$$

where

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

and

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

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

$$\psi_3(x,t) = \sqrt{\rho_3}\exp(iS_3/\hbar), \tag{2.53}$$

where

$$\rho_3 = b \tag{2.54}$$

and

$$S_3/\hbar = -\omega t + kx + \beta, \tag{2.55}$$

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

$$\rho_1(0) = \rho_2(0), \tag{2.56}$$

$$\rho_2(L) = \rho_3(L), \tag{2.57}$$

$$\rho_1'(0) = \rho_2'(0), \tag{2.58}$$

$$\rho_2'(L) = \rho_3'(L), \tag{2.59}$$

$$\rho_1(0)v_1(0) = \rho_2(0)v_2(0), \tag{2.60}$$

$$\rho_2(L)v_2(L) = \rho_3(L)v_3(L), \tag{2.61}$$

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

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

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

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

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

$$2ak\sin\alpha = (c^2 - b^2), \tag{2.66}$$

$$c = de^{-2\bar{q}L}, \tag{2.67}$$

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

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

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

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

which combined to Eq. (2.69) yields

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

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

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

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

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

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

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

Equations (2.68) and (2.69) imply that

$$a^2 = 1 - b^2 \tag{2.76}$$

which inserted into Eq. (2.75) gives

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

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

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

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

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

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

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

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

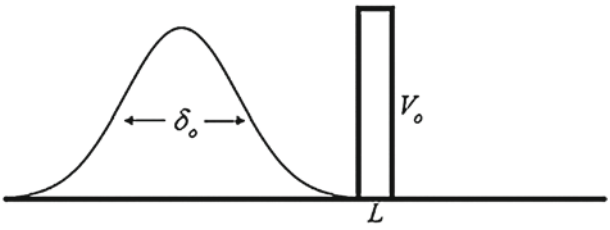

Fig. 2.1 Gaussian wave packet prior to the tunneling through a rectangular potential barrier

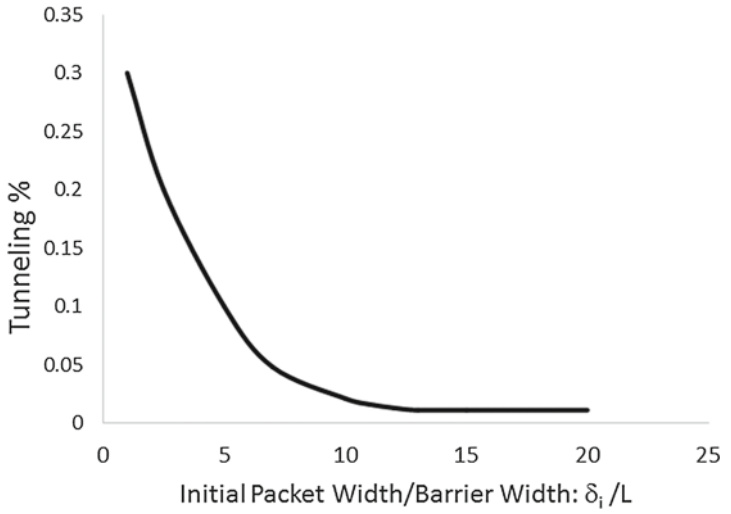

Fig. 2.2 Tunneling versus initial wave packet width

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

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

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

$$\psi(x,t) = \phi(x) \exp\left(i\left[S(x) - Et\right]/\hbar\right) \tag{2.82}$$

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

$$\phi'(x)S'(x) + S''(x)\phi(x) = 0, \tag{2.83}$$

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

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

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

Integration of Eq. (2.83) implies that

$$\rho(x)S'(x) = I_1, \tag{2.86}$$

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

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

we have

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

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

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

or

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

provided that α obeys

$$\alpha''(x) + \lambda^2(x)\alpha(x) = 0. \tag{2.91}$$

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

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

where

$$\alpha_1(x) \equiv \alpha(x) \tag{2.93}$$

and

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

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

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

and

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

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

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

such that we obtain after some manipulations

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

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

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

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

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

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

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

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

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

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

at $x = L$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where

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

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

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

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

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

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

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]

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

and

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

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

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

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

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

where

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

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

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

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

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

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

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

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

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

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v\frac{\partial}{\partial x} \tag{2.127}$$

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

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

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

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

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 $[x - q(t)]^1$

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

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

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

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

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

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

where 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

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

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

and

$$S_0(0) = mv_0x_0. \tag{2.138}$$

Now, the wave packet can be fully written as

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

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

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

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

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

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 Schr̈odinger 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 $x(t)$

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

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 *ith* 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

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

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

and

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

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

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

where

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

By performing the phase change

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

Equation (2.155) reduces further to

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

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

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

where

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

and

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

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

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

$$f_1=\frac{1}{2}m\left[\dot{\delta}^2q^2+\delta^2\dot{q}^2-2q\dot{q}\delta\dot{\delta}\right]. \tag{2.164}$$

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

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

and

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

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

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

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

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

or

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

which upon integration becomes

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

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,

$$\delta_1(t)\equiv\delta(t) \tag{2.171}$$

and

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

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]

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

can be described by a Gaussian wave packet

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

where

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

the complex time dependent spreading is

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

where

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

$$q(t) = q(0) + vt \tag{2.178}$$

and

$$E = \frac{1}{2}mv^2. \tag{2.179}$$

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

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

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]

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

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

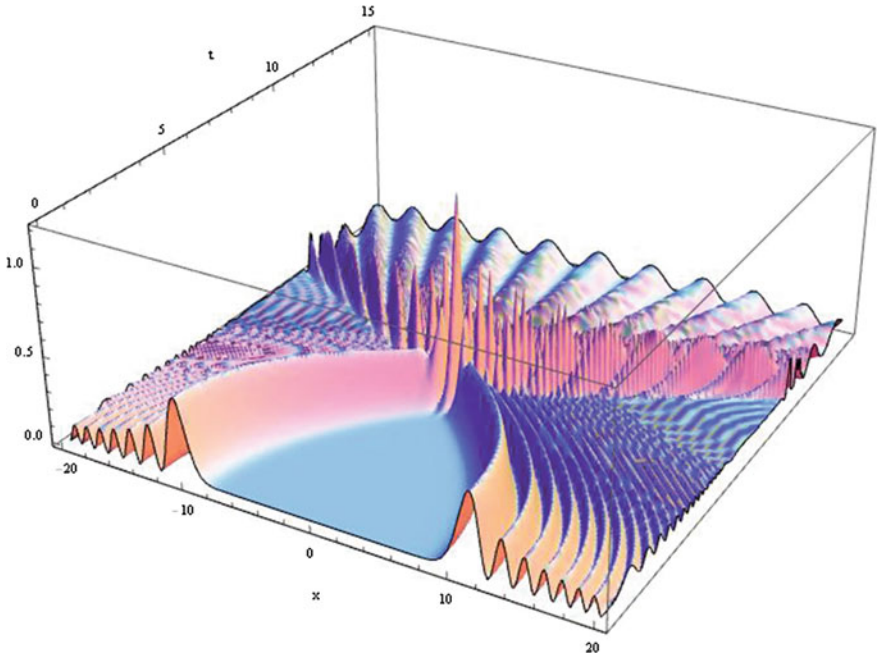

Fig. 2.3 Interference of two initially, widely separated Airy wave packets

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

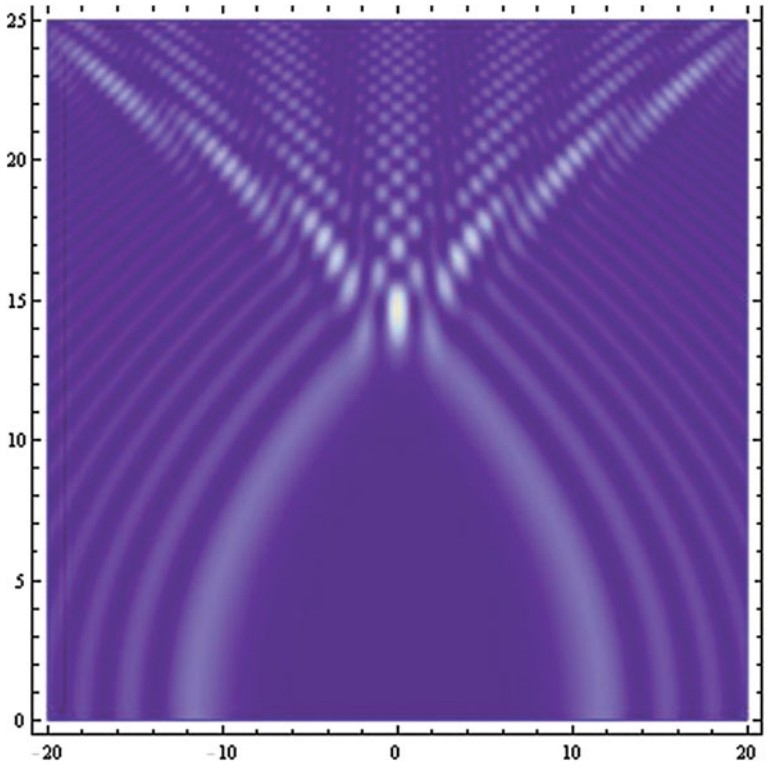

Fig. 2.4 Density plot of the interference of two initially, widely separated Airy wave packets: Quantum focal point

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 threefold: (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

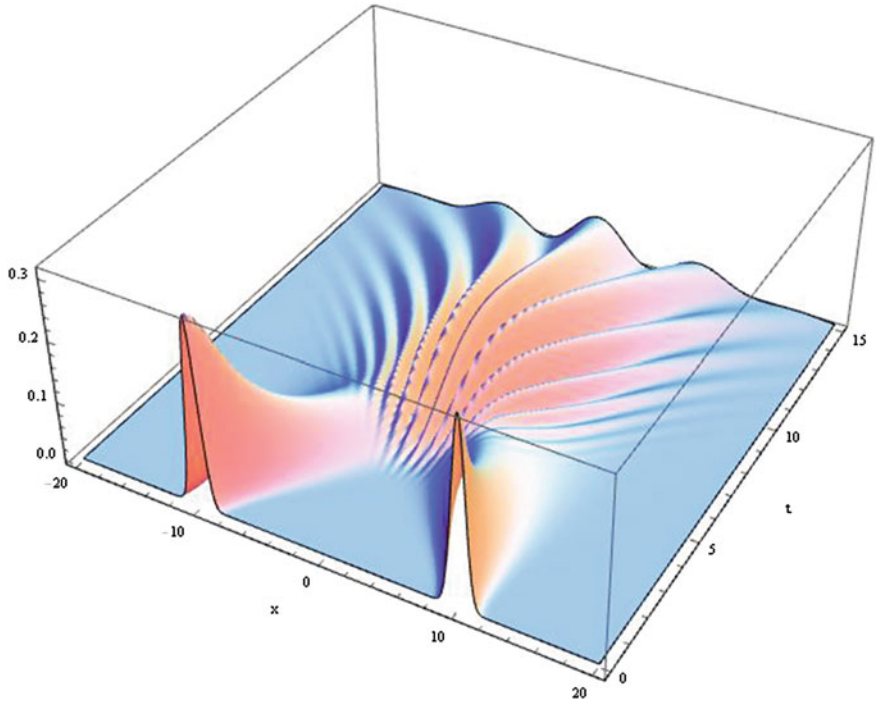

Fig. 2.5 Interference of two initially, widely separated Gaussian wave packets

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 $B = \left(2m_i m_g g\right)^{1/3}$. 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 $\psi(x, t)$

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

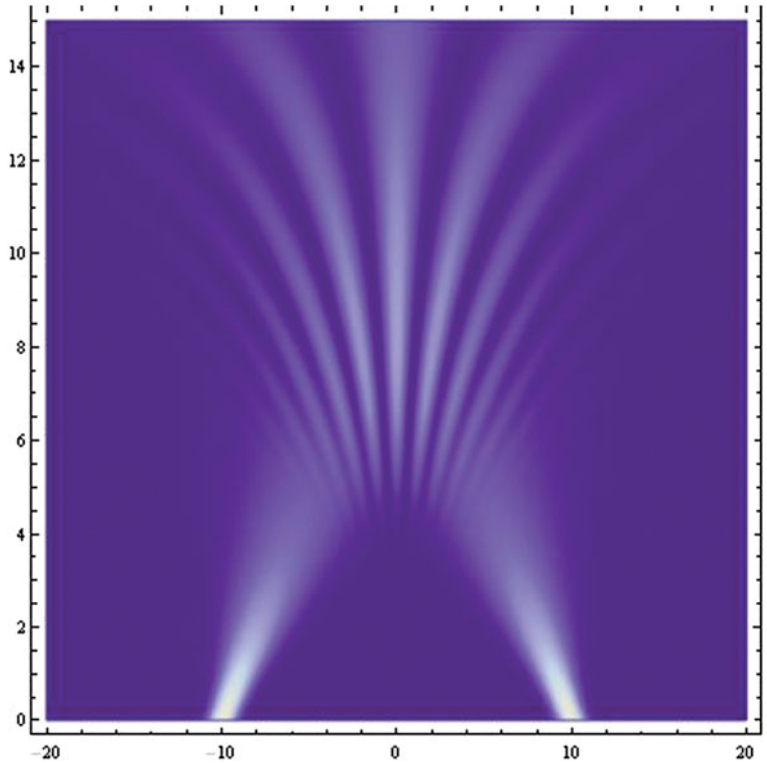

Fig. 2.6 Density plot of the interference of two initially, widely separated Gaussian wave packets: Quantum focal point

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

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

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

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

$$x' = x - q(t), \tag{2.185}$$

and

$$t' = t. \tag{2.186}$$

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

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

where

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

By performing the phase change

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

Equation (2.187) reduces further to

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

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

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

with

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

and

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

Now, the Bohmian trajectories are found to be

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

Thus, we can summarize our main results as follows

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

and

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

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

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

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 $-m_g gx$ 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 *ith* particle of the wave packet ensemble with an initial position x_{0i}. In general, the Bohmian trajectories imply mass-dependent differences in motion, except when the well-known Berry-Balazs constant B is given by $B = \left(2m_i m_g g\right)^{1/3}$. For atoms from a condensate ^{87}Rb [62, 63] this quantity can be related to an inverse scale related to the wave number $k \approx 3.3 \times 10^6\,\mathrm{m}^{-1}$ (k has the same physical units as the familiar wave vector of a plane wave) [54–61, 63–67].

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

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

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

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

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

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

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

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

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

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

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 $S = constant$

$$\oint_C dS = \oint_C \mathbf{p}.d\mathbf{r} + \frac{e}{c}\oint_C \mathbf{A}.d\mathbf{r} = n\hbar \tag{2.203}$$

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

$$\Phi = \int_S \mathbf{B}.d\mathbf{S} = \oint_C \mathbf{A}.d\mathbf{r} \tag{2.204}$$

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

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

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

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

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 funtion 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, $\varphi_{tot} = arg[(\psi(t_1), \psi(t_2)]$, 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]

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

Therefore, the geometric phase is then written as

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

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

$$\varphi_g = \frac{1}{\hbar}\oint_C \mathbf{p}.d\mathbf{r}. \tag{2.209}$$

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]

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

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

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

$$\times\,exp\left[\frac{i\,m\,v}{\hbar}\,(x\;-\;x_o\;-\;v'\,t)\right]. \tag{2.212}$$

where

$$k\;=\;\frac{m\,G}{2\,\hbar^2} \tag{2.213}$$

and

$$v'\;=\;\frac{V_\epsilon\;+\;m\,v^2/2\;-\;\hbar^2\,k^2/2}{m\,v}\,. \tag{2.214}$$

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

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

and

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\dot{X} = \frac{\partial H}{\partial P}, \qquad \dot{P} = -\frac{\partial H}{\partial X}. \tag{2.229}$$

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

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

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

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

leading to the generalized, dissipative Schrödinger equation

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

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

$$\frac{\partial \rho}{\partial t} + \nabla_x J = 0, \tag{2.233}$$

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

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

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

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

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

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]

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

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

$$f_0 = \frac{i\hbar}{4}\,\ln\left[\frac{\pi\hbar}{2\mathrm{Im}\{\alpha_0\}}\right], \tag{2.238}$$

with $\mathrm{Im}\{\alpha_0\} \neq 0$. 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.,

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

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

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

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

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

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

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.,

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

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

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

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

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

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

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 $\hbar \to 0$, but that the wave packet remains relatively localized (i.e., $1/\mathrm{Re}\{\alpha_t\} \to 0$), in agreement with the hypothesis of Ehrenfest's theorem. Furthermore, if $\mathrm{Im}\{\alpha_t\} \to 0$ 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 $\mathrm{Re}\{\alpha_t\}$.

2.12.1 Free Gaussian Wave Packet

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

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

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

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

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

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

$$p_t = p_0 e^{-\gamma t}, \tag{2.250}$$

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

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

where

$$S_{\mathrm{cl},t} = \int_0^t L_{t'}\, dt' \tag{2.253}$$

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

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

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,

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

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

$$\tau = \frac{1 - e^{-\gamma t}}{\gamma} \tag{2.256}$$

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

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

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

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

is its spreading along time, with $\tilde{\sigma}_t^0 = \sigma_0\left[1 + (i\hbar t/2m\sigma_0^2)\right]$. However, with friction, the wave packet undergoes asymptotically (i.e., for $t \to \infty$) 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

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

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

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

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

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

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 $\hbar \to 0$.

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

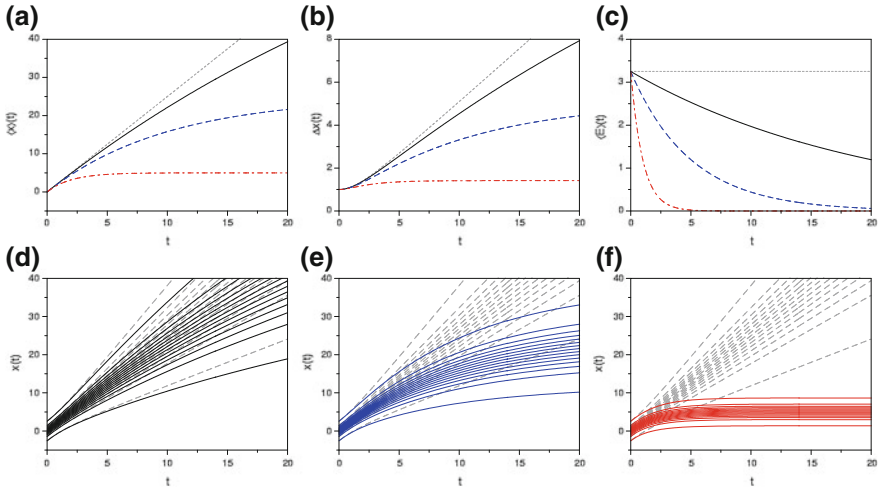

Fig. 2.7 *Top* Average position (**a**), dispersion (**b**), and energy (**c**) for a Gaussian wave packet in free space affected by friction. Different values for the friction coefficient have been considered: $\gamma = 0.025$ (*black solid line*), $\gamma = 0.1$ (*blue dashed line*), and $\gamma = 0.5$ (*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

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

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,

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

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]

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

where $\dot{x}_i$ refers to the equation of motion for the ith 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 ith 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

$$\begin{aligned}
\dot{x} &= \frac{\rho_1}{\rho}\left[\frac{p_{t,1}}{m} + \frac{2\mathrm{Re}\{\alpha_t\}}{m}\,(x - x_0)e^{-\gamma t}\right] + \frac{\rho_2}{\rho}\left[\frac{p_{t,2}}{m} + \frac{2\mathrm{Re}\{\alpha_t\}}{m}\,(x + x_0)e^{-\gamma t}\right] \\
&+ 2\cos\xi_{12}\,\frac{\sqrt{\rho_1\rho_2}}{\rho}\left[\frac{p_{t,1} + p_{t,2}}{2m} + \frac{2\mathrm{Re}\{\alpha_t\}}{m}\,xe^{-\gamma t}\right] \\
&+ 2\sin\xi_{12}\,\frac{\sqrt{\rho_1\rho_2}}{\rho}\left[\frac{2\mathrm{Im}\{\alpha_t\}}{m}\,x_0e^{-\gamma t}\right].
\end{aligned} \tag{2.265}$$

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

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

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

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

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

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)).

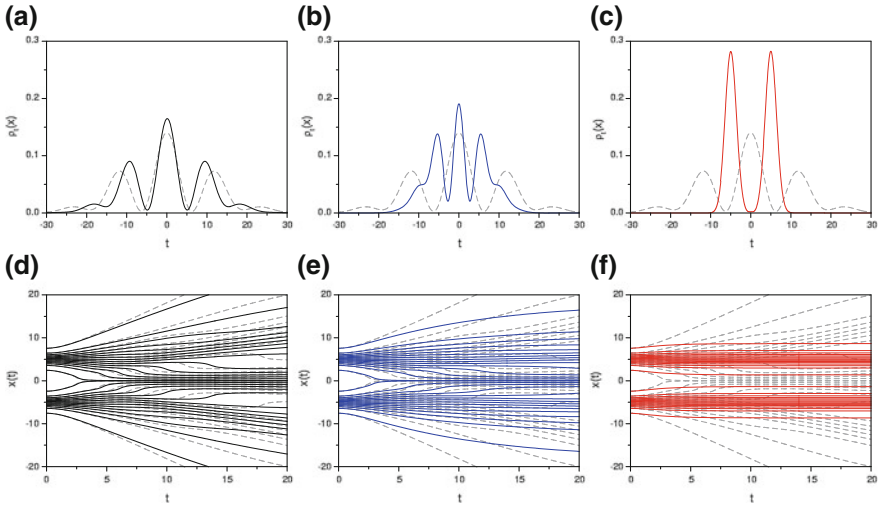

Fig. 2.8 *Top* Final probability density (at $t = 20$) for a coherent superposition of two Gaussian wave packets in free space affected by friction. The same friction values as in Fig. 2.7 have been considered: **a** $\gamma = 0.025$ (*black solid line*), **b** $\gamma = 0.1$ (*blue solid line*), and **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 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

The frictionless limit $\gamma \to 0$ 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

$$x_{t\to\infty} = x_0 + \frac{p_0}{m\gamma} - \frac{a}{\gamma^2} + \frac{a}{\gamma}\,t. \tag{2.269}$$

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

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

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

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

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

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

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],

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

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

$$\dot{x} = -\frac{\gamma}{2}\, x, \tag{2.274}$$

which after integration renders

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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

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

which does not contain exponential terms, and where

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

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

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

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

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

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

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

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 $\gamma \to 0$ the chosen solution has to approach the non-dissipative value, i.e., $\alpha_t \to im\omega_0/2$, which only happens if $g_0 = g_+$. Therefore, we have that

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

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

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

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

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

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

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

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

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

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

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

which is a pure real function. Thus,

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

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

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

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

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

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,

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

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,

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

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

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

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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Chapter 3
Bohmian Stochastic Trajectories

Abstract In the last decades, many nonlinear extensions of the Schrödinger equation have been proposed in literature either to explore the fundamental aspects of quantum mechanics, with the usual linear theory representing only a limiting case, or to describe open quantum systems. For the description of nonconservative quantum systems, Kostin formulated in an heuristic way the so-called Schrödinger–Langevin (SL) equation or Kostin equation, for the Brownian motion. This equation has been subsequently rederived, improved and extended for its use in numerous applications, mainly without including the noise term. Numerous features of this SL equation can be better revealed within the framework of de Broglie–Bohm (quantum hydrodynamical trajectory formulation) of quantum mechanics. Within this formalism, several dissipative problems are presented and discussed: the Ramsauer–Townsend effect, the tunneling dynamics through a barrier, the plasma fluid formulation and the Lorentz–Abraham (extended electron) equation for a point-charge electron. These two last examples are also discussed in order to see the correspondence between classical and quantum dynamics. Very few applications of this SL equation are devoted to stochastic problems in the literature where the noise term needs to be included. The so-called Bohmian–Brownian motion is introduced in the context of surface diffusion with single adsorbates. An extension to interacting adsorbates is discussed within a simple, phenomenological model. Interestingly enough, this study leads us to quantum anomalous diffusion. The harmonic motion is also briefly considered in order to compare with the same open dynamics under the presence of a continuous quantum measurement (Chap. 4). Finally, a generalization of the SL equation is proposed for nonlinear dissipation.

3.1 Introduction

The study of open quantum systems constitutes a very broad and active field of research within quantum mechanics. As it is well known, strictly speaking, real physical systems do not exist in complete isolation in Nature. All physical systems are open systems since the interaction with their environment can never be totally neglected. The energy transfer from the system to the environment is termed quantum

A.B. Nassar and S. Miret-Artés, *Bohmian Mechanics, Open Quantum Systems and Continuous Measurements*, DOI 10.1007/978-3-319-53653-8_3

relaxation or *damping*. If there is no chance for the energy to move backwards into the system, the unidirectional energy flow into the reservoir is then called quantum *dissipation*. On short timescales, the distinction between quantum relaxation and dissipation is obviously unclear. Only when the environment has a small number of degrees of freedom, the energy moves backwards into the system; this phenomenon is called a *recurrence* This interaction also gives rise to a strong quantum correlation or *entanglement* between the system and environment which eventually leads the former to become a statistical mixture (decoherence). The so-called theory of open quantum systems [1–5] encompasses a series of formalisms and approaches developed to deal with the corresponding quantum dynamics. This line of research can be considered as an interdisciplinary field, where very broad branches of physics, chemistry and biology meet together to describe processes that are ubiquitous in nature [1–3, 6–8]. Nevertheless, finding good quantum analogues of classical dissipative systems constitutes a very difficult task and it still remains an important topic because of some problems such as, for example, commutation rules, time ordering and symmetrization can not be neglected in the quantum world.

Irreversible quantum processes take place when dealing with extended systems as environments or, more precisely, with systems displaying an infinite number of degrees of freedom (photon or phonon fields, for example). Quantum noise has its origin in our inability to specify each of all the infinite modes of a given field when considering an environment around a system; noise appears when the reaction of the field back on the system is not neglected. Under certain conditions the duration of the reservoir correlations is very short compared to the dynamical evolution of the system. This leads to a total memory loss of the bath dynamics that gives rise to a subsequent irreversible loss of coherence and energy (or population) relaxation in the system. This is called a *Markovian regime*. Within this regime, the time-evolution of the system does only depend on the present state of the system; this is called a *Markovian process*. As will be seen, when this happens, the system dynamics can be characterized by (relatively) simple Markovian master equations, where one does not need to take into account the reservoir dynamics and its effects on the system are described by means of certain operators. Quantum stochastic methods in the Markovian and non-Markovian regimes have been widely developed in quantum optics [7]. In particular, the non-Markovian dynamics of open quantum systems is being developed very fast in the last years. It has been finally established that there is no quantum Onsager regression theorem and the correct generalization of the Onsager hypothesis is the fluctuation-dissipation theorem [9].

In analogy to open classical systems, three main different approaches to deal with quantum dissipative/stochastic dynamics can also be considered here. First, effective

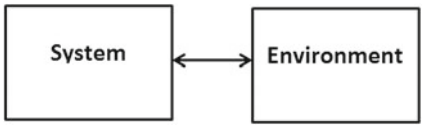

Fig. 3.1 Schematic view of the coupling of a system surrounded by its environment

time-dependent Hamiltonians. The Caldirola–Kanai model is a good example which has been developed shortly in Chap. 2. Second, the system–plus–environment model Hamiltonian where a schematic view is displayed in Fig. 3.1. The whole system (physical system and environment or thermal bath) is considered as an isolated system [2, 3]. Both system and reservoir are in continuous interaction and the effects —quantum coherence loss or decoherence, population transfer, and/or (system–environment) energy exchange— arising from that interaction will depend to a greater or a lesser extent on the coupling strength and its intrinsic nature. Under these conditions, one speaks about the environment induced decoherence. An interesting and very important process is vibrational dephasing of small molecules immersed in a rare gas in liquid phase [10–15]. Fluctuations occur because of random collision events. Due to its interaction with the environment, the system usually behaves quite different with respect to its behavior in isolation. Its time-evolution is not unitary and therefore cannot be described in terms of the Schrödinger equation. However, the powerful standard quantum-mechanical theoretical formalisms developed are at our complete disposal. Dissipation can be described following one of the three standard pictures of quantum mechanics: Schrödinger, Heisenberg, Dirac (interaction). In the first and third pictures, one always tries to find master equations that account for the time-evolution of the so-called reduced system, where the bath degrees of freedom have been traced out. As has been mentioned previously, among this type of equations of motion, the simplest class is that of Markovian character where one assumes that the bath has no memory and the time-evolution of the reduced density matrix depends only on its present time. The Lindblad equation plays a fundamental role in this context. On the contrary, non-Markovian approaches lead to a loss of analytical and conceptual simplicity as well as larger computational times. An alternative way to the density matrix formalism also comes from the path integral formulation of quantum mechanics (fourth picture of quantum mechanics). Many efforts are being addressed along this way with also great success. If the Heisenberg picture is followed, the quantum (generalized or standard) Langevin equation is reached (needless to say that all formulations are equivalent). Essentially, this procedure consists of replacing the reservoir by damping terms in the Heisenberg equations of motion of a conservative system and then adding random forces as driving terms that give rise to fluctuations over the system. These stochastic quantum formalisms are being addressed to more and more complex systems. Finally, if the wave function or vector state is considered as a stochastic process in Hilbert space, the corresponding formulation is given in terms of a time-dependent density functional, the dynamics being described no longer by a master equation but by the Itô stochastic differential equation. The realizations of the underlying stochastic processes are also called quantum trajectories, which have not to be confused with the same denomination used in Bohmian mechanics [4, 5]. And third, nonlinear Hamiltonians. Nonlinear wave mechanics has been sought since the inception of the original linear Schrödinger equation. It constitutes one among the most investigated topics in quantum mechanics. These generalizations emerge from the study of important phenomena occurring in condensed matter physics, for instance, in the propagation of light pulse in an optical fiber and propagation in a nonlinear birefringent medium. Among the many

nonlinear variants of Schrödinger equations proposed in literature [16–25], some of them are applied in order to save the superposition principle of the linear quantum mechanics, or propose the introduction of homogeneous nonlinear terms in order to save, only partially, the superposition principle. The problem of experimental verification has also been studied [26, 27] – and the parameter that defines the coupling constant for nonlinear perturbations of the Schrödinger equation has been estimated. The main problem in applications of results obtained for evaluating the coupling constant is that research in the conventional nonlinear wave mechanics has been mainly concentrated on the equation with log-nonlinearity. As we show in what follows, the conceptual understanding of these equations can be better suited in the framework of Bohmian mechanics and some correspondence between classical and quantum quantities can be carried out [21–24]. The Feynman propagator for eight nonlinear Schrödinger equations within this context have recently been analyzed [28]. Many nonlinear equations have soliton solutions characterized by widths which do not spread in time; in particular, as has been mentioned in Chap. 2, when dealing with the Gross–Pitaevskii equation (see Sect. 2.11). Optical solitons are thought to be very important in optical transmission systems since the soliton pulse can maintain its wave form over long distances. Finally, we should also mention that when considering the measuring process (see Chap. 4), nonlinear equations also play an important role. In any case, without and with the presence of a measurement, the perspective of an open dynamics has to be kept in mind. However, the causal stochastic approach described in Chap. 1, Sect. 1.3.1, is not going to be followed from now on.

In this Chapter, dissipation and stochasticity are discussed within the fifth picture of quantum mechanics due to de Broglie and Bohm (as mentioned in the Preface). Section 3.2 is devoted to the introduction of the so-called nonlinear Schrödinger–Langevin (SL) or Kostin equation for a Brownian particle. This equation has been subsequently rederived, improved and extended for its use in numerous applications, mainly without including the noise term. In Sect. 3.3, this SL equation is derived within the Bohmian formalism, the SLB equation. In this hydrodynamical framework, a Gaussian probability density is considered for potentials up to second order in a Taylor expansion. In particular, for a harmonic potential, the so-called Pinney equation but with an additional friction term is finally obtained for its time spreading. In Sect. 3.4, the Ramsauer–Townsend effect in a dissipative medium is studied and analyzed in very detail by means of the SL and SLB equations. This effect tells us that under certain incident conditions for energy and a given width of the well depth, the reflection coefficient is totally suppressed. Section 3.5 presents the tunneling dynamics through a dissipative barrier. In the next two sections, Sects. 3.6 and 3.7, the plasma fluid formulation and the Lorentz–Abraham equation for a point-charge electron within Bohmian mechanics are also discussed in order see the correspondence between classical and quantum dynamics. Very few applications of this SL equation are devoted to stochastic problems in the literature where the noise term needs to be included. In Sect. 3.8, the so-called Bohmian–Brownian motion is introduced in the context of surface diffusion with single adsorbates. An extension to

interacting adsorbates is discussed within a simple, phenomenological model. Interestingly enough, this study leads us to quantum anomalous diffusion. The harmonic motion is also considered in order to compare with the same open dynamics under the presence of a continuous quantum measurement (Chap. 4). Finally, Sect. 3.9 is devoted to present and discuss a generalization of the SL equation for nonlinear dissipation.

3.2 The Schrödinger–Langevin Equation

In the sixties, Senitzky [29] and Ford et al. [30] showed that a system of coupled harmonic oscillators could model a heat bath. The corresponding Brownian motion was then studied both classically and quantum-mechanically. The corresponding Langevin equation was obtained as a result of reducing the dimensionality of the full problem by tracing out over the bath variables. The heat bath was thus only described by two parameters: the friction coefficient and the temperature through a random force. This random force was shown to be a Gaussian stochastic process. The variables in the quantum Langevin equation were assumed to be operators with order preserved according to the Heisenberg picture. Different orderings are available, such as the symmetric rule, Weyl's rule, etc., in order to construct Hermitian operators. The normal product of the random force was shown to be a Gaussian process, but not Markovian. This point is critical when compared to the classical counterpart. For an Ohmic or constant friction coefficient, the classical Gaussian process is also Markovian. The denomination of Ohmic friction comes from the fact that for a constant field of force F, the average value of the momentum reads like Ohm's law from the Langevin equation, i.e., $\langle p\rangle = \lambda^{-1}F$, where the current described by $\langle p\rangle$ is proportional to the field applied, F, and proportionally inverse to the resistance or friction coefficient.

Kostin [16, 17] derived heuristically the so-called Schrödinger–Langevin (SL) equation for a Brownian particle of mass m subject to an external potential V and interacting with a thermal bath from the corresponding quantum Langevin equation written as

$$m\ddot{\mathbf{r}} = -\gamma\dot{\mathbf{r}} + \mathbf{F}_r(t) + \nabla V(\mathbf{r}) \tag{3.1}$$

where the time random force $\mathbf{F}_r$ is assumed to arise from a random potential linearly dependent on the particle position, V_r. In three dimensions, this equation reads as

$$i\hbar\,\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + \left[V(\mathbf{r}) + V_r(\mathbf{r},t) + V_D(\mathbf{r},t) + G(t)\right]\Psi(\mathbf{r},t), \tag{3.2}$$

where γ is the friction coefficient. The random potential is given by

$$V_r(\mathbf{r},t) = -\mathbf{r}.\mathbf{F}_r(t), \tag{3.3}$$

the so-called damping potential by

$$V_D(\mathbf{r},t) = -\frac{i\hbar\gamma}{2}\ln\left(\frac{\Psi(\mathbf{r},t)}{\Psi^*(\mathbf{r},t)}\right) \tag{3.4}$$

and

$$G(t) = \frac{i\hbar\gamma}{2}\int \Psi^*(\mathbf{r},t)\ln\left(\frac{\Psi(\mathbf{r},t)}{\Psi^*(\mathbf{r},t)}\right)\Psi(\mathbf{r},t)d\mathbf{r} \tag{3.5}$$

is a time dependent function resulting from the average value of V_D by integration with respect to the position variable. It is easy to show that the norm of the corresponding wave function is conserved and the expectation value of the corresponding nonlinear Hamiltonian is, as usual, the sum of the kinetic and potential energies at any time. The rate of change in energy along time is given by $-\gamma\langle p^2\rangle/m$. This $G(t)$ function can be removed from Eq. (3.2) by introducing the transformation

$$\Psi(\mathbf{r},t) = e^{if(t)}\phi(\mathbf{r},t) \tag{3.6}$$

leading to

$$i\hbar\frac{\partial\phi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r},t) + \left[V(\mathbf{r}) + V_r(\mathbf{r},t) + \frac{i\hbar\gamma}{2}\ln\left(\frac{\phi(\mathbf{r},t)}{\phi^*(\mathbf{r},t)}\right)\right]\phi(\mathbf{r},t), \tag{3.7}$$

the $f(t)$ function being given by

$$f(t) = -\hbar^{-1}e^{-\gamma t}\int_0^t e^{\gamma s}G(s)ds. \tag{3.8}$$

The motion of a Brownian particle is strictly described by the nonlinear equation (3.7) when $V = 0$. It is easy to show that with the new transformation

$$\phi(\mathbf{r},t) = e^{iS(\mathbf{r},t)/\hbar} \tag{3.9}$$

and looking for solutions of the type given by

$$S(\mathbf{r},t) = \mathbf{r}.\mathbf{p}(t) + c(t) \tag{3.10}$$

the corresponding quantum Langevin equation is again obtained, the solution being

$$\mathbf{p}(t) = \mathbf{p}(0)e^{-\gamma t} + e^{-\gamma t}\int_0^t F_r(s)e^{\gamma s}ds. \tag{3.11}$$

where the time-dependent function $c(t)$ is given by

$$c(t) = c(0)e^{-\gamma t} - \frac{1}{2m}e^{-\gamma t}\int_0^t |\mathbf{p}(s)|^2 e^{\gamma s}ds. \tag{3.12}$$

We should emphasize that because of the nonlinearity of the SL equation, the superposition principle does not hold. Even more, the general solution of the corresponding equation can not be found and the uniqueness of the solution obtained can not be ascertained. The nonlinear SL wave equation has been received special attention and applied to several problems such as, for example, the damped harmonic oscillator and the motion of a charged particle in the presence of damping while it is moving in an external electromagnetic field [8]. It is also true that some drawbacks are also present when dealing with this equation. For example, the solutions for a damped harmonic oscillator contain the undamped frequency instead of the reduced or renormalized frequency (see below). The analysis of the solutions of the SL equation has been carried out usually without considering the stochastic term, analytically and numerically [8, 31]. For a free particle represented by a plane wave, the SL equation and the corresponding quantum Langevin equation lead to the same solution. However, Messer [32] has studied the evolution of a Gaussian wave function in the free and harmonic potentials and shown that both equations are not strictly equivalent. Very recently, the thermal relaxation given by the SL has been analyzed with white and colored noises (see also Ref. [33]) for an harmonic oscillator [31].

Another heuristic derivation of the equation governing the probability density evolution for the Brownian motion is due to Tsekov [34–36]. In terms of the probability density, the theory becomes nonlinear. Furthermore, the corresponding equations were completed by taking into account thermodynamical functions. A similar Kostin frictional term is found. This procedure is quite similar to that developed in the next section within the Bohmian formalism.

On the other hand, Hasse [37] showed that Kostin's Hamiltonian is a special case of a more general nonlinear Hamiltonian,

$$H = T + V + \gamma W, \tag{3.13}$$

where T and V are the usual kinetic and potential energy operators, and W satisfies the requirements: (i) $\langle W\rangle = 0$ and (ii) $\langle p\rangle = \partial W/\partial q$ according to Ehrenfest's theorem. The second requirement can also be fulfilled for a number of different W operators. For example, Süssmann's Hamiltonian [4] is a special case, originally found by this author in a completely empirical way when studying the force-free motion of wave packets traveling along classical damped paths. W can also be expressed as

$$W = \int_0^q \dot{q}^n dq, \tag{3.14}$$

which, with the usual quantization rule for the momentum, becomes a differential operator of order n. The corresponding Hamiltonian is, in general, complex and non-Hermitian. For linear damping ($n = 1$), the interaction potential becomes complex. This potential, called the *optical potential*, is in general nonlocal and has been widely used in atomic and nuclear physics (for example, in Feshbach's theory). Velocity dependent interactions have also been introduced in nuclear scattering and band theory of solids.

Several alternatives routes to derive the SL or Kostin equation can also be found in the literature (see, for example, Ref. [38]). For nonrandom potentials, the method of Pauli can be used to find the damping potential of the Schrödinger equation which makes the quantum analog of the corresponding classical equations. One can also follow the so-called Schrödinger's procedure to generate a nonlinear wave equation. Without loss of generality, for one dimension, the Hamilton–Jacobi equation for the action S and momentum $p = \partial S/\partial x$ is

$$\frac{\partial S}{\partial t} + H(x, \partial S/\partial x, t) = 0. \tag{3.15}$$

By introducing the wave function Ψ through the relation

$$S(x, t) = -i\hbar \ln \Psi(x, t), \tag{3.16}$$

the continuity equation for $\rho = \Psi^*\Psi$ reads as

$$\frac{\partial \rho}{\partial t} + \frac{1}{m} \nabla (\rho \, \mathrm{Re}\{p\}) = 0, \tag{3.17}$$

where $\mathrm{Re}\{p\}$ stands for the real part of p, which is in general a complex quantity if Ψ is complex, such that

$$\begin{aligned} \mathrm{Re}\{p\} &= -\frac{i\hbar}{2m} \frac{\partial \ln (\Psi/\Psi^*)}{\partial x}, \\ \mathrm{Im}\{p\} &= -\frac{i\hbar}{2m} \frac{\partial \ln \rho}{\partial x}, \end{aligned} \tag{3.18a}$$

with the mean value of the imaginary part always vanishing. Thus, the expression for p does again fulfill Hasse's second requirement. The so-called Kostin *energy dissipation operator* can then be expressed as

$$W = -\frac{i\hbar\gamma}{2} \left[\ln \left(\frac{\Psi}{\Psi^*} \right) - \left\langle \ln \left(\frac{\Psi}{\Psi^*} \right) \right\rangle \right]. \tag{3.19}$$

The density ρ verifies the reversible continuity equation for a system displaying damping which follows an irreversible dynamics. This contradiction was avoided

by Schuch et al. [39–41] by introducing a diffusion term in the continuity equation arriving at the Fokker–Planck equation,

$$\frac{\partial \rho}{\partial t} + \frac{1}{m} \nabla(\rho \, \mathrm{Re}\{p\}) - D \, \frac{\partial^2 \rho}{\partial x^2} = 0, \tag{3.20}$$

D being the diffusion coefficient and with the additional condition

$$-\frac{D}{\rho} \frac{\partial^2 \rho}{\partial x^2} = \gamma(\ln \rho - \langle \ln \rho \rangle) \tag{3.21}$$

to be satisfied in order to achieve separation of the two equations for the amplitudes Ψ and Ψ^*. The mean value on the right–hand side guarantees the normalization. Equations (3.20) and (3.21) can also be seen as a continuity equation with a source term. The so-called logarithmic nonlinear Schrödinger equation is now written as

$$i\hbar \, \frac{\partial \Psi}{\partial t} = [H - i\hbar\gamma(\ln \rho - \langle \ln \rho \rangle)] \, \Psi, \tag{3.22}$$

where Hasse's second requirement comes from considering the irreversible diffusion term. As is well known, the damping motion described by the Fokker–Planck equation can always be expressed in terms of its corresponding Langevin equation [42]. This equation will be again discussed in Chap. 4 but in a different context, the continuous quantum measurement.

Interestingly enough, for the dissipative time dependent harmonic oscillator, Schuch, Chung and Hartmann [40, 41] proposed the following nonlinear Schrödinger equation

$$i\hbar \, \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - i\hbar\gamma(\ln \Psi - \langle \ln \Psi \rangle) + \frac{1}{2} m\omega^2(t) x^2 \right] \Psi, \tag{3.23}$$

$\omega(t)$ being the time-dependent harmonic oscillator frequency. This equation gives the correct reduced frequency of this dissipative motion. It could also be used for a Brownian particle ($\omega = 0$) as an alternative nonlinear equation to the Kostin equation. In passing, it is worth noticing that Eq. (3.23) can be shown to be a special case of Eq. (4.96) from Chap. 4 if one sets $\kappa = \gamma/2$ (where κ characterizes the resolution of the continuous measurement and γ represents the friction coefficient). Chou has studied Eq. (3.23) in the complex plane [43]. In the following chapter, a quantum trajectory analysis of this equation will be carried out.

An extension to the nonlinear Schrödinger equation can be obtained by writing [44]

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi + i\hbar DG(\Psi), \tag{3.24}$$

where $H = T + V$ and the nonlinear term is given by

$$G(\Psi) = \nabla^2 \Psi + \frac{|\nabla \Psi|^2}{|\Psi|^2} \Psi. \tag{3.25}$$

The continuity equation is then modified to a Fokker–Planck equation according to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = D\nabla^2 \rho, \tag{3.26}$$

where $\mathbf{J}$ is the usual quantum probability density current.

A phenomenological nonlinear wave equation with complex interaction was also proposed by Gisin [19, 20] to account for decaying states. This wave equation is

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(1 - \frac{i\kappa}{2}\right) H\Psi + \frac{i\kappa}{2} \langle \Psi | H | \Psi \rangle \Psi, \tag{3.27}$$

where H is the usual Hamiltonian for the undamped system and κ is a dimensionless positive and real damping constant. This wave equation presents some advantages, such as: the norm is independent of time, it reduces to Schrödinger's equation when Ψ is an eigenstate of H, the rate of change of the energy expectation value is negative definite and the equation of motion for the damped harmonic oscillator is obtained in terms of $\langle x \rangle$.

Finally, it is worth mentioning that Razavy [8, 45], Wagner [46] and Schuch [47] have shown a connection between the Caldirola–Kanai Hamiltonian (see Chap. 2) and the log–nonlinear Schrödinger equation following Schrödinger's quantization procedure. This equation has also been derived by Skagerstam [48] and Yasue [49] and has found extensive use in many applications. The Kostin nonlinear logarithmic term has recently been suggested as an appropriate, practical bath functional in time-dependent density functional theory for open quantum systems with unitary propagation [50, 51].

3.3 The Schrödinger–Langevin–Bohm Equation

The purpose of this Section is simply to analyze Eq. (3.2) from a different theoretical (and conceptual) framework, the Bohmian mechanics [23, 52–55]. For the sake of simplicity, let us consider the dynamics of one particle in one dimension. If the wave function is written in polar form as usual

$$\Psi(x, t) = \phi(x, t) e^{iS(x,t)/\hbar} \tag{3.28}$$

where $\phi(x,t)$ and $S(x,t)$ are real valued functions and then is substituted in Eq. (3.2), the resulting Schrödinger–Langevin-Bohm (SLB) equation reads as

$$i\hbar\left[\frac{\partial\phi}{\partial t}+\frac{i}{\hbar}\frac{\partial S}{\partial t}\phi\right]=-\frac{\hbar^2}{2m}\left\{\left[\frac{\partial^2\phi}{\partial x^2}-\frac{\phi}{\hbar^2}\left(\frac{\partial S}{\partial x}\right)^2\right]+\frac{i}{\hbar}\left[2\frac{\partial S}{\partial x}\frac{\partial\phi}{\partial x}+\phi\frac{\partial^2 S}{\partial x^2}\right]\right\}$$
$$+\left[V(x)+V_r(x,t)+\gamma(S-\langle S\rangle)\right]\phi. \tag{3.29}$$

The quantum fluid dynamics description is better illustrated by expressing Eq. (3.29) in a different way, that is, by writing the real and imaginary parts separately. Thus, we have the continuity equation

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho v}{\partial x}=0 \tag{3.30}$$

where $\rho=\phi^2$ and the velocity is defined by $v=(\hbar/m)(\partial S/\partial x)$. The equivalent to the quantum Hamilton–Jacobi equation is now given by

$$\frac{\partial v}{\partial t}+v\frac{\partial v}{\partial x}+\gamma v=-\frac{1}{m}\frac{\partial(V+V_r+Q)}{\partial x}, \tag{3.31}$$

Q being the quantum potential defined in terms of ρ,

$$Q\equiv-\frac{\hbar^2}{2m}\frac{\nabla^2\rho^{1/2}}{\rho^{1/2}}=\frac{\hbar^2}{4m}\left[\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2-\frac{\nabla^2\rho}{\rho}\right]. \tag{3.32}$$

In the following, some simple examples are analyzed under this hydrodynamical formulation when the random potential is neglected (dissipative case). Let us start by writing the probability density as a Gaussian function

$$\rho(x,t)=\frac{1}{\sqrt{2\pi\delta(t)^2}}e^{-(x-q(t))^2/2\delta(t)^2} \tag{3.33}$$

where $\delta(t)$ and $q(t)$ are the width and the center of mass of the wave packet, respectively. From Eq. (3.30), the velocity field turns out to be

$$v(x,t)=\frac{\dot{\delta(t)}}{\delta(t)}(x-q(t))+\dot{q}(t) \tag{3.34}$$

where dots on the variables mean the different orders in time derivation. The time integration of this velocity field is straightforward leading to the equation for the quantum trajectories

$$x(t) = q(t) + (x(0) - q(0))\frac{\delta(t)}{\delta(0)} \tag{3.35}$$

where the friction dependence of these trajectories is through the spreading of the Gaussian wave function in its time evolution and the velocity can be reexpressed as

$$v = \frac{\dot{\delta}}{\delta(0)}(x(0) - q(0)) + \dot{q}. \tag{3.36}$$

Equations (3.35) and (3.36) have the same dressing scheme than previously mentioned in Chaps. 1 and 2: a classical and quantum (nonlocal) contribution.

Consider now the interaction potential expanded in a Taylor series around q as

$$V(x,t) \approx V(q,t) + V'(q,t)(x-q) + \frac{1}{2}V''(q,t)(x-q)^2 + \cdots \tag{3.37}$$

where primes denote derivatives with respect to position and evaluated at $x = q$. By retaining up to quadratic terms in the interaction potential, substituting into Eq. (3.31) and separating terms proportional to $(x-q)^0$ and $(x-q)$ we have that

$$\ddot{q} + \gamma\dot{q} = -\frac{1}{m}V'(q,t) \tag{3.38}$$

and

$$\ddot{\delta} + \gamma\dot{\delta} + \omega^2(t)\delta = \frac{\hbar^2}{4m^2\delta^3} \tag{3.39}$$

where $\omega^2(t) = V''(q,t)/m$ is the frequency of the motion. Thus, the motion of q can be identified with that of the classical particle under the potential V and a linear friction. It should be noticed that Eq. (3.38) is just Ehrenfest's theorem for the potential (3.37) and distribution (3.33). On the other hand, the time evolution of the width is governed by the so-called damped (nonlinear) Pinney equation. This equation is well known to be solvable in terms of the linear time-dependent harmonic oscillator equation for the conservative case, but it only admits approximate solutions for weak damping and slowly varying non-vanishing frequencies $\omega(t)$ [52, 56]. In Chap. 2, Sect. 2.12, the differential equation governing the time evolution of the corresponding Gaussian width is simpler than here because we are in the linear regime of quantum mechanics.

For a free particle, $V = 0$, the dissipative motion given by Eq. (3.38) has a trivial classical solution

$$q(t) = q(0) + \frac{\dot{q}(0)}{\gamma}[1 - e^{-\gamma t}]. \tag{3.40}$$

On the contrary, Eq. (3.39) which is written now as

$$\ddot{\delta} + \gamma\dot{\delta} = \frac{\hbar^2}{4m^2\delta^3} \tag{3.41}$$

or, alternatively,

$$\frac{d}{dt}\left(\frac{\dot{\delta}^2}{2} + \frac{\hbar^2}{8m^2\delta^2}\right) = -\gamma\dot{\delta}^2 \leq 0 \tag{3.42}$$

has apparently no analytical solution. Indeed, for the conservative case, $\gamma = 0$,

$$\delta^2(t) = (\delta(0) + \dot{\delta}(0)t)^2 + \frac{\hbar^2 t^2}{4m^2\delta(0)^2} \tag{3.43}$$

which tells us that the width grows without bound with time (see Chap. 1). This is a problem if we want to use the unperturbed solution (for $\gamma = 0$) to obtain an approximate value of Eq. (3.41). In the overdamped regime, the second derivative or acceleration of the width can be neglected and by integrating the resulting first-order ordinary differential equation, the solution is given by

$$\delta(t) \simeq \left(\frac{\hbar^2 t}{m^2\gamma}\right)^{1/4} \tag{3.44}$$

at long times which is consistent with results found from nonlinear theories of quantum Brownian motion [34, 35]. Moreover, it is straightforward to show that

$$\frac{\ddot{\delta}}{\gamma\dot{\delta}} \simeq -\frac{3}{4\gamma t} \tag{3.45}$$

clearly justifying the omission of the acceleration term as long as $\gamma t >> 1$. In Ref. [52], a first order perturbative solution has been provided to be

$$\delta(t) = (t + c_1^4)^{1/4} + \frac{c_2 + (3/16)\ln(t + c_1^4)}{(t + c_1^4)^{3/4}} \tag{3.46}$$

where $c_1 > 0$ and c_2 are integrations constants, which are determined from the initial conditions

$$\delta(0) = c_1 + \frac{c_2}{c_1^3} + \frac{3\ln c_1}{4c_1^3} \tag{3.47}$$

and

$$\dot{\delta}(0) = \frac{3 - 12c_2 + 4c_1^4 - 9\ln c_1}{16c_1^7} \tag{3.48}$$

to be numerically solved only. A direct numerical integration of this equation should obviously be carried out for an exact evaluation of the time evolution of the width [36]. In any case, a more detail discussion below, when dealing the surface diffusion problem, is presented.

For the time-dependent harmonic oscillator case, $V = (1/2)m\omega^2(t)x^2$, the classical equation is

$$\ddot{q} + \gamma\dot{q} + \omega^2(t)q = 0 \tag{3.49}$$

and the differential equation (3.39) for the width is also valid for this case. In nonlinear dynamics, it is known that the integration of the damped Pinney equation is a real challenge. In fact, several methods have been proposed in the literature to look for approximate solutions within perturbation theory [56]. The perturbation procedure could be carried out to higher orders but the zero order solution is very often sufficient for most purposes. In any case, a direct numerical solution is also easy to be obtained.

On the other hand, by eliminating the frequency $\omega^2(t)$ between Eqs. (3.49) and (3.39), and after some manipulations, the quantity

$$I = \frac{1}{2}e^{2\gamma t}[(\alpha\dot{q} - q\dot{\alpha})^2 + (q/\alpha)^2] \tag{3.50}$$

is no longer an invariant (except in the trivial case $\gamma = 0$) with $\delta = (\hbar/m)\alpha^2$. Thus, Eqs. (3.49) and (3.39) constitute a non-Ermakov system (see Chap. 2).

Once the velocity is known after solving Eq. (3.30) for the probability density given by Eq. (3.33), the phase of the wave function is easily obtained by integrating over the position variable. The wave function is then written as

$$\Psi(x,t) = \frac{1}{(2\pi\delta^2)^{1/4}}e^{-(x-q)^2/4\delta^2}e^{\frac{im}{\hbar}[\frac{\dot{\delta}}{2\delta}(x-q)^2+\dot{q}(x-q)]}. \tag{3.51}$$

An extra arbitrary function of time could have been added to S, but it has been disregarded since it has no effect on the probability density and the probability current. The Wigner function for a pure state defined by

$$f(x,p,t) = \frac{1}{2\pi\hbar}\int dy\, e^{ipy/\hbar}\,\Psi^*(x+\frac{y}{2},t)\Psi(x-\frac{y}{2},t) \tag{3.52}$$

has also a Gaussian shape and is positive defined when Eq. (3.51) is used

$$f(x,q,p,t) = \frac{1}{\hbar\pi}e^{-(x-q)^2/2\delta^2}e^{-\frac{2\delta^2}{\hbar^2}[p-\frac{m\dot{\delta}}{\delta}(x-q)-m\dot{q}]^2}. \tag{3.53}$$

3.4 The Ramsauer–Townsend Effect in a Dissipative Medium

The Ramsauer–Townsend (RT) effect is a quantum phenomenon involving the scattering of low-energy electrons by atoms of a noble gas such as Argon, Krypton, or Xenon [57–59]. The probability of collision between the electrons and gas atoms has a minimum value for electrons with a certain amount of kinetic energy (about 1 eV for Xenon gas). It was shown that when the incident electron wavelength is two times larger than the well width L, there is no reflection and the transmission is complete. In a certain sense, this behavior is just the opposite of the so-called quantum reflection [60, 61] where at very low collisional energies, the transmission can be totally suppressed. Quantum theory predicts the existence of the RT minimum by considering the atom as a finite square potential well [62–66]. Via the de Broglie–Bohm formalism, the RT effect is first analyzed when in the collisional process there is no energy dissipation. Subsequently, the dissipative dynamics of the RT effect is after studied by means of the Kostin equation for small dissipation $\hbar\gamma << (V + E)$ where γ, V and E are the coefficient of friction, the height of the potential and the energy of the particle, respectively.

Let us consider a stationary electronic flux with incident energy E, colliding with a potential well with height V and width L such as

$$V(x) = \begin{cases} 0 & , x \neq 0,\ L \\ -V & , 0 < x < L \end{cases} \tag{3.54}$$

which define the following regions

$$Incidence\ \ Region\ \ (1): \quad x < 0, \tag{3.55}$$

$$Scattering\ \ Region\ \ (2): \quad 0 < x < L, \tag{3.56}$$

$$Transmission\ \ Region\ \ (3): \quad x > L. \tag{3.57}$$

Since E > 0, the solution of Schrödinger's equation

$$i\,\hbar\,\frac{\partial\psi(x,\ t)}{\partial t} = -\frac{\hbar^2}{2\,m}\,\frac{\partial^2\,\psi(x,\ t)}{\partial x^2} + V(x)\,\psi(x,\ t)\ . \tag{3.58}$$

for these three mentioned above regions is given by

$$\psi_1(x,\ t) = (e^{i\,k\,x} + A\,e^{-\,i\,k\,x})\,e^{-\,i\,\omega\,t}\ , \tag{3.59}$$

$$\psi_2(x,\ t) = (C\,e^{i\,q\,x} + D\,e^{-\,i\,q\,x})\,e^{-\,i\,\omega\,t}\ , \tag{3.60}$$

$$\psi_3(x,\ t) = (B\,e^{i\,k\,x})\,e^{-\,i\,\omega\,t}\ , \tag{3.61}$$

where

$$k^2 \;=\; \frac{2\,m\;E}{\hbar^2}\;, \qquad q^2 \;=\; \frac{2\,m\;(E\;+\;V)}{\hbar^2}\;. \tag{3.62}$$

Thus, the reflection $|\;R\;|^2 \;=\; A\;A^*$ and the transmission $|\;T\;|^2 \;=\; B\;B^*$ coefficients are given by

$$|\;R\;|^2 \;=\; \frac{\left(\frac{k^2\,-\,q^2}{2\,k\,q}\right)^2\;sin^2\;(q\;L)}{1\;+\;\left(\frac{k^2\,-\,q^2}{2\,k\,q}\right)^2\;sin^2\;(q\;L)}\;, \tag{3.63}$$

$$|\;T\;|^2 \;=\; \frac{1}{1\;+\;\left(\frac{k^2\,-\,q^2}{2\,k\,q}\right)^2\;sin^2\;(q\;L)}\;. \tag{3.64}$$

Using Eqs. (3.63) and (3.64), a particular case can be considered, that is, when

$$q\;L\;=\;\pi\;. \tag{3.65}$$

Substitution of Eqs. (3.65) into (3.63) and (3.64) results

$$|\;T\;|^2\;=\;1, \qquad |\;R\;|^2\;=\;0, \tag{3.66}$$

which leads to the suppression of the reflection probability.

Let us now turn to the study of the RT effect when in the collision process there is an energy dissipation governed by the Kostin equation [62, 66]

$$i\;\hbar\;\frac{\partial\psi(x,\;t)}{\partial t}\;=\;-\frac{\hbar^2}{2\;m}\;\frac{\partial^2\psi(x,t)}{\partial x^2}\;+\;\left[V(x,\;t)\;+\;\frac{\hbar\;\gamma}{2\;i}\ell n\;\frac{\psi(x,\;t)}{\psi^*(x,\;t)}\right]\;\psi(x,\;t), \tag{3.67}$$

where $\psi(x,\;t)$, $V(x,t)$ and γ represent, respectively, the wave function, the interaction potential and dissipation coefficient of our new system. Equation (3.67) will be studied now within the formalism of de Broglie–Bohm.

First, we write $\psi(x,\;t)$ as

$$\psi(x,\;t)\;=\;\Phi(x)\;exp\;\left[-\;\frac{i\;E}{\hbar\;\gamma}\;(1\;-\;e^{-\;\gamma\;t})\right], \tag{3.68}$$

which yields

$$i\,\hbar\,\frac{\partial\psi(x,\,t)}{\partial t}\;=\;E\,e^{-\,\gamma\,t}\;\psi(x,\,t)\;, \tag{3.69}$$

$$-\,\frac{\hbar^2}{2\,m}\,\frac{\partial^2\psi(x,\,t)}{\partial x^2}\;=\;-\,\frac{\hbar^2}{2\,m}\,\frac{\Phi''(x)}{\Phi(x)}\;\psi(x,\,t)\;, \tag{3.70}$$

$$\frac{\hbar\,\gamma}{2\,i}\;\ell n\;\frac{\psi(x,\,t)}{\psi^*(x,\,t)}\;=\;\frac{\hbar\,\gamma}{2\,i}\;\ell n\;\frac{\Phi(x)}{\Phi^*(x)}\;-\;E\;(1\;-\;e^{-\,\gamma\,t})\;. \tag{3.71}$$

Inserting Eqs. (3.69)–(3.71), into (3.67) and using Eq. (3.68) we obtain

$$\Phi''(x)\;+\;\left[\;q^2\;-\;\frac{m\,\gamma}{i\,\hbar}\;\ell n\;\frac{\Phi(x)}{\Phi^*(x)}\;\right]\;\Phi(x)\;=\;0\;. \tag{3.72}$$

Now, considering the Madelung transformation [67] (for convenience, $\hbar$ has been absorbed in the argument of the phase, $S(x)$)

$$\Phi(x)\;=\;\phi(x)\;e^{i\;S(x)}\;, \tag{3.73}$$

we see that Eq. (3.72) becomes

$$\phi''\;+\;2\,i\,\phi'\,S'\;-\;\phi\,(S')^2\;+\;i\,\phi\,S''\;+\;\left[q^2\;-\;\frac{2\,m\,\gamma}{\hbar}\,S\right]\,\phi\;=\;0\;. \tag{3.74}$$

Separating real and imaginary parts of the above expression we have,

$$\phi''\;+\;\left(q^2\;-\;\frac{2\,m\,\gamma}{\hbar}\,S\right)\,\phi\;=\;(S')^2\,\phi\;,\qquad 2\,\phi'\,S'\;+\;\phi\,S''\;=\;0. \tag{3.75}$$

Defining, as usual,

$$\rho(x)\;=\;\phi^2(x)\;, \tag{3.76}$$

and integrating Eq. (3.75) results

$$\frac{(S')'}{S'}\;=\;-\,\frac{2\,\phi'}{\phi}\;\;\rightarrow\;\;\int\frac{(S')'}{S'}\;=\;-\int\frac{2\,\phi'}{\phi}\;\;\rightarrow$$

$$\ell n\;S'\;=\;-\,2\;\ell n\;\phi\;+\;\ell n\;C\;=\;-\,\ell n\;\phi^2\;+\;\ell n\;C\;=\;\ell n\;\frac{C}{\phi^2}\;\;\rightarrow$$

$$S'(x)\;=\;\frac{C}{\rho(x)}\;,\qquad S(x)\;=\;S(0)\;+\;C\int_0^x\frac{dx'}{\rho}\;. \tag{3.77}$$

Multiplying Eq. (3.75) by ϕ' and using Eqs. (3.76) and (3.77) we reach,

$$\phi''\,\phi' \;+\; [q^2 \;-\; (S')^2]\,\phi\,\phi' \;=\; \frac{2\,m\,\gamma}{\hbar}\,S\,\phi\,\phi' \quad \rightarrow$$

$$\frac{d}{dx}\left[\frac{1}{2}\,(\phi')^2 \;+\; \frac{1}{2}\,q^2\,\phi^2 \;+\; \frac{1}{2}\,\frac{C^2}{\phi^2}\right] \;=\; \frac{2\,m\,\gamma}{\hbar}\,S\,\phi\,\phi' \,. \tag{3.78}$$

Since Eq. (3.76) can be written as

$$\rho' \;=\; 2\,\phi\,\phi' \,, \tag{3.79}$$

Equation (3.78) can be rewritten, using also Eq. (3.76), as

$$I'(x) \;=\; \frac{2\,m\,\gamma}{\hbar}\,S(x)\,\rho'(x) \,, \qquad I(x) \;=\; \frac{[\rho(x)']^2}{4\,\rho(x)} \;+\; q^2\,\rho(x) \;+\; \frac{C^2}{\rho(x)} \,. \tag{3.80}$$

One can readily see that, taking Eq. (3.77), we obtain,

$$\frac{d}{dx}\,(S\,\rho) \;=\; S'\,\rho \;+\; S\,\rho' \;=\; S\,\rho' \;+\; C \;=\; S\,\rho' \;+\; \frac{d}{dx}\,(C\,x) \quad \rightarrow$$

$$S\,\rho' \;=\; \frac{d}{dx}\,(S\,\rho \;-\; C\,x) \,. \tag{3.81}$$

Substituting Eq. (3.81) into (3.80) we have

$$\frac{dI}{dx} \;=\; \frac{2\,m\,\gamma}{\hbar}\,\frac{d}{dx}\,(S\,\rho \;-\; C\,x) \quad \rightarrow \quad \frac{d}{dx}\left[I \;-\; \frac{2\,m\,\gamma}{\hbar}\,(S\,\rho \;-\; C\,x)\right] \;=\; 0 \quad \rightarrow$$

$$I \;-\; \frac{2\,m\,\gamma}{\hbar}\,(S\,\rho \;-\; C\,x) \;=\; constant \;=\; I_0 \quad \rightarrow$$

$$I(x) \;=\; I_0 \;+\; \frac{2\,m\,\gamma}{\hbar}\,[S(x)\,\rho(x) \;-\; C\,x] \tag{3.82}$$

$$I_o \;=\; \frac{[\rho'(x)]^2}{4\,\rho(x)} \;+\; q^2\,\rho(x) \;+\; \frac{C^2}{\rho(x)} \;-$$

$$-\;\frac{2\,m\,\gamma}{\hbar}\left[\rho(x)\left(S(0) \;+\; C\int_0^x \frac{dx'}{\rho(x')}\right) \;-\; C\,x\right] \,. \tag{3.83}$$

By solving the differential Equations (3.80) using a variational-of-parameter technique one has

$$\rho(x) \;=\; \frac{1}{2\,q^2}\,\left[\;I(x)\;+\;\sqrt{I^2(x)\;-\;4\,q^2\,C^2}\;\times\;cos\;\left(\;2\,q\;[x\;-\;\beta(x)]\;\right)\;\right]\,, \tag{3.84}$$

where $\beta(x)$ is a variational unknown function. To determine $\beta(x)$ we take the derivative of Eq. (3.84), that is,

$$\rho'(x) \;=\; \frac{1}{2\,q^2}\,\left(\;I'(x)\;+\;\frac{I(x)\;I'(x)\;cos\;\left(\;2\,q\;[x\;-\;\beta(x)]\;\right)}{\sqrt{I^2(x)\;-\;4\,q^2\,C^2}}\;-\right.$$

$$\left.-\;\sqrt{I^2(x)\;-\;4\,q^2\,C^2}\;sin\;\left(\;2\,q\;[x\;-\;\beta(x)]\;\right)\times 2\,q\;[1\;-\;\beta'(x)]\;\right)\,, \tag{3.85}$$

where the following conditions must be obeyed

$$I'(x)\;+\;\frac{I(x)\;I'(x)\;cos\;[2\;\theta(x)]}{\sqrt{I^2(x)\;-\;4\,q^2\,C^2}}\;+\;\sqrt{I^2(x)\;-\;4\,q^2\,C^2}\;\times$$

$$\times\;2\,q\;\beta'(x)\;sin\;[2\;\theta(x)]\;=\;0\;,\qquad \theta(x)\;=\;q\;[x\;-\;\beta(x)]\;. \tag{3.86}$$

This implies that Eq. (3.85) is written as,

$$\rho'(x)\;=\;-\;\frac{\sqrt{I^2(x)\;-\;4\,q^2\,C^2}}{q}\;sin\;[2\;\theta(x)]\;. \tag{3.87}$$

From Eqs. (3.80) and (3.87) we finally reach

$$\beta'(x)\;=\;\frac{m\;\gamma\;S(x)}{\hbar\;q^2}\;\left(\;1\;+\;\frac{I(x)\;cos\;[2\;\theta(x)]}{\sqrt{I^2(x)\;-\;4\,q^2\,C^2}}\;\right)\,. \tag{3.88}$$

We study now the scattering of a stationary flux of particles with energy E and $k^2\;=\;2\;m\;E/\hbar^2$ by a potential well defined by Eq. (3.54). The particles flux, incident ($x\;<\;0$) and transmitted ($x\;>\;L$), will be given by

$$\psi_I(x)\;=\;e^{i\;k\;x}\;+\;A\;e^{-\;i\;k\;x}\;=\;\phi(x)\;e^{i\;S(x)}\;, \tag{3.89}$$

$$\psi_T(x)\;=\;B\;e^{i\;k\;x}\;=\;\phi(x)\;e^{i\;S(x)}\;. \tag{3.90}$$

Since ψ and $\partial\psi/\partial x$ are assumed to be continuous at the boundaries of the potential well, we have that:
(a) At $x = 0$, Eq. (3.89) becomes

$$\psi_I(x=0) \;\rightarrow\; 1 + A = \phi(0)\, e^{i\, S(0)}\,, \tag{3.91}$$

$$\frac{\partial\psi_I}{\partial x}|_{x\,=\,0} \;\rightarrow\; 1 - A = \frac{e^{i\, S(0)}}{k}\,[-\, i\, \phi'(0) + \phi(0)\, S'(0)]\,. \tag{3.92}$$

Adding Eqs. (3.91) and (3.92), we obtain the following expression

$$2\, k = [cos\; S(0) + i\; sin\; S(0)]\Big(\; \phi(0)\; [k + S'(0)] - i\; \phi'(0)\;\Big),$$

which can be separated again in two parts, real and imaginary,

$$2\, k = cos\; S(0)\; \phi(0)\; [k + S'(0)] + \phi'(0)\; sin\; S(0)\,, \tag{3.93}$$

$$0 = sin\; S(0)\; \phi(0)\; [k + S'(0)] - \phi'(0)\; cos\; S(0). \tag{3.94}$$

Multiplying Eq. (3.93) by $sin\; S(0)$ and Eq. (3.94) by $cos\; S(0)$ and subtracting the expressions, results

$$2\, k\; sin\; S(0) = \phi'(0)\,. \tag{3.95}$$

On the other hand, multiplying Eq. (3.93) by $cos\; S(0)$ and Eq. (3.94) by $sin\; S(0)$ and adding the expressions, we have that

$$2\, k\; cos\; S(0) = \phi(0)\; [k + S'(0)]\,. \tag{3.96}$$

Squaring and adding Eqs. (3.95) and (3.96), the following expression is found

$$4\, k^2 = [\phi'(0)]^2 + \phi^2(0)\; [k + S'(0)]^2. \tag{3.97}$$

(b) At $x = L$, Eq. (3.90) leads to

$$\psi_T(x=L) \;\rightarrow\; B\; e^{i\, k\, L} = \phi(L)\; e^{i\; S(L)}\,, \tag{3.98}$$

$$\frac{\partial\psi_T}{\partial x}|_{x\,=\,L} \;\rightarrow \tag{3.99}$$

$$B\; e^{i\, k\, L} = \frac{1}{k}\; e^{i\; S(L)} \times [-\, i\; \phi'(L) + S'(L)\; \phi(L)]\,. \tag{3.100}$$

Taking the real and imaginary parts of Eqs. (3.98) and (3.100) and using Eq. (3.77)

$$\phi(L) \;=\; \frac{1}{k}\,[-\,i\,\phi'(L) \;+\; S'(L)\,\phi(L)] \;\;\rightarrow\;\; \phi(L) \;=\; \frac{1}{k}\,S'(L)\,\phi(L) \;\;\rightarrow$$

$$S'(L) \;=\; k\;, \qquad \rho(L) \;=\; \frac{C}{k}\;, \tag{3.101}$$

$$\phi'(L) \;=\; 0\;, \qquad \rho'(L) \;=\; 0\;. \tag{3.102}$$

Subtracting Eqs. (3.91) and (3.92) and taking into account Eqs. (3.76), (3.77), (3.79), (3.95) and (3.96), we find

$$2\,A \;=\; e^{i\,S(0)}\left(\phi(0)\left[1 \;-\; \frac{S'(0)}{k}\right] + \frac{i}{k}\,\phi'(0)\right) \;\;\rightarrow$$

$$A \;=\; \frac{2\,i\,[k\,\rho(0) \;-\; C] \;-\; \rho'(0)}{2\,i\,[k\,\rho(0) \;+\; C] \;+\; \rho'(0)}\;. \tag{3.103}$$

Taking the above expression, let us calculate the reflection ($|\;R\;|^2$) and transmission ($|\;T\;|^2$) coefficients

$$|\;R\;|^2 \;=\; A\;A^* \;=\; \frac{4\,[k\,\rho(0) \;-\; C]^2 \;+\; [\rho'(0)]^2}{4\,[k\,\rho(0) \;+\; C]^2 \;+\; [\rho'(0)]^2}\;, \tag{3.104}$$

$$|\;T\;|^2 \;=\; 1 \;-\; |\;R\;|^2 \;=\; \frac{4\,k\,C}{\frac{[\rho'(0)]^2}{4\,\rho(0)} \;+\; \frac{C^2}{\rho(0)} \;+\; k^2\,\rho(0) \;+\; 2\,k\,C}\;. \tag{3.105}$$

Substitution of $x \;=\; 0$ into Eq. (3.83), results

$$I_0 \;=\; \frac{[\rho'(0)]^2}{4\,\rho(0)} \;+ q^2\,\rho(0) \;+\; \frac{C^2}{\rho(0)} \;-\; \frac{2\,m\,\gamma}{\hbar}\,\rho(0)\;S(0)\;. \tag{3.106}$$

Now, substituting Eq. (3.106) into (3.105) the transmission coefficient is written as

$$|\;T\;|^2 \;=\; \frac{4\,k\,C}{I_0 \;+\; [k^2 \;-\; q^2 \;+\; \frac{2\,m\,\gamma}{\hbar}\;S(0)]\;\rho(0) \;+\; 2\,k\,C}\;. \tag{3.107}$$

The above expression can be written in a different form. Indeed, considering Eqs. (3.76) and (3.101), and using Eqs. (3.98) and (3.100) we can write

$$|\;T\;|^2 \;=\; B\;B^* \;=\; \phi^2(L) \;=\; \rho(L) \;=\; \frac{C}{k}\;. \tag{3.108}$$

To obtain the final form for $|\;T\;|^2$ we need to determine the constant C. We find after long calculations [62]

$$|T|^2 \;=\; \frac{1}{1 \;+\; sin^2\,[q\;\beta(0)]\,\left(\frac{1-n^2}{2\,n}\right)^2\left[1 \;+\; \frac{m\;\gamma\;S(0)}{\hbar\,q^2}\left(\frac{n^2+1}{n^2-1}\right)\right]}, \tag{3.109}$$

and

$$|R|^2 = \frac{sin^2\,[q\;\beta(0)]\,\left(\frac{1-n^2}{2\,n}\right)^2\left[1 \;+\; \frac{m\;\gamma\;S(0)}{\hbar\,q^2}\left(\frac{n^2+1}{n^2-1}\right)\right]}{1 \;+\; sin^2\,[q\;\beta(0)]\,\left(\frac{1-n^2}{2\,n}\right)^2\left[1 \;+\; \frac{m\;\gamma\;S(0)}{\hbar\,q^2}\left(\frac{n^2+1}{n^2-1}\right)\right]} \tag{3.110}$$

where $n \equiv q/k$. Note that Eqs. (3.63) and (3.64) are obtained by setting $\gamma \;=\; 0$ into Eqs. (3.109) and (3.110). After substantial calculations we find that

$$\beta(0) \sim L\left(1 - \frac{\gamma\hbar}{V}\left[\frac{kL}{2} + S(0)\right]\right) \tag{3.111}$$

and are in conditions to write the final expression to explain the RT effect. Indeed, as was shown previously, this effect is characterized (see Eq. (3.65)) by

$$q\;L \;=\; \pi\;. \tag{3.112}$$

With the help of Eqs. (3.112) and (3.111), we have

$$q\;\beta(0) \sim \pi \;\;\rightarrow\;\; 2\;q\;\beta(0) \sim 2\;\pi\;. \tag{3.113}$$

Equations (3.86), (3.87) and (3.113) lead us to

$$\rho'(0) \;=\; 0\;, \qquad sin\;[q\;\beta(0)] \;=\; 0\;. \tag{3.114}$$

Equations (3.79), (3.95) and (3.114) yield

$$2\;k\;sin\;S(0) \;=\; \phi'(0) \;=\; \frac{\rho'(0)}{2\;\phi(0)} \;=\; 0 \;\;\rightarrow\;\; S(0) \;=\; 0\;. \tag{3.115}$$

Finally, Eqs. (3.109) and (3.114) show that the coefficients of transmission and reflection are given by

$$|T|^2 \;=\; 1 \;\;\text{and}\;\; |R|^2 \;=\; 0, \tag{3.116}$$

in agreement with Eq. (3.66), which characterizes the RT effect. On the other hand, $|T|^2 \;=\; min$ and $|R|^2 \;=\; max$, provided that $q\;\beta(0) \;\rightarrow\; \pi/2$ where $\beta(0) \approx L\left(1 - \frac{m\gamma kL}{q^2-k^2}\right)$ (Fig. 3.2).

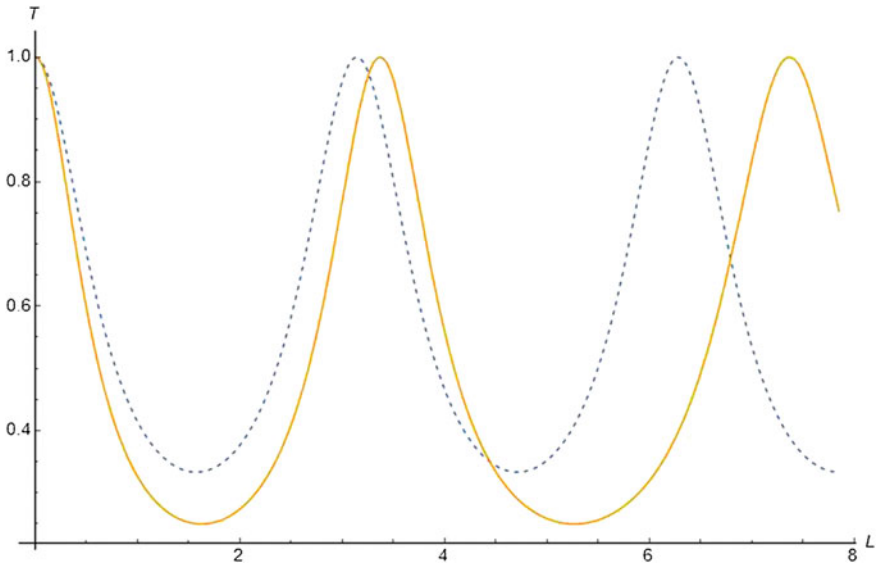

Fig. 3.2 Resonances in Scattering from a square potential: Transmission rate versus width of well with small friction $\gamma << (q^2 - k^2)/mkL$ (*solid line*) and without friction (*dashed line*). Note that the resonances for the dissipative case display a varying periodicity

3.5 Tunneling Through a Dissipative Barrier

Dissipative quantum tunneling is a very important and active field [2]. On the other hand, we have shown in Sect. 2.3 through Bohmian mechanics how more general boundary conditions follow from the continuity of mass, momentum and energy densities. With these new boundary conditions, a novel approach to tunneling through sharp-edged, dissipative potential barriers is presented. The usual boundary conditions are not only more general but the assumption that the wave function and its derivative need to be continuous at a boundary are physically incorrect for dissipative systems. To this end, let us consider the dynamics of a quantum particle in the tunneling region described by the Kostin equation (3.67), expressed the wave function in a polar form $\psi = \phi \exp(iS/\hbar)$ [67]. The proper boundary conditions where the potential undergoes a finite jump read

$$\rho_1(0) = \rho_2(0), \tag{3.117}$$

$$\rho_2(L) = \rho_3(L), \tag{3.118}$$

$$\rho_1{}'(0) = \rho_2{}'(0), \tag{3.119}$$

$$\rho_2{}'(L) = \rho_3{}'(L), \tag{3.120}$$

$$\rho_1(0)v_1(0) = \rho_2(0)v_2(0), \tag{3.121}$$

$$\rho_2(L)v_2(L) = \rho_3(L)v_3(L), \tag{3.122}$$

$$\left(\frac{\partial S_1}{\partial t}\right)_0 = \left(\frac{\partial S_2}{\partial t} + \gamma S_2\right)_0, \tag{3.123}$$

$$\left(\frac{\partial S_2}{\partial t} + \gamma S_2\right)_L = \left(\frac{\partial S_3}{\partial t}\right)_L, \tag{3.124}$$

which show the discontinuity in the phase of the wave function at the boundary (γ represents the friction coefficient as in Sect. 2.3). The potential barrier expressed as

$$V(x) = \begin{cases} 0 & , x \neq 0,\ L \\ V & , 0 < x < L \end{cases} \tag{3.125}$$

defines the following regions

$$Incidence\ \ Region\ \ (1): \quad x < 0, \tag{3.126}$$

$$Scattering\ \ Region\ \ (2): \quad 0 < x < L, \tag{3.127}$$

$$Transmission\ \ Region\ \ (3): \quad x > L. \tag{3.128}$$

Following Sects. 2.3 and 3.4, we find the wave functions for regions 1, 2 and 3 to be (for convenience, in the different interaction regions, $\hbar$ has also been absorbed in the arguments of the corresponding phases, $S_1(x)$, $S_2(x)$ and $S_3(x)$, respectively)

$$\psi_1(x,\ t) \ = \ \sqrt{\rho_1}\ e^{i\ S_1} \ =$$

$$= \sqrt{1 \ + \ a^2 \ + \ 2\ a\ cos\ (2\ k_1\ x \ - \ \alpha)} \ \times exp\left[\ i\ \left(\ - \ \omega_1\ t \ +\right.\right.$$

$$\left.\left. + \ \frac{\alpha}{2} \ + \ tan^{-\ 1}\left[\frac{1\ -\ a}{1\ +\ a} tan\ \left(k_1\ x \ - \ \frac{\alpha}{2}\right)\right]\right)\right], \tag{3.129}$$

$$\psi_2(x) \ = \ \sqrt{\rho_2}\ e^{i\ S_2} \ =$$

$$= \left(\ \frac{1}{\bar{Q}(x)}\left[c^2\ exp\left(2\int_o^x \bar{Q}\ dx\right) \ + \ d^2\ exp\left(\ - \ 2\int_o^x \bar{Q}\ dx\right) +\right.\right.$$

$$+ 2\ c\ d\ cos\ (\gamma\ -\ \delta)\Big]\Big)^{1/2} \times exp\left[\ i\ \left(\ \frac{\gamma\ +\ \delta}{2}\ +\right.\right.$$

$$+ tan^{-1}\left[\ \frac{c\ exp(\int_o^x\ \bar{Q}\ dx)\ -\ d\ exp(-\int_o^x\ \bar{Q}\ dx)}{c\ exp(\int_o^x\ \bar{Q}\ dx)\ +\ d\ exp(-\int_o^x\ \bar{Q}\ dx)} \times\right.$$

$$\left.\left.\times\ tan\left(\frac{\gamma\ -\ \delta}{2}\right)\right]\right)\Bigg] \tag{3.130}$$

$$\psi_3(x,\ t)\ =\ \sqrt{\rho_3}\ e^{i\ S_3}\ =$$

$$=\ \sqrt{b^2}\ exp\ [i\ (-\ \omega_3\ t\ +\ k_3\ x\ +\ \beta)]\ . \tag{3.131}$$

where

$$k_1^2 = \frac{2mE_1}{\hbar^2} \tag{3.132}$$

$$\bar{Q}^2(x)\ =\ \frac{2\ m}{\hbar^2}\ [V\ -\ E_1\ +\ \hbar\ \gamma\ \Delta\ S_2(x)] \tag{3.133}$$

$$k_3^2 = \frac{2mE_3}{\hbar^2}, \tag{3.134}$$

$$\omega_1 = \frac{E_1}{\hbar}, \tag{3.135}$$

$$\omega_3 = \frac{E_3}{\hbar}, \tag{3.136}$$

$$\Delta S_2(0)\ = 0, \tag{3.137}$$

$$\Delta S_2(L)\ =\ -\frac{(\omega_3 - \omega_1)}{\gamma}. \tag{3.138}$$

Thus, E_1,E_2 and E_3 are the energies of the particle in the incident, scattering and transmission regions, Eq. (3.125), and related to the wave numbers k_1, $\bar{Q}$ and k_3, respectively (as expressed above).

After lengthy calculations, we find the tunneling probability to be [62]

$$T^{-2} = b^{-2}\ =\ \frac{1}{D\ +\ 2\ B\ sinh^2\ \alpha}\ \Big(\ A^2\ +\ 2\ A\ B\ sinh^2\ \alpha\ +$$

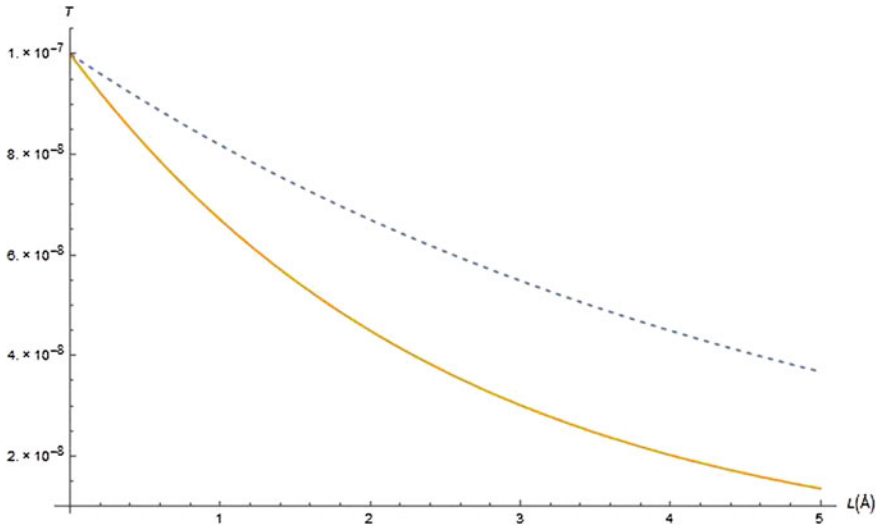

Fig. 3.3 Tunneling through a square potential versus width of well with friction (*solid line*) and without friction (*dashed line*): An electron with kinetic energy $E = 1\,\text{eV}$ tunneling through a barrier with $V = 10\,\text{eV}$, width $L = 0.5\,\text{nm}$ and friction $\hbar\gamma\Delta S = 2\,\text{eV}$

$$+\ 4\ C\ \ sinh^2\ \alpha\ \left[1\ +\ sinh^2\ \alpha\ \left(1\ +\ \frac{k_1^2}{\bar{Q}^2(0)}\right)\right]\ \Big) \tag{3.139}$$

where

$$A\ =\ \frac{1}{2}\left[\ \frac{k_3}{k_1}\ +\ \frac{\bar{Q}(L)}{\bar{Q}(0)}\ \right],\quad B\ =\ \frac{1}{2}\ \frac{\bar{Q}^2(L)\ +\ k_3^2}{\bar{Q}(L)\ \bar{Q}(0)}\ , \tag{3.140}$$

$$C\ =\ \left[\frac{\bar{Q}^2(L)\ +\ k_3^2}{4\ \bar{Q}(L)\ k_1}\right]^2,\quad D\ =\ \frac{\bar{Q}(L)}{\bar{Q}(0)}\ \text{ and }\alpha = \int_0^L \bar{Q}(x)\ dx. \tag{3.141}$$

Finally, by setting $\gamma = 0$, we recover the well-known result

$$T^{-\,2} = b^{-\,2}\ =\ 1\ +\ \frac{(q^2\ +\ k^2)^2}{4\ k^2\ q^2}\ sinh^2\ (\bar{q}\ L) \tag{3.142}$$

where $k^2 = k_1^2 = k_3^2 = \frac{2mE}{\hbar^2}$ and $q^2(x)\ =\ \frac{2\,m}{\hbar^2}\ [V\ -\ E]$ (Fig. 3.3).

3.6 The Plasma Fluid Formulation Within Bohmian Mechanics

In the analysis of correspondence between classical and quantum dynamics, one can find a striking analogy between the quantum mechanics of a point particle and the dynamics of a fluid which has been pursued by a number of authors [68–73]. As shown in Chap. 1, Bohmian mechanics clearly offers an intuitive and appealing understanding of the quantum world in a classical-like fashion by means of trajectories evolving throughout configuration space. It provides an explanation of quantum phenomena in terms of point particles guided by wave functions. As has also been previously reported, Madelung [74] was the first to transform the Schrödinger equation for a particle into two fluid-dynamical equations: a continuity equation and an Euler-type equation. This description involves the density $\rho = \Psi^* \Psi$ and the velocity field v as primary quantities. Thus, the fluid dynamicist can gather experience of its effects by translating some of the elementary situations of the quantum theory into their corresponding fluid mechanical statements and vice versa. This fluid formulation was subsequently refined by de Broglie through his pilot wave theory and further developed by Bohm [75, 76]. The wave function (which satisfies Schrödinger's equation) is an objective field, not just as some ghost wave of information where the particle rides along on the wave at some position $\mathbf{r}(t)$.

In order to illustrate this point, we draw striking similarities with the classical plasma fluid theory describing the motion of charged particles (electrons) in a neutralized (ion) background subject to an external electric field by writing in the three dimensional configuration space [77–79]

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} + \nabla \cdot (\rho(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)) = 0 \tag{3.143}$$

and

$$\frac{\partial \mathbf{v}(\mathbf{r}, t)}{\partial t} + \mathbf{v}(\mathbf{r}, t) \cdot \nabla \mathbf{v}(\mathbf{r}, t) + \gamma \mathbf{v}(\mathbf{r}, t) + \frac{k_B T}{m} \frac{\nabla \rho(\mathbf{r}, t)}{\rho(\mathbf{r}, t)} = -\frac{e\mathbf{E}(\mathbf{r}, t)}{m}, \tag{3.144}$$

where m, e, ρ, $\mathbf{v}(\mathbf{r}, t)$ and $(k_B T/m)^{1/2}$, γ are the particle (electron) mass, charge, density, mean velocity, thermal speed and collision frequency, respectively. In fact, this collision frequency can also be seen as a collisional friction. $\mathbf{E}(\mathbf{r}, t)$ is the electric field and the second part of Eq. (3.144) refers to the Lorentz force.

To obtain the quantum fluid dynamical counterpart of the classical problem described above, we can translate the information into a form that is easier to comprehend by means again from the continuity equation given by (3.143) and

$$\frac{\partial \mathbf{v}(\mathbf{r},t)}{\partial t} + \mathbf{v}(\mathbf{r},t)\cdot\nabla\mathbf{v}(\mathbf{r},t) + \gamma\mathbf{v}(\mathbf{r},t) + \frac{kT}{m}\frac{\nabla\rho(\mathbf{r},t)}{\rho(\mathbf{r},t)} = -\frac{e\mathbf{E}(\mathbf{r},t)}{m} - \nabla\left(\frac{Q}{m}\right), \tag{3.145}$$

where as usual $\rho(\mathbf{r},t) = |\phi(\mathbf{r},t)|^2$ is the quantum fluid-particle density, $\mathbf{v}(\mathbf{r},t) = (\hbar/m)\nabla S(\mathbf{r},t)$ is the quantum fluid-particle velocity, and Q is the quantum potential which is responsible for all the non-local effects predicted by the theory. Equation (3.145) can be interpreted as the Hamilton–Jacobi equation for this new system, with the additional term proportional to $\hbar^2$ defining $Q(\mathbf{r},t)$.

By expressing, as usual, the wave function in the polar form [67] as in Eq. (3.28), the corresponding Schrödinger equation can be obtained

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + \left(\frac{\hbar\gamma}{2i}\ln\frac{\Psi(\mathbf{r},t)}{\Psi^*(\mathbf{r},t)} + kT\ln|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t) + e\mathbf{r}\cdot\mathbf{E}(\mathbf{r},t)\Psi(\mathbf{r},t). \tag{3.146}$$

which is the corresponding SL equation for this dissipative problem. The wave function $\Psi(\mathbf{r},t)$ is that of wave mechanics, but conceived in the tradition of Maxwell and Einstein, as an objective field [80]. The particle rides along on the wave at some position $\mathbf{r}(t)$ with velocity $\dot{\mathbf{r}}(t)$ with the help of the guiding equation

$$\dot{\mathbf{r}}(t) = \frac{\hbar}{m}Im(\nabla\ln\Psi(\mathbf{r},t)), \tag{3.147}$$

which constitutes the simplest first-order evolution equation for the trajectories of the particle – the Bohmian trajectories of an evolving particle of the wave packet ensemble with an initial position $\mathbf{r}_0$ – that is, compatible with the Galilean (and time-reversal) covariance of the Schrödinger evolution.

Interestingly enough, Eq. (3.144) corresponds to the classical standard Langenvin equation

$$\ddot{\mathbf{r}} + \gamma\dot{\mathbf{r}} = -e\mathbf{E}(\mathbf{r},t)/m \tag{3.148}$$

except for the nonlinear term $\mathbf{v}\cdot\nabla\mathbf{v}$ (which is called the inertial term in hydrodynamics) and the pressure term $p = (k_BT/m)\rho$. It only attains the form of Eq. (3.148) if, for instance, $\mathbf{v}$ and its derivatives are small and we consider the cold-plasma approximation. Furthermore, the analogy between Eq. (3.144) and the nonlinear SL Eq. (3.146) renders strong support for the exploration of manifold solutions, based on the well developed mathematical problem solving methods of nonlinear differential equations in the literature.

The term $\mu \equiv Q/m$ had been loosely referred to as a quantum pressure term (see also Chap. 1). This term is a misnomer [73] because: (i) the dimensionality is

incorrect and it would be better regarded as a quantum (chemical) potential per unit mass, (ii) the word pressure suggests a phenomenon that depends only on the local thermodynamics state (here fixed ρ) and (iii) the presence of the derivatives in

$$\nabla_i \mu = -(\nabla_j \sigma_{ij})/\rho \tag{3.149}$$

where

$$\sigma_{ij} = (\hbar^2 \rho / 4m^2) \nabla_i \nabla_j \ln \rho, \tag{3.150}$$

with $i, j = x, y, z$, shows that neighbouring points are involved in its definition. Thus, σ_{ij} is a properly dimensioned contender for the (anisotropic) quantum stress tensor, instead. Even more, the term $(k_B T/m)\rho$ has been proposed by Bialynicki-Birula and Mycielski [18]: a logarithmic Schrödinger-like equation with nonlinearity $b \ln |\Psi|^2$ which possesses soliton-like solutions of Gaussian form (see Sect. 2.11). The term $(\hbar\gamma/2i) \ln(\Psi/\Psi^*)$ in Eq. (3.146) represents quantum dissipation where γ stands for the friction coefficient (collisional friction). Caldeira and Leggett [81] have given support and justification for the use of nonlinear wave functions for the description of non-conservative systems, based on their conclusion that damping tends to destroy interference effects (decoherence) of two Gaussian wavepackets in a harmonic potential. Therefore, the protocol presented above through Bohmian mechanics can be used as a clue to a deeper understanding of nonlinear wave mechanics as well as to encourage usage of the well developed mathematical problem by solving methods of nonlinear differential equations to gather new insights and design some physical models.

Finally, it worth stressing that electron transport studies in nanostructure devices have also been described by the quantum hydrodynamic equations [82, 83].

3.7 The Schrödinger Equation for an Extended Electron via Bohmian Mechanics

About a century ago, Lorentz [84, 85] and Abraham [86] argued that when an electron is accelerated, there are additional forces acting due to the electron's own electromagnetic field. However, the so-called Lorentz–Abraham equation for a point-charge electron

$$m\frac{dV}{dt} = \frac{2e^2}{3c^3}\frac{d^2V}{dt^2} + F_{ext} \tag{3.151}$$

was found to be unsatisfactory because, for $F_{ext} = 0$, it admits runaway solutions. These solutions clearly violate the law of inertia.

Since the seminal works of Lorentz and Abraham, inumerous papers and textbooks have given great consideration to the proper equation of motion of an electron

[87–97]. The problematic runaway solutions were circumvented by Sommerfeld [91] and Page [92] by going to an extended model. In the nonrelativistic case of a sphere with uniform surface charge, such an electron obeys in good approximation the difference-differential equation [93–95]

$$m\frac{dV}{dt} = \frac{e^2}{3L^2c}\left[V(t - 2L/c) - V(t)\right] + F_{ext}. \tag{3.152}$$

This extended model is finite and causal if the electron size L is larger than the classical electron radius $r_e = e^2/\mathrm{mc}^2$. In the following, discussion here is limited to the sphere with uniform surface charge since the case of a volume charge is considerably more complicated and adds nothing to the understanding of the problem.

The dynamics of charges is a key example of the importance of obeying the validity limits of a physical theory. If classical equations can no longer be trusted at distances of the order of (or below) the Compton wavelength $\lambda = h/mc$, c being the speed of light, what is the Schrödinger equation that can replace Eq. (3.152). Within quantum electrodynamics (QED), it has not been able to derive an equation of motion and it is unclear whether QED can actually produce an equation of motion at all. A simple solution to this problem in the nonrelativistic regime is proposed here.

A new quantum mechanical wave equation describing the dynamics of an extended electron is derived via Bohmian mechanics. The solution to this equation is found through a wave packet approach which establishes a direct correlation between a classical variable with a quantum variable describing the dynamics of the center of mass and the width of the electron wave packet. It is shown that the new Schrödinger equation is free of any runaway solutions or any acausal responses. Besides, this approach provides a comparatively clearer picture than the modern time quantum approach carried out by Moniz and Sharp [95]. They derived an infinite order differential equation, i.e., an infinite series of derivatives that apparently can not be summed.

As we know, the Bohmian framework ascribes a particle motion via the de Broglie guidance condition (in one dimension)

$$\frac{dx}{dt} = v(x,t)|_{x=x(t)} = \frac{1}{m}\frac{\partial S}{\partial x}\bigg|_{x=x(t)} \tag{3.153}$$

where v represents the particle velocity and S is the phase of the wave function Ψ written in polar form, [67] Eq. (3.28). In this formalism, Schrödinger's equation can be recast as in Eqs. (3.30) and (3.31). Within this framework, a quantum extension to the Sommerfeld-Page equation (3.152) for an electron sphere with uniform surface charge in the absence of external forces can be accomplished by writing

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = \frac{e^2}{3mL^2c}\left[v(t - 2L/c) - v(t)\right] + \frac{1}{m}\frac{\partial}{\partial x}\left(\frac{\hbar^2}{2m\sqrt{\rho}}\frac{\partial^2\sqrt{\rho}}{\partial x^2}\right). \tag{3.154}$$

Then, Eqs. (3.28) and (3.154) yield

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+\left\{\frac{i\hbar e^2}{6mL^2c}\ln\left(\frac{\Psi(x,t-2L/c)\Psi^*(x,t)}{\Psi^*(x,t-2L/c)\Psi(x,t)}\right)\right\}\Psi(x,t). \tag{3.155}$$

In order to find the most general Gaussian wave packet solution to Eq. (3.155), the usual ansatz is made according to Eq. (3.33). First, Eq. (3.33) is substituted into (3.30) and integrated the result being Eq. (3.34) where the constant of integration must be zero since ρ and $\rho\,(\partial S/\partial x)$ vanish for $|x|\to\infty$. In fact, any well-behaved function of $(x-q)$ multiplied by ρ clearly vanishes as $|x|\to\infty$. Then, substitution of Eqs. (3.33) and (3.145) into (3.154) yields

$$\frac{m}{2a(t)}\left\{\ddot{\delta}(t)-\frac{e^2}{3mL^2c}\left[\dot{\delta}(t-2L/c)-\dot{\delta}(t)\right]-\frac{\hbar^2}{4m^2\delta^3(t)}\right\}[x-q(t)]^2+$$
$$m\left\{\ddot{q}(t)-\frac{e^2}{3mL^2c}\left[\dot{q}(t-2L/c)-\dot{q}(t)\right]\right\}[x-q(t)]=0. \tag{3.156}$$

This polynomial equation is satisfied once the coefficients of $[x-q(t)]$ and $[x-q(t)]^2$ are set equal to zero, namely,

$$\ddot{q}(t)-\frac{e^2}{3mL^2c}\left[\dot{q}(t-2L/c)-\dot{q}(t)\right]=0 \tag{3.157}$$

and

$$\ddot{\delta}(t)-\frac{e^2}{3mL^2c}\left[\dot{\delta}(t-2L/c)-\dot{\delta}(t)\right]=\frac{\hbar^2}{4m^2\delta^3(t)}. \tag{3.158}$$

The wave packet dynamics is now completely determined by Eqs. (3.157) and (3.158). The first equation is the Sommerfeld-Page equation (describing here the time evolution of center of the wave packet) which does not have runaway solutions [95]. The second equation describing the time evolution of the width of the wave packet can be considered as a new result. This equation is free of any runaway solutions or any acausal response due of the restrictive term on the right hand side: physically this means that for $t>2e^2/3mc^3$ (which is the time required for light to traverse the extended electron) this term settles down the dynamics of the wave packet.

To sum up, this new formulation to describe the nonrelativistic quantum dynamics of an extended electron provides then a comparatively clearer picture than other formulations using elaborative manipulation of infinite series of operators. The approach here is also reasonable because the electron is smeared out due to the uncertainty principle and has the appropriate feature of a wave packet. In fact, there exists as yet no proper formulation in QED (and may not be possible within QED as a

perturbation theory). The only calculation by QED was reported by Low [98], who has not been able to derive an equation of motion and it is unclear whether QED can actually produce an equation of motion at all. As far we know, this treatment presents the only nonrelativistic Schrödinger equation available to describe the problem. Further, Eq. (3.155) may be used to investigate quantum tunneling through potential barriers in light of the work developed by Denef et al. on the so-called classical tunneling [99] and described previously.

Finally, Eqs. (3.30) and (3.31) have also been proposed to be macroscopic equations for many superconducting particles in the same state [100]. In this case, the external potential is derived from the Lorentz force when an electric and magnetic field are considered.

3.8 Surface Diffusion

The main purpose of spectroscopic experiments involving a probe and a system at thermal equilibrium with a reservoir (or thermal bath) consists of measuring the system response under the perturbation caused by the probe. As established by the so-called fluctuation-dissipation theorem, the intrinsic properties of matter can be extracted by analyzing the response which many times can be described by first order perturbation theory and determined by the spectrum of the spontaneous fluctuations of the reservoir. Within this linear approximation, the probability per time unit that the full system formed by the probe and reservoir changes from the initial state to the final state is given by the Fermi Golden rule. Within the Born approximation in scattering theory, the nature of the scattered particles as well as the details of the system-probe interaction potential are largely irrelevant, this essentially reducing the scattering problem to a typical statistical mechanics problem [101]. The linear response function of a system consisting of interacting particles, also known as the dynamic structure factor, can then be related to the spontaneous-fluctuation spectrum.

As mentioned in the Introduction, the system–plus–bath approach is perhaps the most successful and useful way to deal with stochastic dynamics, since it starts from the physical system of interest and its environment (or bath) forming all together a conservative system. For open quantum systems, it seems to be the most natural approach. Within this system–plus–bath approach, the corresponding dynamics is commonly described by a total Hamiltonian which is split up into three different parts

$$H = H_S + H_B + H_{SB}, \tag{3.159}$$

where H_S and H_B correspond to the free evolution of the system and the reservoir or bath, respectively, and H_{SB} describes the interaction between them. In this total Hamiltonian, the system usually consists of a few degrees of freedom, while the environment is formed by a huge number of them (even infinity). Moreover, it is reasonable to assume that the coupling between them is a linear function of the bath

coordinates. This property of linearity is very convenient, since it is then very easy to eliminate the bath coordinates in an exact way.

Let us consider briefly the Caldeira-Leggett Hamiltonian model [102, 103]. The role of initial conditions has also been largely discussed in this model since some problems when solving the Langevin equation can appear [104, 105]. This model has been applied (and it is still applying) to physical problems with linear dissipation. In particular, we are going to focus here on atom surface diffusion and the vibrational relaxation of a particle adsorbed (or adsorbate or adparticle) on a surface [106, 107]. Within this context, space–time correlation functions play a key role, since they are used to describe the decay of spontaneous thermal fluctuations at surfaces, this being central to the study of transport phenomena. These functions are defined as the thermodynamic average of the product of two dynamical variables, each one expressing the instantaneous deviation from its corresponding equilibrium value at particular points on the surface and time. A complete description of the particle dynamics in a many–body system is then reached when the behavior of the corresponding correlation functions over the entire wavenumber range (small and long wavelengths) is studied. This range splits into different characteristic regions, each one associated with a different set of properties of the system. Space–time correlation functions can also be used to describe the linear response of a fluid under a weak, external perturbation.

In the quasielastic He atom scattering (QHAS) technique, time–of–flight measurements are converted to energy transfer spectra, from which a wide energy range can be spanned and several peaks are observed. The prominent peak around the zero energy transfer, namely the quasi–elastic peak (Q–peak), gives information about the adsorbate diffusion process. Additional weaker peaks at low energy transfers around the Q–peak are also observed. These peaks are attributed to the parallel (to the surface) frustrated translational motion of the adsorbates (T–mode) and also to the excitations of surface phonons —at positive energy transfers we have creation processes, and annihilation ones at negative energy transfers. The measurable quantity experimentally is the so–called dynamic structure factor or scattering law which gives the lineshapes of all those elementary processes; in particular, those corresponding to the Q and T peaks. The dynamic structure factor provides information about the dynamics and structure of the adsorbates through particle distribution functions and these ones are related to the nature of the adsorbate–substrate and adsorbate–adsorbate interactions.

In QAHS experiments, one is usually interested in the differential reflection coefficient, which can be expressed as

$$\frac{d^2\mathcal{R}(\Delta\mathbf{K},\omega)}{d\Omega d\omega} = n_d F S(\Delta\mathbf{K},\omega) \tag{3.160}$$

in analogy to scattering of slow neutrons by crystals and liquids [108, 109]. This magnitude gives the probability that the probe (He) atoms scattered from the diffusing collective (spread out along the surface) reach a certain solid angle Ω with an energy exchange $\hbar\omega = E_f - E_i$ and a parallel (to the surface) momentum transfer

$\Delta\mathbf{K} = \mathbf{K}_f - \mathbf{K}_i$. In Eq. (3.160), n_d is the (diffusing) surface concentration of adparticles; F is the atomic form factor, which depends on the interaction potential between the probe atoms in the beam and the adparticles on the surface; and $S(\Delta\mathbf{K}, \omega)$ is the dynamic structure factor, which gives the lineshapes of the Q and T peaks — other peaks can also be present, such as the inelastic ones related to surface phonon excitations— and provides a complete information about the dynamics and structure of the adsorbates through particle distribution functions. Experimental information about long distance correlations is obtained from the scattering law when considering small values of $\Delta\mathbf{K}$, while information on long time correlations is available at small energy transfers, $\hbar\omega$.

Surface diffusion is a dynamical problem that can be tackled by means of classical mechanics for heavy adsorbates or adparticles. For light adsorbates, quantum mechanics has to be applied and their positions are replaced by position operator. Thus, let us consider an ensemble of classical/quantum interacting particles on a surface. Their distribution functions are described by means of the so–called van Hove or time–dependent pair correlation function $G(\mathbf{R}, t)$ [108]. This function is related to the dynamic structure factor as

$$S(\Delta\mathbf{K}, \omega) = \iint G(\mathbf{R}, t) e^{i(\Delta\mathbf{K}\cdot\mathbf{R} - \omega t)}\, d\mathbf{R}\, dt. \tag{3.161}$$

Given an adparticle at the origin at some arbitrary initial time, $G(\mathbf{R}, t)$ represents the average probability for finding a particle (the same or another one) at the surface position $\mathbf{R} = (x, y)$ at a time t. Note that this function is a generalization of the well–known pair distribution function $g(\mathbf{R})$ from statistical mechanics [110], since it provides information about the interacting particle dynamics.

Depending on whether correlations of an adparticle with itself or with another one are considered, a distinction can be made between the self correlation function, $G_s(\mathbf{R}, t)$, and the distinct correlation function, $G_d(\mathbf{R}, t)$. The full pair correlation function can then be expressed as

$$G(\mathbf{R}, t) = G_s(\mathbf{R}, t) + G_d(\mathbf{R}, t). \tag{3.162}$$

According to its definition, $G_s(\mathbf{R}, t)$ is peaked at $t = 0$ and approaches zero as time increases because the adparticle loses correlation with itself. On the other hand, at $t = 0$, $G_d(\mathbf{R}, 0) \equiv g(\mathbf{R})$ gives the static pair correlation function (the standard pair distribution function), while it approaches the mean surface number density σ of diffusing particles as $t \to \infty$. Accordingly, Eq. (3.162) can be split up as

$$G(\mathbf{R}, 0) = \delta(\mathbf{R}) + g(\mathbf{R}) \tag{3.163}$$

at $t = 0$, and expressed as

$$G(\mathbf{R}, t) \approx \sigma \tag{3.164}$$

for a homogeneous system with $\|\mathbf{R}\| \to \infty$ and/or $t \to \infty$. At low adparticle concentrations (coverage, $\theta \ll 1$), when interactions among adsorbates can be neglected because they are far apart from each other, the main contribution to (3.162) is G_s (particle–particle correlations are negligible and $G_d \approx 0$). On the contrary, for high coverages, it is expected that G_d presents a significant contribution to (3.162).

Within this theoretical framework, the dynamic structure factor is better written as [108]

$$S(\Delta\mathbf{K}, \omega) = \int e^{-i\omega t}\, I(\Delta\mathbf{K}, t)\, dt, \tag{3.165}$$

where

$$I(\Delta\mathbf{K}, t) \equiv \frac{1}{N}\left\langle \sum_{j,j'}^{N} e^{-i\,\Delta\mathbf{K}\cdot\mathbf{R}_j(0)} e^{i\,\Delta\mathbf{K}\cdot\mathbf{R}_{j'}(t)} \right\rangle \tag{3.166}$$

is the so-called intermediate scattering function —note that this function is the space Fourier transform of $G(\mathbf{R}, t)$. In Eq. (3.166) the brackets denote an ensemble average and $\mathbf{R}_j(t)$ the trajectory of the j adparticle on the surface. This function can be split into two sums, distinct (I_d) and self (I_s), if the crossing terms are taken into account or not, respectively. Following neutron scattering language, the corresponding Fourier transforms of I and I_s give what is called the coherent scattering law, $S(\Delta\mathbf{K}, \omega)$, and incoherent scattering law $S_s(\Delta\mathbf{K}, \omega)$, respectively. In QHAS experiments, and with interacting adsorbates, coherent scattering is always obtained. The corresponding theoretical interpretation of that scattering is usually carried out in terms of the Vineyard convolution approximation [109] where the distinct correlation function G_d is expressed as a convolution of the self correlation function G_s. This approximation is known to fail at small distances where the surface lattice becomes important. Whereas in neutron scattering many attempts to improve the convolution approximation have been developed, in the QHAS context very little effort has been devoted to this goal.

In order to go a step further into the dynamics, a Hamiltonian has to be specified. In surface diffusion, the full system+bath Hamiltonian is usually written as [106, 107]

$$\begin{aligned} H = {} & \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + V(x, y) \\ & + \frac{1}{2}\sum_{j=1}^{N}\left[\frac{p_{x_j}^2}{m_j} + m_j\omega_{x_j}^2\left(x_j - \frac{c_{x_j}}{m_j\omega_{x_j}^2}\,x\right)^2\right] \\ & + \frac{1}{2}\sum_{j=1}^{N}\left[\frac{p_{y_j}^2}{m_j} + m_j\omega_{y_j}^2\left(y_j - \frac{c_{y_j}}{m_j\omega_{y_j}^2}\,y\right)^2\right], \end{aligned} \tag{3.167}$$

where (p_x, p_y) and (x, y) are the adparticle momenta and positions with mass m; and (p_{x_i}, x_i) and (p_{y_i}, y_i) with $i = 1, \ldots, N$ are the momenta and positions of the bath oscillators (phonons), with mass and frequency given by m_i and ω_i, respectively.

Phonons with polarization along the z–direction are not considered. The Hamiltonian was originally considered by Magalinskii and Caldeira and Leggett, who used it for weak and strong dissipation (a general discussion about the Hamiltonian (3.167) can be found in [2]). In surface diffusion, $V(x, y)$ is in general a periodic function describing the surface corrugation at zero temperature. The harmonic frequencies of the bath modes and the coupling coefficients are expressed in terms of spectral densities, defined as

$$J_i(\omega) = \frac{\pi}{2} \sum_{j=1}^{N} \frac{c_{i_j}^2}{m_j \omega_{i_j}^2} \left[\delta(\omega - \omega_{i_j})\right]. \tag{3.168}$$

with $i = x, y$. These densities enable the passage to a continuum model.

In the Heisenberg picture, the time evolution of the position operators is given by the generalized Langevin (GL) equation for each system coordinate

$$m\ddot{x}(t) + m \int_0^t \gamma_x(t - t')\, \dot{x}(t')\, dt' + \frac{\partial V(x, y)}{\partial x} = \xi_x(t), \tag{3.169a}$$

$$m\ddot{y}(t) + m \int_0^t \gamma_y(t - t')\, \dot{y}(t')\, dt' + \frac{\partial V(x, y)}{\partial y} = \xi_y(t), \tag{3.169b}$$

where the associated friction functions are defined through the cosine Fourier transform of the spectral densities,

$$\gamma_i(t) = \frac{2}{\pi m} \int_0^{\infty} \frac{J_i(\omega)}{\omega} \cos \omega t \; d\omega, \tag{3.170}$$

with $i = x, y$. The nonhomogeneity of (3.169) represents a fluctuating or random force ξ (when introducing the SL equation in Sect. 3.2, this force was labeled by F_r) for each degree of freedom which depend on the initial position of the system and initial positions and momenta of the oscillators of each bath [2]

$$\xi_x(t) = -\sum_j c_{x_j} \left\{ \left[x_j(0) + \frac{c_{x_j}(0)}{m_j \omega_{x_j}^2}\, x(0) \right] \cos(\omega_{x_j} t) + \frac{p_{x_j}(0)}{m_j \omega_{x_j}} \sin(\omega_{x_j} t) \right\}. \tag{3.171}$$

and

$$\xi_y(t) = -\sum_j c_{y_j} \left\{ \left[y_j(0) + \frac{c_{y_j}(0)}{m_j \omega_{y_j}^2}\, y(0) \right] \cos(\omega_{y_j} t) + \frac{p_{y_j}(0)}{m_j \omega_{y_j}} \sin(\omega_{y_j} t) \right\}. \tag{3.172}$$

For each cartesian component of the noise, it can be easily shown that its equilibrium (canonical ensemble) expectation value with respect to the heat bath including the

corresponding bilinear coupling to the system vanishes. On the contrary, the noise autocorrelation function (each cartesian component) is a complex quantity because in general it does not commute at different times. In the classical limit $\hbar \to 0$, each noise correlation reduces to $mk_BT\gamma_i(t)$, with $i = x, y$. For Ohmic friction, $\gamma_i(t) = 2\gamma_i\delta(t)$, where γ_i is a constant and $\delta(t)$ is Dirac's δ–function. Under the assumption of Ohmic friction, it can be shown that noise in this model is white. The paradigm of this type of noise is the *Gaussian white noise*. Dealing with large systems (the surface seen as a thermal bath) where the number of collisions between substrate and adsorbate is very high, one of the fundamental theorems of the theory of probability, namely the central limit theorem, ensures that the fluctuations of the bath will be Gaussian distributed. Diffusion can then be described by a Brownian-type motion involving a continuous Gaussian stochastic process. In virtue of the fluctuation–dissipation theorem, such fluctuations can be related to the friction coming mainly from surface phonons: the phonon friction. Electronic friction due to low-lying electron–hole pair excitations is usually neglected in most of cases. Moreover, quantum mechanically [2], for Ohmic friction the imaginary part of each noise function is a step function and its real part goes with $\mathrm{csch}^2(\pi t/\hbar\beta)$. Thus, at zero surface temperature, the noise is still correlated even for long time (it decays as t^{-2}) in contrast to the classical case. These facts give rise to important differences with respect to the classical case such as, for example, the noise and the system coordinates are correlated instead of being zero. In particular, in classical mechanics, the random force can be neglected at zero temperature, but quantum-mechanically this force is always present due to the zero point motion.

In order to simplify this theoretical treatment, only classical noise will be considered, though keeping in mind that the quantum results will be only valid for not too low surface temperatures. Moreover, the motion of only one adsorbate is considered within the so-called single adsorbate approximation since, for very low coverage, adparticles are considered non-interacting. Thus, if Ohmic friction is assumed, Eqs. (3.169) reduce to two coupled standard Langevin equations[1] (Markovian approximation),

$$m\ddot{x}(t) + m\gamma_x(t)\,\dot{x}(t) + \frac{\partial V(x,y)}{\partial x} = \xi_x(t), \tag{3.173a}$$

$$m\ddot{y}(t) + m\gamma_y(t)\,\dot{y}(t) + \frac{\partial V(x,y)}{\partial y} = \xi_y(t). \tag{3.173b}$$

In Fig. 3.4, one classical stochastic trajectory driven by a Gaussian white noise is plotted, which simulates a realization of a two–dimensional Brownian motion. In order to obtain information about the diffusion process, a swarm of these trajectories (i.e., a sampling over many Brownian realizations) should be considered.

[1] The δ–function counts only one half when the integration is carried out from zero to infinity.

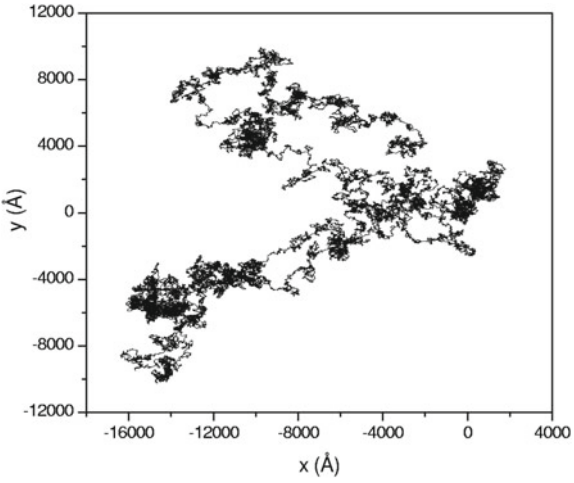

Fig. 3.4 As an example of Brownian motion driven by a Gaussian white noise, the classical stochastic trajectory pursued by a Na atom is displayed here at $T = 300\,\mathrm{K}$, though on a flat surface ($V = 0$). The friction constant is $\gamma = 0.5\ \mathrm{ps}^{-1}$ and the evolution is up to $t = 20,000\,\mathrm{ps}$

When dealing with higher coverages, adsorbate–adsorbate interactions can no longer be neglected. In this case, the adsorbate–surface interaction can still be described as before, but pairwise potential functions accounting for the adsorbate–adsorbate interactions are usually introduced into Langevin molecular dynamics simulations [111]. Moreover, these simulations always result in a relatively high computational cost due to the time spent by the codes in the evaluation of the forces among particles. This problem is even worse when working with long–range interactions, since *a priori* they imply that one should consider a relatively large number of particles in order to get a good numerical simulation. An alternative approach is to consider a purely stochastic description for these interactions [112–115]. This description, which is denominated the interacting single adsorbate approximation, is a fully Langevin approach based on the theory of spectral–line collisional broadening developed by Van Vleck and Weisskopf [116] and the elementary kinetic theory of gases [110]. In this approach, the motion of a single adsorbate is modelled by a series of random pulses within a Markovian regime (i.e., pulses of relatively short duration in comparison with the system relaxation); the pulses simulate the collisions with other adsorbates. In particular, we describe these adsorbate–adsorbate collisions by means of a white shot noise as a limiting case of a colored shot noise [7]. For a good simulation of a diffusion process, one has to consider very long times in comparison to the timescales associated with the friction caused by the surface or with the typical vibrational frequencies observed when the adsorbates keep moving inside a surface well. This means that there will be a considerably large number of collisions during the time elapsed in the propagation, and therefore that, at some point, the past history of the adsorbate could be irrelevant. This memory loss is a signature of a Markovian dynamical regime, where adsorbates have reached what is called the statistical limit. Otherwise, for timescales relatively short, the interaction is not Markovian and it is very important to take into account the effects of the interaction on the particle and its

dynamics (memory effects). The diffusion of a single adsorbate is thus modeled by a series of random pulses within a Markovian regime (i.e., pulses of relatively short duration in comparison with the system relaxation) simulating collisions between adsorbates. In particular, we describe these adsorbate–adsorbate collisions by means of a white shot noise [7] as a limiting case of colored shot noise. In this way, a typical molecular dynamics simulation problem involving N adsorbates is substituted by the dynamics of a single adsorbate, where the action of the remaining $N-1$ adparticles is replaced by a random force given by the white shot noise. Furthermore, the surface coverage can be related to a collisional friction providing the average number of collision per unit time, γ_c [114, 115], where the probability of observing a given number of collisions, after a certain time, follows a Poisson distribution. In brief, the adsorbate is subject to a two white noises, one coming from the substrate and the other from the surrounding adsorbates; both noises being uncorrelated. Thus, the total friction coefficient η for the interacting single adsorbate model is a sum of two friction coefficients, $\eta = \gamma + \gamma_c$ and the total noise is given by $\xi = \xi_G + \xi_S$ (G comes from Gaussian and S from shot) for each degree of freedom (x, y).

In this interacting single adsorbate approximation, and within a classical framework, the distinction between self and distinct time–dependent pair correlation function does not exist and Eqs. (3.161) and (3.165) still hold. The intermediate scattering function reads now as

$$I(\Delta\mathbf{K}, t) \equiv \langle e^{-i\,\Delta\mathbf{K}\cdot[\mathbf{R}(t)-\mathbf{R}(0)]}\rangle = \langle e^{-i\,\Delta\mathbf{K}\cdot\int_0^t \mathbf{v}(t')\,dt'}\rangle \tag{3.174}$$

In order to get some analytical results and therefore a guide for the interpretation of the numerical Langevin simulations, the intermediate scattering function can be expressed as a second order cumulant expansion in $\Delta\mathbf{K}$,

$$I(\Delta\mathbf{K}, t) \approx e^{-\Delta K^2 \int_0^t (t-t')\mathcal{C}_{\Delta\mathbf{K}}(t')dt'}, \tag{3.175}$$

where

$$\mathcal{C}_{\Delta\mathbf{K}}(\tau) \equiv \langle v_{\Delta\mathbf{K}}(0)\, v_{\Delta\mathbf{K}}(\tau)\rangle \equiv \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} v_{\Delta\mathbf{K}}(t)\, v_{\Delta\mathbf{K}}(t+\tau)\, dt \tag{3.176}$$

is the *autocorrelation function* of the velocity projected onto the direction of the parallel momentum transfer (whose length is $\Delta K \equiv \|\Delta\mathbf{K}\|$). Only differences between two times, τ, are considered because this function is *stationary*. This is the so–called *Gaussian approximation* [110], which is exact when the velocity correlations at more than two different times are negligible, thus allowing to replace the average acting over the exponential function by an average acting over its argument. These approximation results of much help in the interpretation of the numerical results as well as in getting an insight into the underlying dynamics.

The decay of $\mathcal{C}_{\Delta\mathbf{K}}(\tau)$ allows to define a characteristic time, the so-called correlation time,

$$\tilde{\tau} \equiv \frac{1}{\langle v_0^2 \rangle} \int_0^\infty \mathcal{C}_{\Delta \mathbf{K}}(\tau)\, d\tau, \tag{3.177}$$

where $\sqrt{\langle v_0^2 \rangle} = \sqrt{k_B T/m}$ is the average thermal velocity in one dimension —though the dimensionality is two, note that $\mathcal{C}_{\Delta \mathbf{K}}$ is defined along a particular direction (that given by $\Delta \mathbf{K}$) and therefore $\mathcal{C}_{\Delta \mathbf{K}}(0) \equiv k_B T/m$, i.e., the thermal velocity in one direction. The correlation time is related to the lineshape broadening in the sense that it provides a timescale for the decay of the intermediate scattering function and therefore information about the width of the Q–peak in the dynamic structure factor.

On the contrary, if we are dealing with quantum position operators, Eq. (3.174) is not longer valid due to the fact that the position operators at two different times do not commute. However, it is possible to factorize the intermediate scattering function in two factors, one of them being precisely that given by Eq. (3.174) [107].

In order to better understand the shape and broadening of the Q and T peaks within the SLB equation formalism, two simple cases are considered. In the first case, the simplest illustration for the Q-peak is to assume a Brownian motion of the adsorbates with $V(x, y) = 0$; that is, the diffusion of adsorbates on a flat surface. And the second one, for the T-peak, a good model is that provided by the harmonic oscillator motion in a potential well of a periodic corrugated surface.

3.8.1 The Bohmian–Brownian Motion

Apart from considering the interaction potential zero, one also can assume the diffusion of adsorbates on low corrugated surfaces where the energy provided by the surface temperature can easily surmount the corresponding energy barrier. Thus, the adparticle motion can be regarded as quasi–free since it is not ruled by a potential, but only influenced by stochastic forces. It can be shown [115])

$$\mathcal{C}(\tau) = \frac{k_B T}{m}\, e^{-\eta \tau}. \tag{3.178}$$

Unless the relaxation of the collisional effects can be of relevance, these effects and those caused by the surface should be indistinguishable and therefore (3.178) would describe accurately the loss of correlation, with $\tilde{\tau} = \eta^{-1}$.

The expression for the intermediate scattering function that results from (3.178) is

$$I(\Delta K, t) = \exp\left[-\chi^2 \left(e^{-\eta t} + \eta t - 1\right)\right], \tag{3.179}$$

where the so–called shape parameter χ is defined as

$$\chi^2 \equiv \frac{\langle v_0^2 \rangle \Delta K^2}{\eta^2} = \frac{D \Delta K^2}{\eta}. \tag{3.180}$$

From this relation we can extract both the mean free path, $\bar{l} \equiv \tilde{\tau}\sqrt{\langle v_0^2 \rangle}$, and the self–diffusion coefficient D which is also given by Einstein's relation

$$\begin{aligned} D &= \lim_{t\to\infty} \int_0^t \mathcal{C}(t')dt' \\ &= \frac{k_B T}{m\eta}. \end{aligned} \tag{3.181}$$

This ensures that the adparticle velocity distribution becomes Maxwellian asymptotically. The same result is reached from the mean squared displacement (MSD)

$$D = \lim_{t\to\infty} \frac{1}{4t} < (\mathbf{R}(t) - \mathbf{R}(0))^2 > . \tag{3.182}$$

When the coverage increases, the collisions among adsorbates are also expected to increase, and so λ and therefore η. As can be easily shown, (3.179) displays a Gaussian decay at short times that does not depend on the particular value of η, while at longer times it decays exponentially as ηt. Thus, two dynamical regimes can be clearly distinguished depending on the value of ηt. For $\eta t << 1$, collision events are rare and the adparticle shows an almost free motion with relatively long mean free paths. This is the ballistic or free-diffusion regime characterized by the MSD

$$\langle q^2(t) \rangle \sim \frac{k_B T}{m} t^2. \tag{3.183}$$

On the other hand, for $\eta t << 1$, there is no free diffusion since the effects of the stochastic force are dominant. This is the diffusive regime where the MSD is linear with time according to

$$\langle q^2(t) \rangle \sim \frac{2k_B T}{m\eta} t = 2Dt \tag{3.184}$$

which is an alternative way to express Einstein's law.

The type of decay is important concerning the width and shape of the dynamic structure factor which is analytically obtained from the time Fourier transform of Eq. (3.179),

$$S(\Delta K, \omega) = \frac{e^{\chi^2}}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n \chi^{2n}}{n!} \frac{(\chi^2 + n)\eta}{\omega^2 + [(\chi^2 + n)\eta]^2} . \tag{3.185}$$

As can be seen in the high friction limit, this function becomes a Lorentzian function which its full width at half maximum (FWHM) is $\Gamma = 2\eta\chi^2$. Thus, D is experimentally extracted from this width and following Eq. (3.180). Furthermore, Γ is approaching zero as η increases (narrowing effect). This in sharp contrast to what one could expect - as the frequency between successive collisions increases one would expect that the line shape gets broader (effect of the pressure in the spectral

line shapes of gases [116]). The physical reason for this effect is relatively simple: as η increases the particle's mean free path decreases and therefore correlations are lost more slowly. In the limit case where friction is such that the particle remains in the same place, the space-time correlation function becomes a δ, the intermediate scattering function remains equal to one and the dynamic structure factor will also consist of a δ–function at $\omega = 0$. Conversely, in the low friction limit, the line shape is given by a Gaussian function whose width is $\Gamma = 2\sqrt{2\ln 2}\sqrt{k_B T/m}\,\Delta K$, which does not depend on η. This is precisely the case of a two dimensional free gas. This gradual change of the line shapes as a function of the friction and/or the parallel momentum transfer leading to a change of the shape parameter is known as the motional narrowing effect. Remember that in this formalism the friction is related to the coverage. Thus, at higher coverages a narrowing effect is predicted for a flat surface [115].[2]

In the quantum regime within the Heisenberg representation, the standard quantum Langevin equation has the following formal solution

$$\mathbf{R}(t) = \mathbf{R}(0) + \frac{\mathbf{P}(0)}{m\eta}\Phi(\eta t) + \frac{1}{m\eta}\int_0^t \Phi(\eta t - \eta t')\xi(t')dt' \tag{3.186}$$

where $\mathbf{P}(0)$ is the initial adparticle momentum operator and $\Phi(\eta t) = 1 - exp(-\eta t)$ and ξ is the sum of the two noises (ξ_G and ξ_S) for (x, y). As mentioned above, the operators $\mathbf{R}(t)$ and $\mathbf{R}(0)$ do not commute each other, leading to a much more involved diffusion dynamics according to Eq. (3.174); for example,the velocity autocorrelation function is complex with several decaying constants.

In Fig. 3.5, the real and imaginary parts of Eq. (3.174) for Na diffusion on a flat surface are plotted at two different surface temperatures, 50 and 100 K, and two coverages, 0.028 and 0.18 [107]. As can be clearly seen, the real part of $I(t)$ decreases faster with temperature and slower with coverage. On the other hand, the imaginary part of $I(t)$ displays maxima between 4–6% of the corresponding real part, depending on the temperature. It starts linearly with time and, after passing through a maximum, decays smoothly to zero. The corresponding quasielastic line shapes (around the zero energy exchange) will then display narrowing with the coverage and broadening with the surface temperature. This behavior could be experimentally confirmed for those systems where the diffusion barrier is smaller than the thermal energy $k_B T$. For light particles, the imaginary part is expected to be much more important keeping the same shape. The scattering law for the Q-peak is no longer a simple sum of Lorentzian functions [107]. However, quantum effects are mainly important at low surface temperatures, except if the adorbate is very light.

[2] At finite coverages, one usually distinguishes between two diffusion coefficients: the tracer and the collective diffusion constants [117]. The first one refers to the self–diffusion process and focuses on the motion of a single adsorbate. On the contrary, the second is related to the collective motion of all adsorbates which is governed by Fick's law. In any case, a Kubo–Green formula relates both diffusion coefficients with the velocity autocorrelation function of a single adsorbate or with the corresponding of the velocity of the center of mass, respectively.

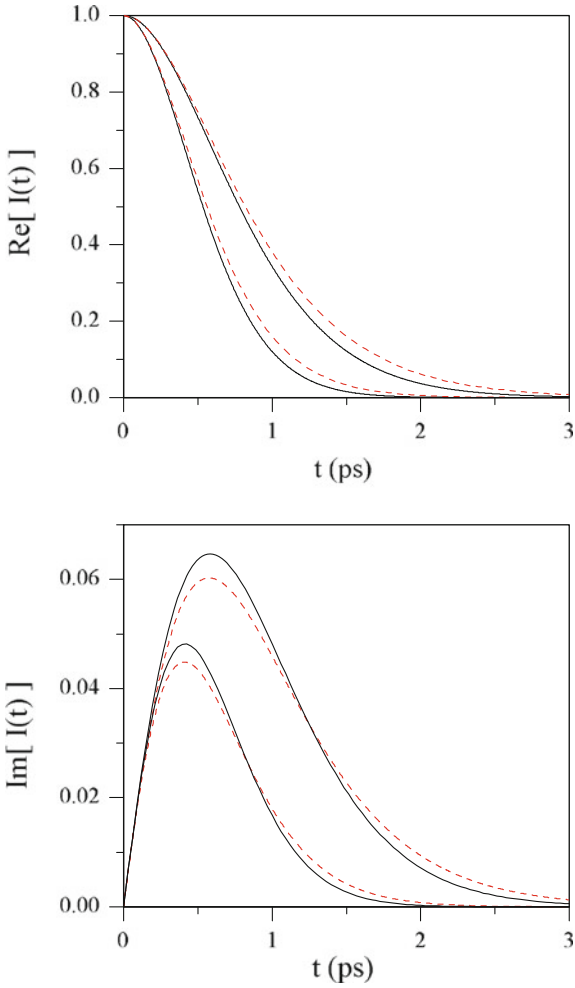

Fig. 3.5 Quantum intermediate scattering function (3.174) for Na diffusion on a flat surface at 50 and 100 K: **a** real part and **b** imaginary part. Two coverages are considered: $\theta = 0.028$ (*black solid line*) and $\theta = 0.18$ (*red dashed line*)

Once the simplest description of the surface diffusion (Brownian motion regime) is introduced, the next step is to see how the SLB formalism is applied to this very fundamental quantum process. In Sect. 3.3, we have discussed the free regime problem $V = 0$ with no random force. For simplicity and without loss of generality, we are going to deal with a one dimensional quantum surface diffusion (light adparticles). By starting from Eq. (3.29), and assuming a Gaussian probability density given by Eq. (3.33) for an adsorbate, the quantum trajectories are expressed by Eq. (3.38), which comes from a direct integration of Eq. (3.36) in time, and Eq. (3.39) ruling the time evolution of the wave packet width. Under the presence of noise, the quantum trajectory has the following expression

$$x(t) = q(0) + \frac{\dot{q}(0)}{\eta}\Phi(\eta t) + \frac{1}{m\eta}\int_0^t \Phi(\eta t - \eta t')\xi(t')dt' + (x(0) - q(0))\frac{\delta(t)}{\delta(0)} \tag{3.187}$$

where the classical trajectory $q(t)$ has been rewritten from Eq. (3.186).

In this diffusion problem, a critical function is the velocity autocorrelation function $\mathcal{C}_{\Delta\mathbf{K}}(\tau)$ which is defined along with the direction given by $\Delta\mathbf{K}$. For a flat surface, diffusion is isotropic (however, for a corrugated surface, that direction can be determined by a symmetry direction of the surface). After Eq. (3.36), we have that the quantum autocorrelation function is

$$\mathcal{C}_{\Delta\mathbf{K}}(t) \equiv \langle v(0)v(t)\rangle = \langle \dot{q}(0)\dot{q}(t)\rangle + \langle (x(0) - q(0))^2\rangle \frac{\dot{\delta}(0)}{\delta(0)^2}\dot{\delta}(t) \tag{3.188}$$

since $\langle \dot{q}(0)(x(0) - q(0))\rangle = 0$ and $\langle (x(0) - q(0))\dot{q}(t)\rangle = 0$, keeping the same structure than the quantum velocity, that is, a classical contribution given by the classical autocorrelation function and a quantum contribution governed by the time derivative of the Gaussian wave packet width (dressing scheme). Interestingly enough, when the initial velocity of spreading of the wave packet is zero, the quantum contribution disappears. In the long time limit, the classical contribution is simply given by Eq. (3.178). In this limit, the overdamped regime is established and therefore the acceleration term of the differential equation (3.41) for this width can be neglected. Thus, Eq. (3.188) is finally expressed

$$\langle v(0)v(t)\rangle = \frac{k_B T}{m} e^{-\eta\tau} + \langle (x(0) - q(0))^2\rangle \frac{\dot{\delta}(0)}{\delta(0)^2}\frac{\hbar^2}{4m\eta\delta(t)^3} \tag{3.189}$$

where $\delta(t)$ is asymptotically given by Eq. (3.44). Remember that the time dependence of $\delta(t)^{-3}$ comes from the quantum potential. Several important consequences are deduced from this time behavior. First, the line shape of the Q-peak is no longer a Lorentzian function; it is modified by the quantum contribution which goes with $t^{-3/4}$ according to Eqs. (3.175) and (3.165). Second, the relation of Einstein for the diffusion constant is also no longer valid. In fact, from Eq. (3.182),

$$< (x(t) - x(0))^2 > \propto t^{\alpha} \tag{3.190}$$

with $\alpha = 1/2$, indicating an anomalous diffusion process [118, 119]. In general, when the MSD is not linear in time, Einstein's relation is violated and the diffusion process can be described by a subdiffusion regime ($\alpha < 1$) or a superdiffusion regime ($\alpha > 1$), that is, slower or faster than ordinary Brownian motion [120]. Superdiffusion is originated by anomalous long jumps of a random walker while diffusion can be associated with unusually long waiting times between successive walks. A useful model to describe these processes is the so-called continuous time random walk. And third, this way is still completely unexplored and new studies need to be carried

out for a better understanding of this quantum anomalous diffusion. An open question is if for very light adparticles, surface diffusion can exhibit this anomalous behavior.

3.8.2 The Harmonic Oscillator Motion

The harmonic potential model is an appropriate working model to understand the bound motion inside the wells of a corrugated surface and, therefore, to also understand the behavior associated with the T-mode (observed through the so-called T-peak). This mode comes from the oscillating behavior undergone by the adparticle when the diffusional motion is temporarily frustrated.

In contrast with the case of a dynamics where the interaction potential with the surface does not play a relevant role, we can devise a particle fully trapped within a harmonic potential well. The velocity autocorrelation function can be expressed [107, 115] as

$$\mathcal{C}(\tau) = \frac{k_B T}{m} e^{-\eta\tau/2} \left(\cos \bar{\omega}\tau - \frac{\eta}{2\bar{\omega}} \sin \bar{\omega}\tau \right), \tag{3.191}$$

where

$$\bar{\omega} \equiv \sqrt{\omega_0^2 - \frac{\eta^2}{4}} \tag{3.192}$$

and ω_0 is the harmonic frequency. Equation (3.191) can also be recast as

$$\mathcal{C}(\tau) = \frac{k_B T}{m} \frac{\omega_0}{\bar{\omega}} e^{-\eta\tau/2} \cos(\bar{\omega}\tau + \delta), \tag{3.193}$$

with

$$\delta \equiv (\tan)^{-1} \left(\frac{\eta/2}{\bar{\omega}} \right). \tag{3.194}$$

Note that Eq. (3.178) can be easily recovered after some algebra in the limit $\omega_0 \to 0$ from either Eq. (3.191) or (3.193). For anharmonic potentials, ω_0 represents the corresponding approximate harmonic frequency.

The only information about the structure of the lattice is found in the shape parameter through ΔK. When large parallel momentum transfers are under consideration, both the periodicity and structure of the surface have to be taken into account. Consequently, the shape parameter should be changed for different lattices. The simplest model including the periodicity of the surface is that developed by Chudley and Elliott [121] who proposed a master equation for the pair–distribution function in space and time assuming instantaneous discrete jumps on a two–dimensional Bravais lattice. Very recently, a generalized shape parameter has been proposed to be [122]

$$\chi_l(\Delta\mathbf{K}) \equiv \sqrt{\frac{\Gamma_\nu(\Delta\mathbf{K})}{2\gamma}}, \tag{3.195}$$

where

$$\Gamma_\nu(\Delta\mathbf{K}) = \nu \sum_{\mathbf{j}} P_{\mathbf{j}} \left[1 - \cos(\mathbf{j} \cdot \Delta\mathbf{K})\right], \tag{3.196}$$

ν being the total jump rate out of an adsorption site, and $P_{\mathbf{j}}$ the relative probability that a jump with a displacement vector $\mathbf{j}$ occurs.

Introducing now Eq. (3.193) into (3.175), this leads to the following expression of the intermediate scattering function

$$I(\Delta K, t) = \exp\left\{-\frac{\chi_l^2 \eta^2}{\bar{\omega}\omega_0}\left[\cos\delta - e^{-\eta t/2}\cos(\bar{\omega}t - \delta)\right]\right\}. \tag{3.197}$$

The argument of this function displays an oscillatory behavior around a certain value with the amplitude of the oscillations being exponentially damped. This translates into an also decreasing behavior of the intermediate scattering function, which also displays oscillations around the asymptotic value. This means that after relaxation the intermediate scattering function has not fully decayed to zero unlike the free–potential case. It can be easily shown that in the limit $\omega_0 \to 0$, Eq. (3.197) approaches the result given by Eq. (3.179).

From (3.197) it is now straightforward to derive an expression for the dynamic scattering factor (the time Fourier transform of the corresponding intermediate scattering function), which results

$$S(\Delta K, \omega) \propto \sum_{m,n=0}^{\infty} \frac{(-1)^{m+n}}{m!\,n!}\, \chi_l^{2(m+n)}\, \frac{(2\chi_l^2 + m + n)\eta/2}{[\omega - (m-n)\bar{\omega}]^2 + [(2\chi_l^2 + m + n)\eta/2]^2}. \tag{3.198}$$

For a harmonic potential, there is no diffusion and, therefore, the line shapes (or scattering law) are only observed when $m \neq n$ consisting of Lorentzian functions related to vibrational excitations (creation and annihilation events of the T-mode). These Lorentzians are characterized by a width given by $\Gamma = (2\chi_l^2 + m + n)\eta/2$, which increases as η becomes larger. This broadening (proportional to η) undergone by the dynamic structure factor is thus contrary to the narrowing effect observed for a flat surface. It can be then assigned to the confined or bound motion displayed by the adparticle ensemble when trapped inside the potential wells. Hence, in order to detect broadening of the lineshapes in surface diffusion experiments, adparticles must spend some time confined inside potential wells, since it is induced by the presence of temporary vibrational motions.

On the other hand, the corresponding quantum trajectory in one-dimension has the following expression

$$x(t) = \left[q(0)cos(\bar{\omega}t) + \left(\frac{\dot{q}(0)}{m\bar{\omega}} + \frac{\gamma}{2\bar{\omega}} q(0) \right) sin(\bar{\omega}t) \right] e^{-\eta t/2} + \int_0^\infty \chi(t-t')\xi(t')dt' + (x(0) - q(0)) \frac{\delta(t)}{\delta(0)} \tag{3.199}$$

where the standard classical trajectory $q(t)$ is written in terms of the response function

$$\chi(t) = \Theta(t) \frac{1}{m\bar{\omega}} e^{-\eta t/2} sin(\bar{\omega}t) \tag{3.200}$$

with $\Theta(t)$ being the Heaviside function to ensures causality and $\delta(t)$ the width of the Gaussian wave packet which is governed by Eq. (3.39).

As said above, the velocity autocorrelation function has also two contributions, classical and quantum. Unfortunately, analytical expressions for this function as well as for the T-peak are no longer possible.

3.9 The Generalized Schrödinger–Langevin–Bohm Equation

As mentioned previously in the Introduction, in the system-plus-bath model, the dynamics is carried out in a conservative scenario. The so–called Caldeira-Leggett Hamiltonian [102] is the starting point leading to the generalized Langevin equation (GLE). One of the key issues is the interaction term which by construction is linear in the bath coordinates. For example, in one dimensional systems, the dependence on the system variable is through a function $f(x)$ which usually is separable and linear (linear dissipation). This scenario is known as a state–independent dissipation and can be seen as a measurement of particle's position by a reservoir in von Neumann's sense [2]. This function also appears in an additional term in the total Hamiltonian in order to avoid the renormalization of the interaction potential. In the Markovian regime with Ohmic (constant) friction, this GLE becomes the standard Langevin equation for a Brownian particle where noise is additive. As we have seen along this Chapter, Kostin [16, 17] established the link between this standard Langevin equation with the Schrödinger equation. The resulting logarithmic nonlinear equation is quite different from others existing in the literature such as the so–called stochastic Schrödinger equation and the Linblad equation for the density matrix [3].

For a nonlinear function $f(x)$, the open quantum system displays a state dependent dissipation process and the corresponding GLE exhibits multiplicative noise [33, 123]. Typical examples of nonlinear functions take place, for example, in rotational tunneling systems [124], quasi-particle tunneling in Josephson systems [125], in the Langevin canonical formulation of chiral two level systems [126], in atom surface

scattering [127] and so on. Within the Markovian regime, the standard Langevin equation with multiplicative noise is reached. The main purpose of this Section is to derive a generalization of the SLB equation for nonlinear dissipation.

Without loss of generality, a one dimensional problem is again considered. As mentioned at the beginning of this Chapter and in the previous section, for open systems, it is usual to split the total Hamiltonian into three parts including system, bath and mutual coupling after Eq. (3.159). Let us consider explicitly the different Hamiltonians

$$H_S = \frac{p^2}{2m} + V(x) \tag{3.201}$$

which stands for the Hamiltonian of the isolated system in presence of a force field given by the potential $V(x)$;

$$H_B = \frac{1}{2}\sum_i \left(\frac{p_i^2}{m_i} + m_i\omega_i^2 x_i^2\right) \tag{3.202}$$

is the Hamiltonian for the bath, which acts as a reservoir, and can be represented as an infinite set of harmonic oscillators; and

$$H_{SB} = \sum_i \left[\frac{f^2(x)d_i^2}{m_i\omega_i^2} - 2d_i f(x)x_i\right] \tag{3.203}$$

expressing the interaction term between the isolated system and the bath, d_i being appropriate coupling constants. The function $f(x)$ is, in general, a nonlinear function of the system variable x. The term with the squared of $f(x)$ gives the so–called counter term introduced to compensate the renormalization of the potential. Following the standard procedure where the bath degrees of freedom are eliminated, the equation of motion for the corresponding system dynamics in the Heisenberg picture of quantum mechanics is given by the GLE [102]

$$\begin{aligned} f'[x(t)]\,\xi(t) &= m\ddot{x}(t) + V'(x) \\ &+ mf'[x(t)]\int_0^t dt'\gamma(t-t')f'\left[x(t')\right]\dot{x}(t') \end{aligned} \tag{3.204}$$

where the time–dependent friction (memory kernel) is given by

$$\gamma(t) = \frac{1}{m}\sum_i \frac{d_i^2}{m_i\omega_i^2}\cos(\omega_i t) \tag{3.205}$$

and the external force (noise term) is expressed as (written in Sect. 3.2 as F_r)

$$\xi(t) = -\sum_i d_i \left[\left(x_i(0) + \frac{d_i}{m_i \omega_i^2} f(0) \right) \cos(\omega_i t) \right] - d_i \sum_i \left[\frac{p_i(0)}{m_i \omega_i} \sin(w_i t) \right]. \tag{3.206}$$

In the Markovian regime, the memory kernel is a δ–function in time, giving place to an Ohmic dissipation with a time–independent friction. Within this regime and for a nonlinear coupling, the corresponding standard Langevin equation reads as

$$m\ddot{x}(t) + m\gamma \left[f'(x) \right]^2 \dot{x}(t) + V'(x) = f'[x(t)]\, \xi(t). \tag{3.207}$$

Notice that the random force is multiplied by the derivative of the function $f(x)$ giving place to a stochastic process with multiplicative noise. When the system–bath coupling is linear, that is, for $f(x) = x$, the standard Langevin equation for additive noise (that is, when the noise term is not multiplied by any system function) with Ohmic friction is recovered

$$m\ddot{x}(t) + m\gamma \dot{x}(t) + V'(x) = \xi(t). \tag{3.208}$$

Following the Kostin procedure [16], the generalized SL equation (that is, for any $f(x)$) can be obtained by writing first the Schrödinger equation as

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[\frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x} \right)^2 + V(x) + V_D + V_r \right] \Psi, \tag{3.209}$$

where the random potential V_r is given by

$$V_r(x, t) = -f(x)\xi(t). \tag{3.210}$$

and V_D is the damping potential, Eq. (3.4). On the other hand, the quantum mechanical current is defined as

$$J = \frac{1}{2m} \left[\Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi + \Psi \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi^* \right] \tag{3.211}$$

Then, from $\partial\Psi/\partial t$ and $\partial\Psi^*/\partial t$ and Eq. (3.209) we have that

$$\frac{d}{dt}\langle x \rangle = \int J dx$$
$$\frac{d^2}{dt^2}\langle x \rangle = \int \frac{\partial J}{\partial t} dx. \tag{3.212}$$

where $< . >$ is the expectation value of a given operator. Now, by performing the same type of averaging into Eq. (3.207)

$$m\langle\ddot{x}(t)\rangle + m\gamma\langle\left[f'(x)\right]^2\dot{x}(t)\rangle + \langle V'(x)\rangle = \langle f'(x)\xi(t)\rangle, \tag{3.213}$$

and comparing it with Eq. (3.209) and using Eq. (3.212), we can identify terms leading to

$$\int \Psi^*\left(-\frac{\partial V_D}{\partial x}\right)\Psi dx = \gamma m\int f'(x)^2 J dx. \tag{3.214}$$

Thus, the damping potential is a functional of the wave function and can be expressed as

$$V_D\left[\Psi, \Psi^*, f\right] = -m\gamma\int\frac{\tilde{J}}{\Psi\Psi^*}dx, \tag{3.215}$$

where the new quantum mechanical current is now

$$\tilde{J} \equiv f'(x)^2 J \tag{3.216}$$

which is coupling–dependent. Finally, the corresponding generalized SL equation can then be expressed as [54]

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + V(x) - m\gamma\int\frac{\tilde{J}}{\Psi\Psi^*}dx - f(x)\xi(t) - W(t)\right]\Psi. \tag{3.217}$$

where $W(t) = \langle V_D\rangle$ arises from the requirement that the integration of Eq. (3.215) with respect to x must be equal to the expectation values of the kinetic and potential energies through the total Hamiltonian. As mentioned previously, this term can be removed from Eq. (3.217) by introducing the transformation of the wave function given by Eq. (3.6). We also note that when the coupling function f is assumed to be linear in the system variable, Eq. (3.217) reduces to the standard Kostin equation.

Equation (3.217) can also be written in terms of the quantum trajectory formulation by expressing the wave function in polar form [67] as in Eq. (3.28). Doing this, Eq. (3.209) can be split into a system of two coupled equations,

$$\frac{\partial S}{\partial t} = -\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - (V + V_d + V_r + Q) \tag{3.218}$$

$$\frac{\partial\phi^2}{\partial t} = -\frac{1}{m}\frac{\partial S}{\partial x}\frac{\partial\phi^2}{\partial x} - \frac{\phi^2}{m}\frac{\partial^2 S}{\partial x^2}. \tag{3.219}$$

Moreover, the current density is expressed in this formalism as

$$J = \frac{\Psi\Psi^*}{m}\frac{\partial S}{\partial x}. \tag{3.220}$$

By differentiating Eq. (3.218) with respect the position, the time evolution of $p(x,t)$ is given by

$$\frac{\partial p}{\partial t} = -\frac{p}{m}\frac{\partial p}{\partial x} - \frac{\partial}{\partial x}\left(V + V_d + V_r + Q\right). \tag{3.221}$$

According to Eq. (3.207), which can be interpreted in terms of the Lagrangian framework of hydrodynamics, the corresponding quantum Newton–Langevin equation including the dissipative and random sources can be expressed as

$$\begin{aligned}\frac{\partial p}{\partial t} = &-\frac{p}{m}\frac{\partial p}{\partial x} - \frac{\partial}{\partial x}\left(V + Q\right)\\ &- \gamma f'(x)^2 p - f'(x)\xi(t).\end{aligned} \tag{3.222}$$

Then, by integrating Eq. (3.222) with respect to x, we obtain [54]

$$\begin{aligned}-\frac{\partial S}{\partial t} = &\frac{p^2}{2m} + V + Q + \gamma\int f'(x)^2 p dx\\ &+ f(x)\xi(t) + C(t),\end{aligned} \tag{3.223}$$

where $C(t)$ is an arbitrary time function resulting from the space integration to be specified later on. This equation gives the evolution of the wave function phase in presence of damping which corresponds to a generalized Caldeira–Leggett coupling.

Furthermore, the partial integration in Eq. (3.223) leads to

$$\int\left(\frac{df}{dx}\right)^2 p dx = \left(\frac{df}{dx}\right)^2 S - 2\int S\frac{df}{dx}\frac{d^2 f}{dx^2}dx, \tag{3.224}$$

which gives place naturally to the coupling–dependent phase

$$\tilde{S} \equiv \left(\frac{df}{dx}\right)^2 S - 2\int S\frac{df}{dx}\frac{d^2 f}{dx^2}dx. \tag{3.225}$$

which can be straightforwardly expressed as

$$\tilde{S} = m\int\frac{\tilde{J}}{\Psi\Psi^*}dx \tag{3.226}$$

with

$$V_D\left[\Psi, \Psi^*, f\right] = -\gamma\tilde{S}. \tag{3.227}$$

Importantly, Eq. (3.227) includes, as a special case, the Bohmian version of the Kostin equation when the coupling is linear. In this case, $\tilde{J} \rightarrow J$ and $V_D[\Psi, \Psi^*, f] \rightarrow V_D[\Psi, \Psi^*, x] = -\gamma S$, which is the dissipative potential expressed within the Bohmian formalism [8, 53, 128].

The constant of integration $C(t)$ can be defined in such a way that the overall phase of the wave function should not affect its evolution. This requirement is satisfied when $C(t) = -\gamma\langle\tilde{S}\rangle$. Therefore, $C(t) \equiv W(t)$ and for a general nonlinear coupling, the generalized SLB equation can be rewritten in terms of the modified quantum action, $\tilde{S}$, as

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + V(x) - \gamma\left(\tilde{S} - \langle\tilde{S}\rangle\right) - f(x)\xi(t)\right]\Psi. \tag{3.228}$$

Thus, the corresponding generalized Hamilton–Jacobi equation for the nonlinear dissipation is given by Eq. (3.218) with V_D given by Eq. (3.227) and V_r by Eq. (3.210). Notice, however, that the continuity equation is the same expressed by Eq. (3.219).

A similar theoretical analysis could be carried out with the nonlinear Eq. (3.22) where the continuity equation has an extra term, a source or sink term.

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Chapter 4
Continuous Quantum Measurements in the Bohmian Framework

Abstract Following a phenomenological approach for continuous measurement, a general theory for decoherence in the framework of restricted path integrals (RPI) has been proposed by Mensky. The corresponding propagator is modified according to the information provided by the measurement through the so-called quantum corridors, which correspond to different readouts of the measurement. The measured system is also considered in this theory as an open system since the back reaction of the environment, considered as a measuring apparatus, is taken into account implicitly. In this chapter, the RPI formulation is briefly presented and discussed since our approach is inspired from Mensky's procedure. The linear time dependent Schrödinger equation derived from this formulation is reached for a non-Hermitian (complex) effective Hamiltonian which takes into account the measurement readout. The RPI formulation is equivalent to a master equation, a special case of the Linblad equation, and to a stochastic Schrödinger equation. Within the Kostin framework, a logarithmic nonlinear Schrödinger equation is proposed and discussed by extending Mensky's approach to be analyzed in terms of Bohmian trajectories, the so-called SLB equation for continuous measurement. When a time-dependent Gaussian shape is assumed for the probability density, soliton-like solutions are first analyzed in order to establish the dividing line between the quantum and classical trajectories, leading to the concept of Bohmian time. Afterwards, the solutions of the Schrödinger–Langevin–Bohm (SLB) equation for continuous measurement are analyzed in terms of mathematical stability for three simple cases, that is, the free particle and the linear and harmonic potentials. In particular, the continuous position measurement is seen that it is no longer governed by a standard continuity equation. The sign of the extra source/sink term appearing in this new equation is critical for the stability of the solutions. Two types of general solutions are found: (i) the stationary wave packet considered becomes unstable (that is, this solution is not a physically acceptable solution for that process since, as time evolves, the width of the corresponding wave packet becomes more delocalized) and (ii) the probability density becomes more and more localized at asymptotic times (the stationary wave packet is then an attractor of the corresponding width dynamics); in terms of trajectories, this analysis indicates that the Bohmian trajectories are not approaching the corresponding

A.B. Nassar and S. Miret-Artés, *Bohmian Mechanics, Open Quantum Systems and Continuous Measurements*, DOI 10.1007/978-3-319-53653-8_4

classical ones. These conclusions are also corroborated by carrying out an analysis of the entropy. Finally, it is also briefly discussed the question of coupling classical variables (apparatus) to quantum ones (system) in terms of Lyapunov exponents.

4.1 Introduction

It is well known that the path integral formulation is equivalent to the Schrödinger picture of quantum mechanics. Thus, the restricted path integral (RPI) formalism due to Mensky [1, 2] is also directly related to a linear Schrödinger equation but with complex Hamiltonian and the measuring process can then be described in terms of wave functions. A straightforward extension to a master equation in terms of the density matrix can also be carried out. Doing this, the *non-selective* description of the measurement is reached when the concrete readout is not known. In other words, the summation or integration is carried out over the set of alternatives readouts. Furthermore, dealing with open systems, it is natural to ask oneself if the RPI formulation is related to a stochastic (nonlinear) Schrödinger equation [3, 4].

Inspired by Mensky's work, Nassar has proposed that the evolution of the wave function of the quantum system under continuous measurement can also be described in terms of a logarithmic nonlinear Schrödinger equation [5]. This equation clearly provides a good starting point for a hydrodynamical description of the measuring process in terms of quantum trajectories. We would like to show that one of the fundamental aspects of Bohmian mechanics is its ability to tackle more intuitively the quantum measurement problem. Following the same theoretical scheme, Nassar and Miret-Artés [6] have also proposed that the time evolution of the wave function of a quantum dissipative system under continuous measurement can also be described in terms of a more general nonlinear Schrödinger equation. The logarithmic nonlinearity for the dissipative part is the same one proposed by Kostin when considering open quantum systems (see Chap. 3) [7]. Recently, this nonlinear Schrödinger equation has been investigated by Zander et al. [8].

As pointed out by Bell [9], the lack of clarity in regards to where the transition between the classical and quantum regimes is located is one aspect of the measurement problem. This problem represents one of the most important conceptual difficulties in quantum mechanics. A solution to the challenge posed by Bell on the dividing line between the quantum and classical regimes in a measurement problem is proposed here within the Bohmian context. Via the quantum trajectory method, a solution to this equation reveals a novel result: it displays a time threshold which establishes the dividing line between the quantum and classical trajectories. It is shown that continuous measurements and damping not only disturb the particle but compel the system to converge in time to a Newtonian regime without any assumption of collapse. In particular, it is shown that damping tends to suppress further quantum effects on a time scale shorter than the relaxation time of the system following also a gradual decoherence process. The solution to this equation is found through a wave packet approach which establishes a direct correlation between a classical

variable with a quantum variable describing the dynamics of the center of mass and the width of the wave packet. The approach presented here gives a comparatively clearer picture than approaches using restricted path integrals and master equation.

For these goals, this chapter is organized as follows. In Sect. 4.2, the so-called characteristic function of a quantum measurement which is very convenient for the RPI formulation is described. In Sect. 4.3, since our approach is inspired from Mensky's procedure, a very short introduction to path integrals and restricted path integrals is presented In Sect. 4.4, some equations derived from the RPI formalism are presented and discussed, such as the linear time dependent Schrödinger equation for a non-Hermitian (complex) effective Hamiltonian which takes into account the measurement readout, a master equation which is a special case of the so-called Linblad equation, and a stochastic Schrödinger equation. In Sect. 4.5, a logarithmic nonlinear Schrödinger equation for continuous measurement is proposed and discussed by extending Mensky's approach within the Bohmian formalism which is equivalent to the one presented in Chap. 3, Eq. (3.22). In Sect. 4.6, this nonlinear equation is again extended within the Kostin framework to be analyzed in terms of Bohmian trajectories, resulting the Schrödinger–Langevin–Bohm equation for continuous measurement. Some important consequences are also analyzed when considering Eq. (3.22) instead. In Sect. 4.7, it is established the dividing line between the quantum and classical trajectories, leading to the concept of Bohmian time. Section 4.8 is devoted to the analysis of the solutions of the Schrödinger–Langevin–Bohm in terms of mathematical stability for three simple cases, that is, the free particle and the linear and harmonic potentials. When a time-dependent Gaussian shape is assumed for the probability density, the continuous quantum measurement process (in particular, the continuous position measurement) is no longer governed by a standard continuity equation. The extra source/sink term is mainly dependent on the sign (positive/negative) of such a parameter. Two types of general solutions are found: (i) the stationary wave packet considered becomes unstable (that is, this solution is not a physically acceptable solution for that process since, as time evolves, the width of the corresponding wave packet becomes more delocalized) and (ii) the probability density becomes more and more localized at asymptotic times (the stationary wave packet is then an attractor of the corresponding width dynamics). In terms of stochastic trajectories, this analysis indicates that the corresponding Bohmian trajectories are not approaching the corresponding classical ones. These conclusions are also corroborated by carrying out an analysis of the entropy. Finally, Sect. 4.9 sets out the question of coupling classical variables (apparatus) to quantum ones (system) in terms of Lyapunov exponents.

4.2 Measurement and the Characteristic Function

As is well known, the Heisenberg uncertainty principle (HUP) has a double interpretation. First, it concerns the relationship between two observables in a given quantum state or, in general, between the so-called conjugate observables. And, second, when dealing with *instantaneous* quantum measurements, it asserts that it is impossible

to measure simultaneously two conjugate observables with arbitrary precision. The most general expression of this principle is given by

$$\Delta A \Delta B \geq \frac{1}{2}\langle \Psi | [A, B] | \Psi \rangle \tag{4.1}$$

where A and B are two Hermitian operators. When these two operators are canonically conjugate to each other, or their commutation relation is the same as for the coordinate and momentum, the usual expression is obtained.[1] The squared of the uncertainty or quantum variance of an operator A is defined as

$$\Delta A^2 = \langle \Psi | A^2 | \Psi \rangle - \langle \Psi | A | \Psi \rangle^2. \tag{4.2}$$

Following Mensky [2], if the uncertainties ΔA and ΔB characterize the state before the measurement, and δA and δB refer to the state after the measurement, and DA is the measurement error or resolution, then

$$\delta B \geq \frac{1}{2}\frac{\hbar}{DA} \tag{4.3}$$

for two canonically conjugate observables. If, on the contrary, $[A, B] = iC$, then

$$\delta B \geq \frac{1}{2}\frac{|\langle C \rangle|}{DA} \tag{4.4}$$

where the mean value of C is over the final state, that is, after the measurement. These expressions are no longer valid when continuous quantum measurements are carried out. For example, when monitoring the position up to a certain error, information about the momentum can not be expressed as dictated by the Heisenberg principle.

It is very well known that when a quantum system is measured, its corresponding dynamics is unavoidably affected. Following the standard theory due to von Neumann about quantum measurements, an idealized measurement is described by the reduction postulate or collapse of the wave function. The conversion of a superposition of states to the mixture of the same states is called decoherence. Interaction between the system and its environment or measuring apparatus leads to entanglement or quantum correlation. When the measurement is carried out, the measured system decoheres. This measurement in standard quantum mechanics is described in terms of projection operators, a complete set of orthogonal projectors.

In general, when dealing with composite systems (for example, $S = S_1 + S_2$), the corresponding Hilbert space is the tensor product space of the Hilbert spaces describing its subsystems ($\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$). The corresponding density matrix when both subsystems are uncorrelated takes also the form of a tensor product, $\rho = \rho_1 \otimes \rho_2$,

[1] As $[q, p] = i\hbar$, then $\Delta q \Delta p \geq \frac{1}{2}\hbar$ and, therefore, $\Delta A \Delta B \geq \frac{1}{2}\hbar$.

and the corresponding expectation value of any tensor product of operators pertaining to the subsystems factorizes. The reduced density matrix of one of the subsystems is obtained by tracing over the second Hilbert space, $\rho_1 = \mathrm{Tr}_2\rho$. This is called a coarse grained description since very often we are not interested in all details of one of the subsystems, usually the more extended one which is considered as the environment. A state of $\mathcal{H}$ is a product state if and only if the reduced density matrices ρ_1 and ρ_2 describe pure states. On the other hand, if a state of $\mathcal{H}$ can not be written as a tensor product of states of the subsystems is said to be *entangled*.

The physical process leading to the transition from the density matrix (describing the pure state $|\psi\rangle$) $\rho = |\psi\rangle\langle\psi|$ to the density matrix of a mixed state where all the coherences are zero (or when phase relations are lost) is an alternative way to describe *decoherence*. The off-diagonal terms are typically decaying as an exponential function where the decoherence time is inversely proportional to the squared difference between the measured values of the corresponding observable. In other words, decoherence appears when quantum interference is destroyed or suppressed. In a certain sense, it could be said that decoherence leads to the emergence of a classical world in quantum mechanics. Environment induced decoherence [10] is omnipresent and, in general, it is a short time phenomenon. When measuring, the dynamics of the system tends to be decoherent. In the weak coupling approximation between the system and environment, the trace operation carried out to obtain the reduced density matrix is key to the existence of any master equation. However, this operation is questionable when the system and environment are entangled at all times, including the initial state. The role of the initial conditions has also be widely discussed in the corresponding literature.

In a measurement, the physical mechanism leading to decoherence consists of the interaction of the measured system with its environment (for example, a measuring device). As mentioned above, this interaction also leads to their entanglement or quantum correlation of the two systems. Thus, the information about the system is somehow recorded in the state of the environment. This process can also be described by the reduced density matrix of the measured system (when tracing over the degrees of freedom of the device). Doing this, it can easily be shown (starting from a product state of wave functions), that one more property is needed for decoherence, the orthogonality of the measuring device wave functions before and after the measurement. This condition is satisfied for macroscopically distinct states and the decoherence is irreversible. When dealing with microscopic environments where such a condition is not satisfied, the decoherence process is reversible. An alternative way of seeing this is by considering the environment split into two parts, one microscopic part directly interacting with the system, usually called a *meter* or (*pointer*), and this, in turn, interacts with a macroscopic part usually named *reservoir*. Thus, decoherence induced by entanglement through a unitary evolution of both the system and meter is practically reversible. When the reservoir is also present, decoherence may be considered reversible, in principle, but it is irreversible from a practical point of view. However, the *many-worlds* interpretation by Everett is an attempt to overcome irreversibility completely. It seems to be impossible to verify it or to be testable; in other words, to be falsified.

When one wants to obtain information on the state of the system by means of the measurement on the meter, we speak about the indirect (or *ancilla*) measurement [11, 12]. As said before, in this composite system, correlations between the measured system and the meter are built up during their interaction. The time-dependent interaction Hamiltonian is assumed to vanish outside the time interval $[0, \tau]$. If the time interaction is sufficiently small to suppose that only the interaction Hamiltonian is acting, the unitary time evolution operator takes a very simple form in terms of the integrated coupling strength G (given by the integration of the time-dependent coupling $g(t)$ in that time interval). For example, if the position operator Q, canonically conjugate to the momentum operator P of the meter, is coupled to an observable A the interaction Hamiltonian is given by

$$H_I(t) = g(t)AQ \tag{4.5}$$

the evolution operator being then written as

$$U = \exp(-iGAQ). \tag{4.6}$$

It is a straightforward exercise to show that the variance of the inferred eigenvalue of A (through one the measurement outcomes of P) is the sum of the variance of A and the variance of P in the initial state divided by G^2. Thus, the measurement is the more accurate the lower the momentum uncertainty of the meter and the stronger the coupling between the system and meter.

In standard textbooks, the measurement is introduced through the projection procedure due to von Neumann (the so-called von Neumann's reduction postulate). In this ideal or instantaneous measurement, the system is projected onto one of the possible eigenstates of a given observable. In a given basis set of the observable A, the state of the system is expressed as

$$|\psi\rangle = \sum_m c_m |m\rangle. \tag{4.7}$$

The probability that the system is projected onto $|m\rangle$ is $|c_m|^2$. In other words, the transition from the state given by Eq. (4.7), before the measurement, to one of its eigenstates, after the measurement, is the simplest form of the state reduction or wave function collapse. This collapse is considered to be an irreversible process. In this sense, it is claimed that this type of measurement is complete. If $P_m = |m\rangle\langle m|$ is the projection operator onto the eigenstate $|m\rangle$ and the initial state of the system is $\rho = |\psi\rangle\langle\psi|$, the m possible outcome of the final state is given by

$$\rho_f = |m\rangle\langle m| = \frac{P_m \rho P_m}{\mathrm{Tr}\, P_m \rho P_m} \tag{4.8}$$

with probability $P(m) = \mathrm{Tr}(P_m \rho P_m) = |c_m|^2$ and $\mathrm{Tr}\rho_f = 1$. This is the well-known von Neumann–Lüders projection postulate. Under the collapse condition, one may ask for the density matrix after the measurement to have a particular measurement outcome or alternative (*selective measurement*) or, for one reason or another, one does not register the outcomes or alternatives (*Nonselective measurement*). In this case, we have to sum over all possible outcomes.

The von Neumann–Lüders postulate can be generalized to a set of operators Ω_m with the condition $\sum_{m=1}^{M} \Omega_m^\dagger \Omega_m = I$, I being the identity operator. The different outcomes can be again written as

$$\rho_f = \frac{\Omega_m \rho \Omega_m^\dagger}{\mathrm{Tr}(\Omega_m \rho \Omega_m^\dagger)} \tag{4.9}$$

with $P(m) = \mathrm{Tr}(\Omega_m \rho \Omega_m^\dagger) = \mathrm{Tr}(\Omega_m^\dagger \Omega_m \rho)$, being the probability of having the mth outcome. These generalized measurements are referred to as *positive- operator-valued measure*. The measurements described by such operators are minimally disturbing. Furthermore, the positive operator $F = \sum_{m=a}^{b} \Omega_m^\dagger \Omega_m$ determines the probability for obtaining an outcome lying in the range of real numbers $[a, b]$. This positive operator is also called the *effect* and the operator $\Omega_m \rho \Omega_m^\dagger$ is called an *operation*. A measurement is a quantum non-demolition (QND) measurement for the observable A if the operators Ω_m describing the change of the quantum system induced by the measurement commute with A. This condition is always fulfilled for an ideal measurement of the observable A. Moreover, in a composite system, if A is a constant of motion under the free evolution of a quantum system, a general sufficient condition for a QND measurement takes place when the commutator of A and the interaction Hamiltonian is zero. The more general forms for operations and effects are established by the so-called representation theorem for quantum operations. The reader interested in more details about the properties of such operators are addressed to Refs. [10–17]

The Ω operators could be thought to be a weighted (for example, a Gaussian function; the weight function is also called a *characteristic function* of the measurement) sum of projectors onto the eigenstates $|m\rangle$, each one peaked around a different value of the observable such as

$$\Omega_m = \frac{1}{\bar{N}} \sum_n e^{-(n-m)^2/2\sigma_0^2} |n\rangle\langle n| \tag{4.10}$$

where $\bar{N}$ is a normalization constant chosen to fulfill the normalization condition for $\Omega_m^\dagger \Omega_m$ previously established, the mean value is given by m and the variance by σ_0^2. After the measurement, with an outcome m, the state of the system is given by

$$\rho_f = \frac{\Omega_m \rho \Omega_m^\dagger}{\mathrm{Tr}(\Omega_m \rho \Omega_m^\dagger)} = \frac{1}{\bar{N}} \sum_n e^{-(n-m)^2/2\sigma_0^2} |n\rangle\langle n| \tag{4.11}$$

that is, the final state is peaked around the eigenvalue m with a width given by the variance σ_0^2. The width σ_0 of this function corresponds to the resolution of the measurement; sometimes, we also speak about the uncertainty of the observable. For large variances, we have *fuzzy, soft or unsharp measurements* (sometimes, the adjective *weak* is also used but we are going to reserve this adjective for the weak measurement due to Aharonov et al. [18]); conversely, *strong, projecting or sharp measurements* are obtained for small variances. Measurement devices have in general a finite resolution, given by the variance in the example above. If the eigenvalues of a given observable are not too closely spaced, one can measure such an observable with a very small uncertainty, provided the experimental resolution is sufficiently large. However, if such a resolution is not high enough to distinguish neighbouring eigenvalues, our measure is quite approximate [11, 12]. The renewed interest in coupling classical systems to quantum ones has been revived by a number of authors [2, 19, 20] who have examined continuous quantum measurements. Nowadays, continuous or repeated (prolonged in time) measurements of a quantum system is a very active field mainly for two reasons. First, it is a direct way to look into the intrinsic features of quantum theory and second, such measurements are gaining step by step a predominant role in typical experimental setups [2]. In this context, one of the most well known illustrations is the so-called quantum Zeno effect [21], as well as the anti-Zeno effect [22], where the decaying of an unstable system can be delayed or accelerated, respectively. This process is carried out in a series of projecting (sharp, hard or strong) measurements. In fact, the Zeno effect is a nice illustration of the reduction or collapse postulate of the wave function due to von Neumann. Each observation collapses the wave function, resetting the clock and allowing to delay, in principle, indefinitely or freezing a given decaying process. Clearly, this series of measurements has to be carried out under certain conditions.

A continuous measurement is performed when information is continually extracted from the system, by reducing such an information with the duration of the measurement. This time is divided into a sequence of intervals of length Δ where a fuzzy measurement is carried out. If, for example, the observable we want to measure is the position of a particle, X, which displays a continuous spectrum of eigenvalues x with $\langle x|x'\rangle = \delta(x-x')$, one can consider a fuzzy measurement in each time interval Δt described by the operators [23]

$$\Omega(\alpha) = \left(\frac{1}{\pi\sigma_0^2\Delta t}\right)^{1/4} \int_{-\infty}^{\infty} e^{-(x-\alpha)^2/2\sigma_0^2\Delta t}|x\rangle\langle x|dx \tag{4.12}$$

where each operator is a Gaussian-weighted sum of projectors onto the eigenstates of X peaked at α, which is a real number. In other words, the continuum of measurement outcomes is labelled by α. The probability density $P(\alpha)$ of the outcome α, when Δt is small, is then given by

$$P(\alpha) = \mathrm{Tr}(\Omega(\alpha)^\dagger\Omega(\alpha)|\psi\rangle\langle\psi|) = \frac{1}{\sigma_0\sqrt{\pi\Delta t}} \int_{-\infty}^{\infty} e^{-(x-\alpha)^2/\sigma_0^2\Delta t}|\psi(x)|^2 dx \tag{4.13}$$

and the mean value by

$$\langle X\rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2 dx = \int_{-\infty}^{\infty} \alpha P(\alpha) d\alpha = \langle \alpha\rangle \tag{4.14}$$

For Δt sufficiently small, the Gaussian function is much broader than $|\psi(x)|^2$, which could be replaced by a delta function centered at the expected position of X. Thus,

$$P(\alpha) = \frac{1}{\sigma_0\sqrt{\pi\Delta t}} e^{-(\alpha-\langle\alpha\rangle)^2/\sigma_0^2\Delta t}. \tag{4.15}$$

Now, following Ref. [23], the probability density given by Eq. (4.15) can be transformed in the corresponding of a Wigner process if

$$\alpha - \langle\alpha\rangle = \frac{\sigma_0^2 \Delta W}{\sqrt{2}} \tag{4.16}$$

where ΔW denotes the small displacement of a Brownian particle [24].

A different approach is by considering a fuzzy measurement which results from the generalization of von Neumann's projector theory. For example, when measuring the position of a particle, a certain finite resolution should be considered. The simplest way of describing this fact is by means of an indicator or characteristic function of the measurement. Thus, by considering the interval $[x_i - \Delta x, x_i + \Delta x]$ where x_i is the center of the interval and Δx the finite resolution, the projector P_i is defined as a function to be unity inside the points of the above interval, and zero otherwise. Then, the projector simply multiplies the wave function by one inside that interval

$$P_i\Psi(q) = \begin{cases} \Psi(q) & , if\ |q - q_i| < \Delta a \\ 0 & , otherwise. \end{cases} \tag{4.17}$$

Obviously, this characteristic function which is discrete and rectangular can be improved by considering a more general scheme [2]. Let us define a set of non-orthogonal characteristic functions $\{R_i\}$ with $\sum_i R_i^\dagger R_i = 1$ such that

$$|\Psi_i\rangle = R_i|\Psi\rangle \tag{4.18}$$

with

$$P_i = ||\Psi_i||^2 = \langle\Psi|R_i^\dagger R_i|\Psi\rangle \tag{4.19}$$

and

$$\sum_i P_i = 1. \tag{4.20}$$

If these characteristic functions are assumed to be continuous functions (for example, a Gaussian function), the index i is replaced by a continuous index x_c in such a

way that the continuous set of operators is now given by $\{R_{x_c}\}$ with $\int dx_c R_{x_c}^{\dagger} R_{x_c} = 1$ and

$$|\Psi_{x_c}\rangle = R_{x_c}|\Psi_{x_c}\rangle \tag{4.21}$$

with

$$P_{x_c} = ||\Psi_{x_c}||^2 = \langle\Psi|R_{x_c}^{\dagger} R_{x_c}|\Psi\rangle \tag{4.22}$$

and

$$\int dx_c P_{x_c} = 1. \tag{4.23}$$

In the literature, the set of positive operators $\{R_{x_c}^{\dagger} R_{x_c}\}$ represents a positive-operator-valued measure on the set $\{x_c\}$ of all possible values of such a parameter.[2] For a Gaussian function, we have

$$R_{x_c}\Psi(x) = R(x - x_c)\Psi(x) \tag{4.24}$$

where x_c is the center of the Gaussian and its width gives the resolution of the measurement (or fuzziness of the measurement). The measurements described by such operators are called *minimally disturbing* since only the amplitude of the wave function is rescaled, but not its phase. When the characteristic function includes a phase of the momentum, a transition of the linear momentum is accompanied with the measurement.

The characteristic function can be generalized to any observable. Thus, if the observable A has a spectrum $\{a_i\}$, the wave function in the representation of A is written as

$$|\Psi\rangle = \sum_i c_i|a_i\rangle \tag{4.25}$$

and

$$R_{a_c}|\Psi\rangle = \sum_i R(a_i - a_c)c_i|a_i\rangle. \tag{4.26}$$

The next interesting step is to consider the effect of repeated fuzzy measurement and free evolution in the intervals between the measurements at each instant. Decoherence is settled down after a measurement has been carried out. Obviously, in the limit of many, many measurements during a finite time interval, we have a continuous measurement with the corresponding gradual decoherence. Each fuzzy measurement has a poor resolution leading to a poor information about the observable to be measured. However, the repetition of this type of measurement improves the resolution of the eigenvalues of the corresponding observable by projecting more and more the state of the system onto one of the eigenvectors. Thus, with a long

[2] A Hermitian operator is called positive, $R \geq 0$, if for an arbitrary state $|\phi\rangle$ then $\langle\phi|R|\phi\rangle \geq 0$.

series of fuzzy measurements, a model for gradual decoherence is provided leading to von Neumann's projection. The sequence thus defined by the measurements can be seen as a stochastic process [2].

4.3 A Short Introduction to Restricted Path Integrals

When dealing with classical systems, each individual trajectory or path forms a complete description of its time evolution. However, for quantum systems, only the sum or integration over all paths according to certain rules describes its corresponding evolution.

The time evolution of a closed system in terms of its wave function is described by the so-called propagator (or evolution operator), starting at t_0, according to

$$\Psi(t) = U(t, t_0)\psi(t_0) \tag{4.27}$$

which is equivalent to solve the time-dependent Schrödinger equation. For a time-independent Hamiltonian, this operator is defined as

$$U(t, t_0) = \theta(t - t_0) \exp\left[-\frac{iH(t - t_0)}{\hbar}\right] \tag{4.28}$$

where θ is the step function (1 for positive argument and 0, otherwise). In one-dimension, its matrix elements are given by

$$U(q'', t''; q', t') = \langle q''|U(t'', t')|q'\rangle \tag{4.29}$$

with $q(t') = q'$ and $q(t'') = q''$. The evolution of the wave function is then given by

$$\Psi(q'', t'') = \int dq' U(q'', t''; q', t')\Psi(q', t'). \tag{4.30}$$

The combined effect of all possible paths is defined by means of a propagator, which acts according to *Huygens' principle*. That is, following an optical analogy, the (quantum) wave function at the time t'' is formed by the interference of a series of secondary wavelets starting from a wave function at a previous time t'.

As is well known, this propagator can also be expressed as an integral over all paths connecting the initial and final points [1, 2, 25, 26], the so-called Feynman path integral, which in the one dimensional configuration space, is written as

$$U(q'', t''; q', t') = \int d\,[q]\, e^{iS[q]/\hbar}, \tag{4.31}$$

where the integral is understood over all paths of the coordinate q fulfilling the condition

$$[q] = \{q(t) | t' \leq t \leq t''\},$$

and the action S of the corresponding system is given by

$$S\,[q] = \int_{t'}^{t''} L(q, \dot{q}, t) dt \tag{4.32}$$

$L(q, \dot{q}, t)$ being its Lagrangian, which is related to the Hamiltonian as

$$H(p, q, t) = p\dot{q} - L(q, \dot{q}, t), \tag{4.33}$$

with $p = \partial L/\partial \dot{q}$. In the phase space, the path integral for U is written as

$$U(q'', t''; q', t') = \int d\,[p] \int d\,[q]\; e^{\frac{i}{\hbar}\int_{t'}^{t''}(p\dot{q} - H(p,q,t))dt}, \tag{4.34}$$

where the paths of the momentum are defined as

$$[p] = \{p(t) | t' \leq t \leq t''\},\ p(t') = p',\ p(t'') = p''.$$

Equation (4.31) can be written in a more explicit way by means of the so-called discretization. This procedure consists of replacing the continuous paths by continuous piecewise linear curves or broken lines. The nodes of the broken line lie on the path and are at the time and space positions $q_j = q(t_j)$ and $q_{j+1} = q(t_{j+1})$ with $t_j = j\Delta t$. Thus, the integration over continuous path $d\,[q]$ is replaced by integration over all possible node positions

$$\prod_{j=1}^{N-1} dq_j$$

leading to the correct value of the integral when the time interval between nodes of the broken lines tends to zero, i.e., $\Delta t = (t'' - t')/N \to 0$ or $N \to \infty$. For example, for a particle of mass m with a Lagrangian of the form

$$L(q,\dot{q},t)=\frac{1}{2}m\dot{q}^2-V(q,t) \tag{4.35}$$

the propagator given by Eq. (4.31) is finally expressed as

$$U(q'',t'';q',t')=\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2}\int\prod_{j=1}^{N-1}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2}dq_j$$
$$.\exp\left(\frac{i}{\hbar}\sum_{j=1}^{N}\left[\frac{1}{2}m\frac{(q_j-q_{j-1})^2}{\Delta t}-V(q_j,t_j)\Delta t\right]\right) \tag{4.36}$$

where a normalization factor has been introduced.

For Eq. (4.34), the measure $d[q]\,d[p]$ is discretized as

$$\prod_{j=1}^{N-1}dq_j\prod_{j=1}^{N}\frac{dp_j}{2\pi\hbar}$$

where piecewise constant curves are used for paths $[p]$. The resulting expression for the propagator is finally given by

$$U(q'',t'';q',t')=\lim_{N\to\infty}\int\prod_{j=1}^{N-1}dq_j\prod_{j=1}^{N}\frac{dp_j}{2\pi\hbar}$$
$$.\exp\left(\frac{i}{\hbar}\sum_{j=1}^{N}\left[p_j(q_j-q_{j-1})-\left(\frac{p_j^2}{2m}-V(q_j,t_j)\right)\Delta t\right]\right). \tag{4.37}$$

For an n-dimensional system, where q and p are n-vectors, the generalization of the propagator is straightforward by taking into account the corresponding measures [1, 2, 25, 26].

The next step is to describe sequential measurements of, for example, the position of the system, in order to reach the continuous quantum measurement. If the output of the measurement is q', with an error equal to Δq, by simulating the device by a rectangular characteristic function,[3] we could write this operation by a set of operators $\{R_{q'}\}$ proportional to projectors as

$$R_{q'}=\frac{1}{\sqrt{2\Delta q}}P_{q'}, \tag{4.38}$$

where $P_{q'}$ is defined as in Eq. (4.17)

[3]Real devices correspond to smoother characteristic functions such as a Gaussian one.

$$P_{q'}\Psi(q) = \begin{cases} \Psi(q) & , if\ |q - q'| < \Delta q \\ 0 & , otherwise \end{cases}, \tag{4.39}$$

with the probability density

$$P(q') = \langle \Psi | R_{q'}^2 | \Psi \rangle, \tag{4.40}$$

the normalization relation being

$$\int_{-\infty}^{+\infty} P(q')dq' = 1. \tag{4.41}$$

Usually, the sequence of measurements is carried out with intervals of free evolution of the system between them. Thus, after $N-1$ measurements with outputs $\{q_1, q_2, \ldots, q_{N-1}\}$ during the period T, we have that

$$\Psi(N) = U_{q_1,q_2,\ldots,q_{N-1}}\Psi(0) \tag{4.42}$$

where

$$U_{q_1,q_2,\ldots,q_{N-1}} = U(t_N, t_{N-1})R_{q_{N-1}} \cdots U(t_2, t_1)R_{q_1}U(t_1, t_0) \tag{4.43}$$

and the probability density of the outputs of the sequential measurement is

$$P(q_1, q_2, \ldots, q_{N-1}) = P(q_1)P(q_2)\cdots P(q_{N-1}) = \langle \Psi(N) | \Psi(N) \rangle \tag{4.44}$$

due to the unitarity of the free evolution. Finally, the normalization condition is

$$\int \cdots \int P(q_1, q_2, \ldots, q_{N-1})dq_1 dq_2 \cdots dq_{N-1} = 1. \tag{4.45}$$

In the limit $N \to \infty$, $\Delta t = T/N \to 0$, the continuous measurement process in the finite time interval T is reached. As seen in Fig. 4.1, the sequence of outputs determines in this limit a quantum corridor or band of width $2\Delta q$. It is clear why path integrals can be used to calculate characteristics of continuous measurements.

The limit of the operator $U_{q_1,q_2,\ldots,q_{N-1}}$ is the propagator for a system under continuous quantum measurement. This propagator can also be expressed in this limit as

$$U(q'', t''; q', t') = \int dq_1 \int dq_2 \cdots \int dq_{N-1} U(q'', t''; q_{N-1}, t_{N-1}) \cdots U(q_2, t_2; q_1, t_1)U(q_1, t_1; q', t') \tag{4.46}$$

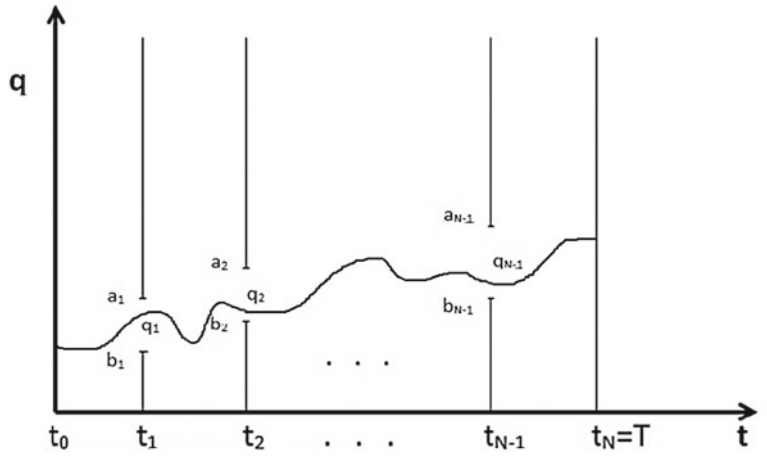

Fig. 4.1 The discretization procedure of both space and time required to evaluate the propagator (4.31) is plotted which is analogous to carrying out a Riemannian integral

which satisfies the Chapman–Kolmogorov condition

$$U(q'', t''; q, t) = \int dq' U(q'', t''; q', t') U(q', t'; q, t). \tag{4.47}$$

As shown by Kac [26, 27], the connection between path integration and Brownian motion is so close that they are nearly indistinguishable. The Brownian motion leads us to the Wiener integral which is a *bona fide* integral on the space of paths, this being defined from a Wiener measure. The space on which the proposed measure is imposed is that of the continuous functions $[q]$ where $q(0) = 0$ and $q(t) = q$. The σ-algebra is built by forming countable unions and intersections of *cylinder sets* (in our case, quantum corridors) defined as follows

$$K[a_1, b_1, t_1; a_2, b_2, t_2; ...; a_n, b_n, t_n] = \{q(.) | a_j < q(t_j) < b_j, j = 1, \ldots, N\}$$

and the measure is the probability that a particle starting at $q(0) = 0$ is between a_1 and b_1 at time t_1, is between a_2 and b_2 at $t_2, \ldots,$ and is between a_N and b_N at time t_N with $a_j < b_j$ and $t_j < t_{j+1}$, that is,

$$\int_{a_1}^{b_1} dq_1 ... \int_{a_N}^{b_N} dq_N G(q_1, t_1) G(q_2 - q_1, t_2 - t_1) ... G(q_N - q_{N-1}, t_N - t_{N-1})$$

where the G-functions are Gaussian functions.

4.3.1 Quantum Corridors

Opposite to strong measurements, fuzzy (unsharp, soft or weak) continuous measurements have also been proposed for monitoring quantum transitions leading to a new and deeper insight of the measuring process. In this chapter, when discussing about weak measurements is to be understood as a fuzzy one, not to be confused with the weak measurement due to Aharonov et al. discussed in Chap. 1. For fuzzy continuous measurements, the theory technically developed by Mensky provides a general phenomenological theory of gradual decoherence in the framework of restricted path integrals (RPI) [2]. This notion of restricted path integral was originally proposed by Feynman [25], the propagator being modified according to the information provided by the measurement through the so-called *quantum corridor*, which corresponds to a given readout of the measurement. The measured system is then considered in the RPI theory of measurements as an open system since the interaction with the environment is taken into account implicitly. In general, interaction of the system with its environment may be interpreted as measuring the system, the corresponding information being recorded in the environment. A phenomenological approach is sometimes preferred since no model for such interaction or measurement is chosen and the rather cumbersome procedure of considering first explicitly the environment and afterwards excluding it turns out to be unnecessary. In this theory, no special postulate is introduced in order to take into account the measuring process, it is just derived from the Feynman formulation of quantum mechanics.

In the path integral formalism, one does not deal with quantum states but with alternatives or paths and it results a quite natural framework to describe continuous quantum measurements. The analogue of the HUP under these conditions is the so called action uncertainty principle (AUP) [2]. In particular, the RPI formalism turns out to be very convenient for such a goal. This formalism takes into account the measuring process without explicit reference to the apparatus or environment, the back influence of the environment being considered implicitly. It makes the emphasis on the dynamical role of information issued from the continuous measurement as treated as an open quantum system. Thus, in the coordinate representation, the evolution operator or propagator is written as

$$U_{[a]}(q'', q') = \int_{I_{[a]}} d[q] e^{iS[q]/\hbar} \tag{4.48}$$

where the integral is restricted to the set $I_{[a]}$ of paths $[q] = \{q(t)|t' \leq t \leq t''\}$ (with $q'' = q(t'')$ and $q' = q(t')$) representing the measurement readout $[a]$ of a given observable A. A similar expression can be written in the phase space. This measurement readout may be expressed by the function or curve $[a] = \{a(t)|0 \leq t \leq T\}$ during the measuring period of time T and characterized by an error or resolution $[\Delta a] = \{\Delta a(t)|0 \leq t \leq T\}$, establishing a quantum corridor between $[a - \Delta a, a + \Delta a]$ (see Fig. 4.2). In this way, $|q(t) - a(t)| \leq \Delta a$. In principle, this resolution could also be a time dependent function. This evolution operator $U_{[a]}$ can

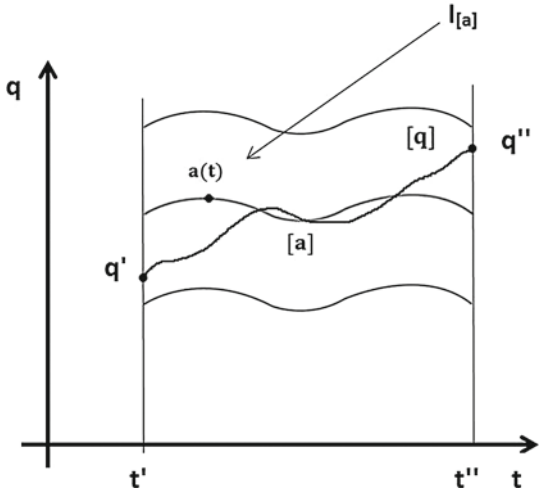

Fig. 4.2 Restriction of a path integral to the quantum corridor $I_{[a]}$ which corresponds to the readout $[a]$ when monitoring the position. The quantum corridor is defined by $[a - \Delta a, a + \Delta a]$

be interpreted as an amplitude for the measurement to give the readout $[a]$. The most probable measurement output always corresponds to the classical trajectory $[q]_{class}$. However, due to the quantum effects, outputs may differ with a large probability. The variance we are dealing with in the HUP is with respect to the classical output. The simplest (and weakest) way to express this AUP is

$$\delta S \geq \hbar, \tag{4.49}$$

which means that a continuous measurement produces information such that the uncertainty in the action is not less than the quantum of action. Thus, the most probable output corresponds to the classical output $[a]_{class}$ and to the minimum of the action. However, outputs different from the classical one with larger values of the action are also probable but different from the minimum action by a term of the order of the quantum action, $\hbar$. Therefore, the variance of the action δS should be not less than $\hbar$.

The AUP is an inequality allowing one to specify the subset of the measurement readout $[a]$ having comparatively high probabilities. When monitoring a coordinate, this principle (in a stronger form) is given by the condition [2]

$$max|\int_0^T \frac{\delta S[q]}{\delta q(t)} \Delta q(t) dt| \leq \hbar \tag{4.50}$$

where the functional derivative is taken at $[q] = [a]$ and the maximum should be taken for all $[\Delta q]$ such that $[a + \Delta q] \in I_{[a]}$ (condition for the measurement readout $[a]$ to be highly probable). When monitoring an observable $A(t) = A(p(t), q(t), t)$ such as $|A(t) - a(t)| \leq \Delta a(t)$, then the AUP is expressed as [2]

$$max|\sum_i \int_0^T dt \left[\Delta p_i \left(\dot{q}_i - \frac{\partial H}{\partial p_i}\right) - \Delta q_i \left(\dot{p}_i + \frac{\partial H}{\partial q_i}\right)\right]| \leq \hbar \tag{4.51}$$

where $H(p, q, t)$ is the Hamiltonian of the system with components q_i and p_i for the coordinate and momentum, respectively. Again, the maximum is taken for $|\Delta A(t)| = |A(p'(t), q'(t), t) - A(p(t), q(t), t)| \leq \Delta a(t)$. If we write an effective Hamiltonian as $H_e(p, q, t) = H(p, q, t) - \delta F(t) A(p, q, t)$, then the AUP can be reexpressed as

$$\int_0^T |\delta F(t)| \Delta a(t) \leq \hbar \tag{4.52}$$

the function $\delta F(t)$ being the deviation of the measured system from the classical behavior. This can be seen as a fictitious force describing the measurement process on the system of interest. The readout then follows a Langevin-type equation where $\delta F(t)$ plays the role of noise.

4.3.2 Some Simple Applications of the RPI Formalism

When a continuous measurement is performed in the interval $[t', t'']$, the information of this measurement is then expressed by the positive-valued functional $0 \leq \omega_{[a]} \leq 1$, the measurement output being $[a]$. Thus, paths $[q]$ for which this functional is close to unity are probable. Then, the so-called measurement amplitude is defined by

$$U^{[a]}(q'', q') = \langle q'|U^{[a]}|q''\rangle = \int_{q'}^{q''} d\,[q]\,\omega_{[a]}[q] e^{iS[q]/\hbar}, \tag{4.53}$$

which its modulus squared roughly estimates the probability of the corresponding output or readout, through the probability density $P_{[a]} = |U^{[a]}|^2$. For the classical output, this probability is maximum. Furthermore, we have also the following inequality

$$|q(t) - a(t)| \leq \Delta a \tag{4.54}$$

where the output is given by the curve $[a] = \{a(t)|t' \leq t \leq t''\}$, the quantum corridor being defined by $[a - \Delta a, a + \Delta a]$ and symbolized by $I_{[a]}$.

If the $\omega_{[a]}$ functional is considered to be Gaussian as described by the following expression

$$\omega_{[a]}[q] = \exp\left(-\frac{2}{T\Delta a^2}\int_0^T ((q(t)-a(t))^2 dt\right) \tag{4.55}$$

the position monitoring may be called measurement of a path. The error Δa is usually taken to be a constant. Let us consider now a driven harmonic oscillator of mass m [1]. The Lagrangian is given by

$$L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2 + qF(t) \tag{4.56}$$

where ω is its frequency and $F(t)$ the driving force. The measurement amplitude is then written as

$$U_{[a]}(q'', q') = e^{-\frac{2}{T\Delta a^2}\int_0^T a(t)^2 dt}\int_{q'}^{q''} d[q]e^{i\tilde{S}[q]/\hbar} \tag{4.57}$$

since an effective action and effective Lagrangian can be defined as

$$\tilde{S}[q] = \int_0^T \tilde{L}(q, \dot{q}, t) \tag{4.58}$$

and

$$\tilde{L} = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\tilde{\omega}^2 q^2 + q\tilde{F}(t), \tag{4.59}$$

respectively. This also leads to an effective driven harmonic oscillator with complex frequency

$$\tilde{\omega}^2 = \omega^2 - i\nu^2 \tag{4.60}$$

and new driving force

$$\tilde{F}(t) = F(t) - im\nu^2 a(t). \tag{4.61}$$

The imaginary part of the complex frequency is governed by the error of the measurement,

$$\nu^2 = \frac{4\hbar}{mT\Delta a^2} \tag{4.62}$$

showing that a very precise measurement leads to very high contributions of the imaginary parts of the frequency and driving force and, therefore, to a strong influence on the measured system.

When spectral measurements are considered, the theoretical procedure is different [1]. The path of an oscillator is clearly periodic and it can be expanded in a Fourier series as

$$q(t) = \sum_{n=1}^{\infty} q_n sin\frac{n\pi}{T}t \tag{4.63}$$

in the time interval $[0, T]$. The continuous measurement is carried out for the q_n components with the errors Δa_n for the frequencies $\Omega_n = n\pi/T$. If a given device is effective in the range $I = [\Omega_a, \Omega_b]$, only those frequencies Ω_n inside such an interval with the corresponding errors are considered a spectral measurement. The weight functional can then be written for one of the n components as

$$\omega_{a_n,\Delta a_n}[q] = \exp\left(-\frac{(q_n - a_n)^2}{\Delta a_n^2}\right). \tag{4.64}$$

and for all components inside that interval of frequencies as a product of exponential functions as written above. The measure for the measurement amplitude is given by

$$d[q] = \prod_{n=1}^{\infty} dq_n. \tag{4.65}$$

A detailed account of this problem can be found in Mensky's book [1],

An interesting and illustrative result is also when we want to measure the momentum of a free particle. It can be shown [1] that the variance of the linear momentum at the instant T after continuous measurement is given by

$$\Delta p = \sqrt{\Delta p_0^2 + \frac{2\hbar^2}{\Delta a^2}} \tag{4.66}$$

which shows that it does not change with time because of the momentum conservation. When there is no measurement, $\Delta a = \infty$. However, when a measurement is carried out by monitoring the position, the variance is higher due to the error of the measurement. In a certain sense, the particle undergoes scattering as a result of the continuous measurement. The second sum inside the square root can be easily understood from the uncertainty principle.

Finally, another aspect of the measurement process is worth commenting. The variance of the outputs or readouts of a precise measurement can be considered to be a quantum measurement noise. For a certain level of precision, this noise becomes an inconvenient. For a class of continuous measurements, this fact is not valid and they have been called quantum non-demolition (QND) leading to no absolute restriction on observability. In other words, the idea of the QND measurement is to measure a variable such that the unavoidable disturbance of the complementary one does not disturb the evolution of the chosen variable. This is clearly seen when measuring the linear momentum of a free particle since it is a conserved property, even disturbing the position. In general, a given variable is quantum nondemolition (as the linear momentum for a free particle) when the commutation relation of this observable at two different times is zero. Mensky has clearly shown the radical difference between the linear momentum and the velocity of a particle when considering this quantum property.

4.4 Some Equations Derived from the Restricted Path Integral

4.4.1 The Schrödinger Equation

Using Mensky's notation, his quantum corridor approach can be outlined as follows. If the system of interest undergoes a continuously prolonged in time measurement (time interval T) and, therefore, is considered as being open, the propagator can then be expressed by restricted path integrals. When monitoring an observable $A = A(p, q, t)$ by continuous measurement, the measurement readout may be given by the curve

$$[a] = \{a(t)|0 \leq t \leq T\}, \tag{4.67}$$

characterizing the values of this observable in different time moments (see Fig. 4.2 where the position is measured). However, due to the finite resolution of the measurement, Δa, the actual value of A at t may differ from $a(t)$. In this sense, a quantum corridor can be defined by including all curves or paths which differ from $[a]$ by not more than Δa. In general, the width of the corridor also depends on time performing the measurement, Δa_T. Thus, the restricted path integral representing the monitoring of A has to be taken over paths in the corridor around $[a]$.

If the squared average deflection

$$\left\langle (A-a)^2 \right\rangle_T = \frac{1}{T} \int_0^T [A(t) - a(t)]^2 dt \tag{4.68}$$

is seen as a measure of the deviation of the observable $A(t) \equiv A(p(t), q(t), t)$ from the readout $a(t)$, then the most natural weight functional describing the measurement may be written in the Gaussian form as

$$\omega_{[a]}[p, q] = \exp\left[-\kappa \int_0^T [A(t) - a(t)]^2 dt \right]. \tag{4.69}$$

In general, $\omega_{[a]}$ is a positive-valued functional fulfilling $0 \leq \omega_{[a]} \leq 1$. The constant κ characterizes the resolution of the measurement and may be expressed in terms of the "measurement error" Δa_T which is achieved during the period T of the measurement

$$\kappa = \frac{1}{T \Delta a_T^2}, \tag{4.70}$$

where Δa_T decreases if its duration T increases. In general, the κ parameter can also be a time dependent function. For small values of κ, the measurement is weak or fuzzy; on the contrary, for large values, a sharp measurement is settled down.

The measurement amplitude (partial evolution operator) in the phase space representation is then given by

$$U_T^{[a]}(q'', q') = \int_0^T d[p]d[q] \exp\left\{ \frac{i}{\hbar} \int_0^T (p\dot{q} - H)dt - \kappa \int_0^T [A(t) - a(t)]^2 dt \right\}, \tag{4.71}$$

where $q'' = q(t'')$, $q' = q(t')$ and H the corresponding Hamiltonian. This integration is carried out over the subset of paths compatible with the $[a]$ readout. However, the time evolution of a continuously measuring system (open system) is described, in general, by a set of partial evolution operators $\{U_T^{[a]}\}$. Each partial evolution operator is not unitary because it describes only one curve of the total evolution. Therefore, a summation or integration over all possible alternatives or measurement readouts gives rise to what is known *non-selective* description of the measurement (that is, without fixing a certain measurement readout) and it is given only in terms of the density matrix,

$$\rho_T = \int d[a]\rho_T^{[a]} = \int d[a] U_T^{[a]} \rho_0 (U_T^{[a]})^\dagger, \tag{4.72}$$

with $d[a] = \prod_{t=0}^{T} da(t)$. Obviously, the generalized unitary condition or normalization of the RPI is

$$\int d[a](U_T^{[a]})^\dagger U_T^{[a]} = 1, \tag{4.73}$$

and the probability density of the readout $[a]$ is given by

$$P([a]) = Tr(U_T^{[a]} \rho_0 (U_T^{[a]})^\dagger). \tag{4.74}$$

Equation (4.71) has the form of a conventional Feynman path integral but with the non-Hermitian (complex) effective Hamiltonian

$$H_{[a]}(p, q, t) = H(p, q, t) - i\kappa\hbar[A(p, q, t) - a(p, q, t)]^2. \tag{4.75}$$

Now, instead of calculating a restricted path integral, one may solve the corresponding (linear) Schrödinger equation with the effective Hamiltonian given by

$$\frac{\partial}{\partial t}\Psi(q, t) = -\frac{i}{\hbar} H_{[a]} \Psi(q, t) = \left(-\frac{i}{\hbar} H - \kappa[A - a(t)]^2 \right) \Psi(q, t). \tag{4.76}$$

If this equation is solved for the initial wave function Ψ_0 describing the initial state of the measured system, then the solution Ψ_T in the final time moment represents the state of the system after the measurement, under the condition that the measurement readout is $[a]$.

A special case is when considering the monitoring of the energy where $A \equiv H_0$ is the free evolution of the system for a total Hamiltonian given by $H = H_0 + V$, V being the interaction term responsible for transitions between stationary states. Similarly, $[a] \equiv [E]$ and $[E] = \{E(t), 0 \leq t \leq T\}$. The fuzziness or resolution of the measurement is better characterized by

$$\Delta_T = \frac{1}{\kappa T} \tag{4.77}$$

than by κ since it takes also into account the duration T (the corresponding resolution clearly decreases when increasing the duration of the measurement). The weight functional is then expressed as

$$\omega_{[E]} = \exp\left(-\frac{\langle (H_0 - E)^2 \rangle_T}{\Delta E_T^2}\right) \tag{4.78}$$

with

$$\langle (H_0 - E)^2 \rangle_T = \frac{1}{T}\int_0^T (H_0(q, p, t) - E(t))^2 dt \tag{4.79}$$

and the repetition of this fuzzy measurement improves the sharpness of the measurement. This analysis allows one to deal with the monitoring of a transition between two stationary states. If the characteristic difference between energy levels is ΔE, the T duration can then be controlled in order to monitor a given energy transition (when $\Delta E_T \ll \Delta E$). The corresponding linear Schrödinger equation is now expressed as

$$\frac{\partial}{\partial t}\Psi(q, t) = \left(-\frac{i}{\hbar}H - \kappa[H_0 - E(t)]^2\right)\Psi(q, t). \tag{4.80}$$

Interestingly enough, each partial evolution operator describes only one channel of the evolution. The probability of a single curve $[a]$ ($P[a] = \langle \Psi(T)|\Psi(T)\rangle$) is zero since, strictly speaking, the pure state evolution of the corresponding Schrödinger equation, Eq. (4.76), is not possible. Finite probabilities are only adscribed to a bundle $\mathcal{A}$ of curves $[a]$

$$P_{[a]\in\mathcal{A}} = \int_{\mathcal{A}} P[a]d[a]. \tag{4.81}$$

Thus, the state of the system has to be represented by a density matrix and its time evolution is written as follows

$$\rho_T = \int_{\mathcal{A}} d[a]\rho_T^{[a]} = \int_{\mathcal{A}} d[a]U_T^{[a]}\rho_0(U_T^{[a]})^\dagger. \tag{4.82}$$

When the bundle $\mathcal{A}$ is quite narrow and the initial state is pure, the final state may be considered to be pure to a good approximation, being represented by Eq. (4.76).

Several weight functionals $\omega_{[a]}$ can be envisaged leading to different generalizations of the concept of monitoring an observable. Thus, for example, we can write

$$\omega_{[a]}[p,q] = \exp\left[-\kappa \int_0^T W(A,a)dt\right], \tag{4.83}$$

where $W(A,a)$ is an arbitrary complex-valued function of two multidimensional variables A and a, when simultaneous continuous measurements of several observables with different resolutions are carried out. The corresponding effective Hamiltonian has then the expression

$$H_{[a]} = H - i\kappa\hbar W(A, a(t)). \tag{4.84}$$

As a final remark of Mensky's approach it is worth mentioning that this theoretical framework is always considered within a linear theory where the Schrödinger equation is valid.

4.4.2 The Master Equation

The description of the RPI in terms of the density matrix opens the door to link this formalism with the master equation theory. If the weight functional is chosen to be a Gaussian function, it simplifies enormously this correspondence. Mensky [2] proved that the non-selective RPI description of the measurement is

$$\begin{aligned}\rho_t(q',q'') &= \int d[a]\langle q'|U_t^{[a]}\rho_0(U_t^{[a]})^\dagger|q''\rangle \\ &= \int d[p']d[q']d[p'']d[q'']\exp\left\{\frac{i}{\hbar}\int_0^t (p'\dot{q}' - H(p',q',t))dt\right\} \\ &\quad .\exp\left\{-\frac{i}{\hbar}\int_0^t (p''\dot{q}'' - H(p'',q'',t))dt\right\} \\ &\quad .\exp\left\{-\frac{\kappa}{2}\int_0^t (A(p',q',t) - A(p'',q'',t))^2 dt\right\}\rho_0(q_0',q_0'').\end{aligned} \tag{4.85}$$

In order to derive a master equation, within the system-plus-device framework, the density matrix of the system may be obtained by tracing out degrees of freedom

of the device (or apparatus). The simplest master (phenomenological) equation is given by

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] - \frac{\kappa}{2}[A, [A, \rho]] \tag{4.86}$$

for monitoring of the observable $A(p, q)$. This equation is a special case of the so-called Linblad equation which was derived without using any particular model and under the assumption of the Markovian character of the process. The first term results from the dynamical properties of the free system and the second term provides the decay of the off-diagonal matrix elements. It is a straightforward exercise to prove that Eq. (4.85) satisfies the above master equation.

When dealing with Hermitian and positive operators representing the fuzziness or the characteristic function of the measurement, the modulus of the wave function is scaled, but not its phase. This kind of measurements carried out by such operators is minimally disturbing. Mensky also showed the equivalence between the corresponding RPI density matrix and a much more involved master equation.

Finally, from a practical point of view, the assumption that the measuring device resolves time with absolute accuracy is an approximation (Markovian approximation). In this sense, the weight functional used in the RPI formalism has to be changed and no differential equation in time exits for the resulting density matrix due to non-local character in time [2]. The replacement of the value of an observable $A(t)$ by its time coarse graining $\langle A \rangle_t$ has to be carried out (non-Markovian approach).

4.4.3 The Stochastic Schrödinger Equation

Dealing with open systems, it is natural to ask oneself if the RPI formulation is related to a stochastic Schrödinger equation. With appropriate change of variables, it has been shown by several authors [3, 4] that the resulting equation is written as

$$d|\Phi\rangle = \left[-\frac{i}{\hbar}H - \kappa(A - c)^2\right]|\Phi\rangle dt + \sqrt{2\kappa}(A - c)|\Phi\rangle dW \tag{4.87}$$

with $a = c + (\xi/\sqrt{2\kappa})$, $\Phi = exp[(1/2)\int_0^t dt\xi^2]\Psi(0)$ and $dW = \xi dt$. W is a Wiener stochastic process with the property $dW^2 = dt$. To have the norm of the wave function conserved, it should occur that $c = \langle\Phi|A|\Phi\rangle$. Therefore, this stochastic differential equation is of Itô type and non-linear. Different stochastic equations

have also been proposed in the literature for the description of continuous quantum measurements [28–30].

4.4.4 The Bohmian Equations

The Bohmian formalism could obviously be applied to Eq. (4.76) in order to obtain the counterpart of this linear Schrödinger equation in terms of the quantum action coming from the phase of the wave function. Thus, by writing the wave function in one dimension in the usual form as

$$\Psi(x,t) = \rho^{1/2}(x,t)e^{iS(x,t)/\hbar}, \tag{4.88}$$

and after introducing Eq. (4.88) into the time-dependent Schrödinger Eq. (4.76), the following two real, coupled partial differential equations are obtained from the resulting imaginary and real parts, respectively

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial x} = -2\kappa(x-q)^2\rho, \tag{4.89a}$$

$$\dot{v} + \frac{1}{m}\frac{\partial V_{\text{eff}}}{\partial x} + vv' = 0, \tag{4.89b}$$

where the effective potential is again

$$V_{\text{eff}}(x,t) = V(x) + Q(x,t). \tag{4.90}$$

Q being the standard quantum potential and v' is the first derivative of the velocity with respect to x. Notice that Eq. (4.89a) is no longer the standard continuity equation since the source term $(-2\kappa(x-q)^2\rho)$ is added due to the continuous quantum measurement process. Furthermore, Eqs. (4.76) and (4.89) do not exhibit important properties such as separability of noninteracting systems, normalization, etc.

4.5 The Nonlinear Schrödinger Equation for Continuous Measurement

By considering only position measurements, monitoring a quantum particle by the measure of the deviation of the actual path $x(t)$, from the classical trajectory $q(t)$, may be given by the negative of the logarithmic of a weight functional $w_{[x]}$ as follows

$$[x(t) - q(t)]^2 \propto -\ln w_{[x]}. \tag{4.91}$$

Now, the back influence of the selective measuring device onto the measured system can be explicitly taken into account by the non-Hermitian effective Hamiltonian

$$H_{[x]}(x,t) = H(x,t) - i\hbar\kappa \ln w_{[x]}, \tag{4.92}$$

where κ measures the strength of the interaction between the measuring apparatus and the measured system and the choice of the weight functional depends on the class of measurements under consideration. Nassar have proposed that the evolution of the wave function of the quantum system $\Psi(x,t)$ under continuous measurement can be described in terms of the logarithmic nonlinear Schrödinger equation [5]

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left(H(x,t) - i\hbar\kappa\left[\ln|\Psi(x,t)|^2 - \left\langle\ln|\Psi(x,t)|^2\right\rangle\right]\right)\Psi(x,t). \tag{4.93}$$

which is identical to Eq. (3.22) of Chap. 3. This generalization can be better understood from the following arguments. If we start from a minimum-uncertainty wave packet solution around the measurement readout or record $q(t)$ written as

$$|\Psi(x,t)| = [2\pi\delta^2(t)]^{-1/4}\exp\left(-\frac{[x(t)-q(t)]^2}{4\delta^2(t)}\right) \tag{4.94}$$

where $\delta(t)$ is the total width of the Gaussian wave packet, then $\ln|\Psi(x,t)|^2 \propto [x(t)-q(t)]^2$ by considering that continuous position measurements produce and maintain localization as a necessary result of the information it provides. This minimum-uncertainty wave packet solution is further supported by recent, alternative stochastic approaches [31] which have demonstrated that individual trajectories remain minimum-uncertainty localized wave packets for all times, the localization being stronger the smaller $\hbar$ becomes.

The last term of Eq. (4.93) arises from the requirement that the integration of this equation, with respect to the variable x, under the condition that for a particle the expectation value of the energy $< E(t) >$ must be equal to the expectation values of the kinetic and potential energies where

$$< E(t) > \equiv \int_{-\infty}^{+\infty} \Psi^*(x,t)E(t)\Psi(x,t)dx. \tag{4.95}$$

as seen in the Schrödinger–Langevin or Kostin equation discussed in Chap. 3. Furthermore, Eq. (4.93) has several unique properties easy to prove. First, it guarantees the separability of noninteracting subsystems. Other nonlinear modifications can introduce an interaction between two subsystems even when there are no real forces acting between them. Second, the stationary states can always be normalized. For other nonlinearities, stationary solutions have their norms fully determined and after multiplication by a constant they cease to satisfy the equation. Third, this equation possesses simple analytical solutions in a number of dimensions, especially non-spreading wave packet solutions. A remarkable feature of this equation is the existence of exact soliton-like solutions of Gaussian shape. Hefter [32] has given physical grounds for the use of this logarithmic nonlinear equation by applying it to nuclear physics and obtaining qualitative and quantitative positive results. He argues that this type of equation can be applied to extended objects such as nucleons and alpha particles. Fourth, it is fundamentally different from the equation proposed by Bialynicki-Birula and Mycielsky due to the imaginary coefficient in front of the logarithmic terms and the last term $\langle \ln |\Psi(x,t)|^2 \rangle$ [33]. Fifth, as mentioned in Chap. 3, the irreversible dynamics in this case due to the continuous measurement leads to fulfil a Fokker–Planck equation. And sixth, it provides a good starting point for a hydrodynamical description of the measuring process in terms of quantum trajectories. In fact, we want to show that one of the fundamental aspects of Bohmian mechanics is its ability to tackle more intuitively the quantum measurement problem. As we know, the wave function plays a dual role in the Bohmian framework; it determines the probability of the actual location of the particle and choreographs its motion. As pointed out by Bell [9], in physics the only observations we must consider are position observations - a definite outcome in an individual measurement is determined by the relevant position variable associated with the apparatus. It is a great merit of the Bohmian picture to force us to consider this fact.

4.6 The Schrödinger–Langevin–Bohm Equation for Continuous Quantum Measurement

For simplicity, let us consider again a one-dimensional problem. The time evolution of the wave function $\Psi(x,t)$ of a quantum stochastic system under continuous measurement can also be described in terms of a more general nonlinear Schrödinger equation. This equation has to combine two types of logarithmic nonlinearities [6]: (i) For the description of a system under continuous measurement, Eq. (4.93) is used with the logarithmic nonlinear term $-i\hbar\kappa \ln|\Psi|^2$ and (ii) For the description of quantum stochastic processes, Eq. (3.2) is also used but with the logarithmic nonlinear term $(i\gamma\hbar/2)\ln(\Psi/\Psi^*)$. Thus, by combining both nonlinearities, the resulting equation now reads

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left[H(x,t) + i\hbar\left(W_\kappa(x,t) + W_\gamma(x,t)\right)\right]\Psi(x,t), \quad (4.96)$$

where

$$H(x,t) = -\frac{\hbar^2}{2m}\nabla^2 + V(x) + V_r(x,t) \quad (4.97)$$

V_r being the random potential (see Chap. 3),

$$W_\kappa(x,t) = -\kappa\left[\ln|\Psi(x,t)|^2 - \left\langle\ln|\Psi(x,t)|^2\right\rangle\right], \quad (4.98)$$

and

$$W_\gamma(x,t) = \frac{\gamma}{2}\left[\ln\frac{\Psi(x,t)}{\Psi^*(x,t)} - \left\langle\ln\frac{\Psi(x,t)}{\Psi^*(x,t)}\right\rangle\right], \quad (4.99)$$

and where, as we know, the coefficient κ characterizes the resolution of the continuous measurement and the coefficient γ represents the friction coefficient. The terms in $< . >$ arise from the requirement that the integration of Eq. (4.96) with respect to the variable x must be equal to the expectation values of the kinetic and potential energies through the Hamiltonian H, see Eq. (4.95). Equation (4.96) has the same unique properties than Eq. (4.93) mentioned before.

Equation (4.96) can now be further developed via the method of quantum trajectories. In order to simplify the resulting equations and discussion, let us consider $V = 0$ and $V_r = 0$ (or zero temperature, no thermal fluctuations or noise is involved) and whence only a dissipative free dynamics is present. To this end, the wave function is again expressed in the polar form as in Eq. (4.88) After substitution of this equation into Eq. (4.96), we obtain the Schrödinger–Langevin–Bohm (SLB) equation

$$i\hbar\left[\frac{\partial\phi}{\partial t} + \frac{i}{\hbar}\frac{\partial S}{\partial t}\phi\right] =$$

$$= -\frac{\hbar^2}{2m}\left\{\left[\frac{\partial^2\phi}{\partial x^2} - \frac{\phi}{\hbar^2}\left(\frac{\partial S}{\partial x}\right)^2\right] + \frac{i}{\hbar}\left[2\frac{\partial S}{\partial x}\frac{\partial\phi}{\partial x} + \phi\frac{\partial^2 S}{\partial x^2}\right]\right\}$$

$$- i\hbar\kappa\left[\ln\phi^2 - < \ln\phi^2 >\right]\phi + \gamma\left[S - \langle S\rangle\right]\phi. \quad (4.100)$$

As we have carried out in similar contexts, Eq. (4.100) can be separated into real and imaginary parts. By defining the quantum hydrodynamical density ρ, velocity v and quantum potential Q respectively as

$$\rho(x,t) = \phi^2(x,t), \tag{4.101}$$

$$v = \frac{1}{m}\frac{\partial S}{\partial x}, \tag{4.102}$$

$$Q = -\frac{\hbar^2}{2m\phi}\frac{\partial^2 \phi}{\partial x^2}, \tag{4.103}$$

we have the corresponding splitting of the SLB equation into

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + \gamma v = -\frac{1}{m}\frac{\partial Q}{\partial x} \tag{4.104}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) + 2\kappa\left[\ln\rho - \langle \ln\rho\rangle\right]\rho = 0. \tag{4.105}$$

Equation (4.104) is again an Euler-type equation describing trajectories of a fluid particle, with momentum $p = mv$. On the other hand, Eq. (4.105) describes the evolution of the quantum fluid density ρ but it is no longer a continuity equation since a source term is added due to the presence of the continuous measurement. 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 that the wave packet is initially centered at $x = 0$ and $\rho(x,0) = \left[2\pi\delta^2(0)\right]^{-1/2}\exp\left[-x^2/2\delta^2(0)\right]$ and ρ vanishes for $|x| \to \infty$ at any time, it can be written as Eq. (4.94) Now, Eq. (4.94) can be readily used to demonstrate that

$$\int_{-\infty}^{+\infty} \left([x - q(t)]^2\right) \rho(x,t)dx = \delta^2(t). \tag{4.106}$$

Substitution of Eq. (4.94) into (4.105) yields

$$\frac{\partial \rho}{\partial t} = \left[-\frac{\dot{\delta}}{\delta} + \frac{(x-q)}{\delta^2}\dot{q} + \frac{1}{\delta^3}(x-q)^2\dot{\delta} \right] \rho, \tag{4.107}$$

and

$$\frac{\partial(\rho v)}{\partial x} = \left(\frac{\dot{\delta}}{\delta} - \kappa\right)\rho + \left[\left(\frac{\dot{\delta}}{\delta} - \kappa\right)(x-q) + \dot{q}\right]\left(-\frac{(x-q)}{\delta^2}\right)\rho, \tag{4.108}$$

which implies that

$$v(x,t) = \left(\frac{\dot{\delta}}{\delta} - \kappa\right)(x-q) + q \tag{4.109}$$

according to the standard dressing scheme.

Analogously, substitution of Eq. (4.109) into (4.104) yields

$$\left(\ddot{\delta}(t) + (\gamma - 2\kappa)\dot{\delta}(t) + (\kappa^2 - \kappa\gamma)\delta(t) - \frac{\hbar^2}{4m^2\delta^3(t)}\right)(x-q)^1 + \delta(\ddot{q}(t) + \gamma\dot{q})(x-q)^0 = 0, \tag{4.110}$$

which implies that

$$\ddot{\delta}(t) + (\gamma - 2\kappa)\dot{\delta}(t) + (\kappa^2 - \kappa\gamma)\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)} \tag{4.111}$$

and

$$\ddot{q}(t) + \gamma\dot{q} = 0. \tag{4.112}$$

Equations (4.111) and (4.112) show that a continuous measurement of a quantum dissipative wave packet gives specific features to its evolution: the appearance of distinct classical and quantum elements, respectively. This measurement consists of monitoring the position of the quantum dissipative system and the result is the measured classical trajectory $q(t)$ for t within a quantum uncertainty $\delta(t)$. If the random potential is included (temperature different from zero), the above derivation changes slightly the resulting equations. Thus, in Eq. (4.104) the extra random force has to be added and Eq. (4.112) becomes the standard Langevin equation with the noise

term. When $\kappa = 0$, the same coupled partial differential equations for the amplitude and phase of the wave function, as seen in Chap. 3, are recovered. Furthermore, when $\gamma = 0$, the corresponding Bohmian equations for continuous measurements are finally obtained.

As far as the Schuch–Chung–Hartmann equation (3.23) is concerned, notice that if we set

$$\kappa = \frac{\gamma}{2} \tag{4.113}$$

in Eq. (4.111), we obtain such an equation and results as a special case, such that

$$\ddot{\delta}(t) - \frac{\gamma^2}{4}\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)} \tag{4.114}$$

or for the harmonic oscillator

$$\ddot{\delta}(t) - \left(\omega^2 - \frac{\gamma^2}{4}\right)\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)} \tag{4.115}$$

with the corrected reduced frequency for the dissipative harmonic oscillator, as well as

$$\ddot{q}(t) + \gamma\,\dot{q} + \omega^2 q(t) = 0. \tag{4.116}$$

Interestingly enough, a new starting point is the following differential equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left[H(x,t) + i\hbar\left(W_\kappa(x,t) + W_\gamma(x,t)\right)\right]\Psi(x,t), \tag{4.117}$$

where W_κ is defined as in Eq. (4.98) but the dissipative operator is now given by

$$W_\gamma(x,t) = -\gamma\left[\ln|\Psi(x,t)|^2 - \left\langle\ln|\Psi(x,t)|^2\right\rangle\right], \tag{4.118}$$

according to Eq. (3.22). Now, following the same theoretical procedure as before, the final important equations are

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{1}{m}\frac{\partial Q}{\partial x} \tag{4.119}$$

and

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) + 2(\kappa+\gamma)\left[\ln\rho - \langle\ln\rho\rangle\right]\rho = 0. \tag{4.120}$$

Again, starting from the Gaussian shape for the density given by Eq. (4.94), the differential equations fulfilled by the width and center of the Gaussian wave packet are, respectively,

$$\ddot{\delta}(t) - 2(\kappa+\gamma)\dot{\delta}(t) + (\kappa+\gamma)^2\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)} \tag{4.121}$$

and

$$\ddot{q}(t) = 0 \tag{4.122}$$

and the velocity is written as

$$v(x,t) = \left(\frac{\dot{\delta}}{\delta} - (\kappa+\gamma)\right)(x-q) + \dot{q}\,. \tag{4.123}$$

As can be seen from Eq. (4.122), the classical dissipative motion is not recovered. The dissipative operator can not have the same nonlinearity term than that of the continuous measurement; in other words, as expected, the two mechanisms (measurement and friction) have to be different source.

The same theoretical analysis carried out here for Gaussian wave packets could be extended to Airy packets introduced in Sect. 2.7 and given by Eq. (2.149),

$$\psi(x,t) = Ai^2\left[\frac{B}{\hbar^{2/3}}\left(x - \frac{B^3t^2}{4m^2}\right)\right]\exp\left[i\left(\frac{B^3t}{2m\hbar}\right)\left(x - \frac{B^3t^2}{6m^2}\right)\right]. \tag{4.124}$$

where Ai is the Airy function, m is the mass of the particle and B an arbitrary constant. As we know, Airy wave packets continue to propagate without spreading even when a spatially uniform and time-varying force is acting.

4.7 Bohmian Time: Dividing Line Between Quantum and Classical Trajectories

As pointed out by Bell [9], the lack of clarity in regards to where the transition between the classical and quantum regimes is located is one aspect of the measurement problem. This problem represents one of the most important conceptual difficulties in quantum mechanics. Consequently, this topic of research has gained considerable interest in the last decades [2, 5]. The presence of a classical apparatus considerably affects the behavior of the observed quantum system and measurements typically fail to have outcomes of the sort the theory was created to explain.

The solution to a challenge posed by Bell on the dividing line between the quantum and classical regimes in a measurement problem is proposed here from the theory developed in the previous Section. It is shown that continuous measurements and damping not only disturb the particle but compel the system to converge in time to a Newtonian regime without any assumption of collapse. While the width of the wave packet may reach a stationary regime, its quantum trajectories converge exponentially in time to classical trajectories. In particular, it is shown that damping tends to suppress further quantum effects on a time scale shorter than the relaxation time of the system.

The associated Bohmian trajectories of an evolving i^{th} particle of the ensemble with an initial position x_{oi} can be calculated by first substituting

$$\dot{x}_i(t) = v_i(x,t) \tag{4.125}$$

into Eq. (4.109) to obtain (dressing scheme)

$$x_i(t) = q(t) + (x_{0i} - q_{0i})\frac{\delta(t)}{\delta_0}e^{-\kappa t}, \tag{4.126}$$

where $\delta(0) = \delta_0$ is the initial width. The position of the center of mass of the wave packet (the classical trajectory) is represented by $q(t)$ and its initial value q_{0i}, while x_{0i} is the initial position of the i^{th} individual particle in the Gaussian ensemble corresponding to the wave function given by Eq. (4.88). Now, Eq. (4.111) admits analytic Gaussian-shaped soliton-like solution or gausson where the width is constant and, therefore, $\dot{\delta} = \ddot{\delta} = 0$. For $\kappa \neq 0$, a stationary regime can be reached and the width of the wave packet can be related to the resolution of measurement as follows

$$\kappa = \frac{\gamma}{2} \pm \sqrt{\frac{\gamma^2}{4} + \frac{\hbar^2}{4m^2\delta_0^4}}, \tag{4.127}$$

which means that if an initially free wave packet is kept under a certain continuous measurement, its width may not spread in time. The two basic existing decoherence mechanisms are put on equal footing. The contribution $\hbar/2m\delta_0$ is exactly the same associated with the spreading velocity of a free Gaussian wave packet [34]. Equation (4.127) displays a very similar form to that found for the renormalized frequency of a damped harmonic oscillator (see below) [35]. It is worth stressing that when the friction mechanism is added, the resolution of the apparatus is changed, showing the intertwining role played by both mechanisms when Eq. (4.127) holds.

The main characteristic of the transition from quantum to classical trajectories can then be defined as the Bohmian time constant as $\tau_B \equiv \kappa^{-1}$ and Eq. (4.126) can be further simplified to

$$x_i(t) = q(t) + x_{0i}e^{-t/\tau_B}. \tag{4.128}$$

It follows from Eq. (4.128) that if $x_{0i} = 0$, then the particle follows the Newtonian trajectory at any time. If, however, 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. Nevertheless, there is only a temporary asymmetry in the Bohmian velocities between any two symmetric particles since the rate of the asymmetry diminishes with time. After a short time, the distance in position space shifted by the particles initially lying at positive and negative $x_{0i}{}'s$ converges to a constant value. Thus, continuous measurements not only disturb the particle but compel it to eventually converge to a classical position leading to the violation of the noncrossing rule of quantum trajectories. It is also noticeable that damping tends to suppress further quantum effects on a time scale shorter than the relaxation time of the system. For a small friction coefficient ($\gamma < \hbar/m\delta_0^2$), the Bohmian time constant can be expressed as

$$\tau_B \simeq \frac{2m\delta_0^2}{\hbar}\left(1 - \frac{\nu m\delta_0^2}{\hbar}\right). \tag{4.129}$$

Further, from Eqs. (4.103) and (4.126) we have that the quantum force is given by

$$F_{qu} = -\frac{\partial Q}{\partial x} = -\frac{\partial}{\partial x}\left[-\frac{\hbar^2}{8m\delta_0^4}(x-q)^2 + \frac{\hbar^2}{4m\delta_0^2}\right] = \frac{\hbar^2}{4m\delta_0^4}x_{0i}e^{-t/\tau_B}. \tag{4.130}$$

Thus, the convergence of the quantum particle trajectories to classical trajectories is due to the influence of the measuring apparatus and friction through the quantum force. From Eq. (4.94), we note that the expectation value of the quantum force vanishes at all times since $-1/m\langle\partial Q/\partial x\rangle = [\hbar^2/(2m\delta^2)]\langle x - q(t)\rangle = 0$. The quantum force is directly proportional to the initial position of the i^{th} particle and decays exponentially in time (it drops 63% of its initial value after a time constant τ_B). Likewise, the quantum position $x_i(t)$ - the initial position of the i^{th} individual particle in the Gaussian ensemble - approaches its classical value. In this way, friction

and continuous observation of a wave packet may lead to a gradual freezing (gradual decoherence) of the quantum features of the particle. This is translated in a gradual violation of the noncrossing rule of quantum trajectories.

Finally, if the initial wave packet width for an electron is taken to be equal to 2.8×10^{-15} m (the approximate size of an electron [36]) and the coefficient of friction is made very small ($\gamma \ll \frac{\hbar}{m\delta_0^2}$), the Bohmian time constant is found to have an upper limit

$$\tau_B \simeq 10^{-26}\,\text{s}. \tag{4.131}$$

This result provides an answer to a challenge posed by Bell [9, 37] on the lack of clarity about the line between the quantum and classical regimes in a measurement problem: The Bohmian time constant above may establish that dividing line.[4]

4.8 Some Simple Applications

As seen previously, the logarithmic nonlinear Schrödinger equation proposed for continuous measurement in a dissipative environment for a one-dimensional problem is given by Eq. (4.96). The corresponding Hamiltonian and the nonlinear operators involving the action of the continuous measurement and the stochastic part are expressed by means of Eqs. (4.97)–(4.99), respectively. In Fig. 4.3, a schematic view of such a measurement is displayed. Following the work by Zander et al. [8], the parameter characterizing the continuous measurement κ is going to be considered a free real (mathematical) parameter and noted as χ. Doing this, the new nonlinear differential equations to be analyzed is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left[H(x,t) + i\hbar\left(W_\chi(x,t) + W_\gamma(x,t)\right)\right]\Psi(x,t), \tag{4.132}$$

where

$$W_\chi(x,t) = \chi\left[\ln|\Psi(x,t)|^2 - \left\langle\ln|\Psi(x,t)|^2\right\rangle\right], \tag{4.133}$$

Some of the interesting properties of this equation have already been previously mentioned; in particular, the breakdown of the superposition principle in this theoretical framework. Two important aspects are also worth commenting. First, along

[4] One of the most interesting uses of an RC circuit is the electronic pacemaker, which can make a stopped heart start beating again. The electrodes are implanted in the heart, and the circuit contains a capacitor and resistor. The pulsing rate depends on the time constant $\tau = RC$, which regulates the frequency of the heartbeat.

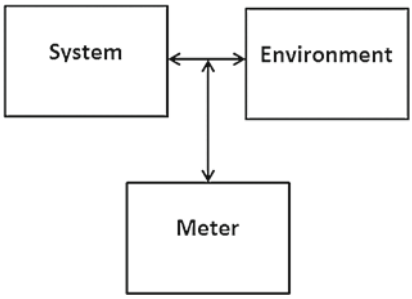

Fig. 4.3 Schematic view of the continuous measurement process on a system surrounded by an environment

this monograph (in particular, see Chap. 3), it has been pointed out several times that the environment also plays the role of a measuring device. However, it is clear from Eq. (4.132) that the sources of the two nonlinearities are drastically different; the one coming from the continuous measurement goes with the amplitude of the wave function and the one coming from the environment goes with the phase of the wave function. The second aspect concerns the interaction potential. For example, when the particle is considered free, these two nonlinearities play the role of a certain interaction potential (imaginary potential) and the corresponding dynamics is no longer "free", apart from the random potential arising from thermal fluctuations of the environment (monitoring the position of the Brownian particle).

On the other hand, the Bohmian description of the measuring process under the presence of an environment is easily reached when the wave function is, as usual, expressed in the polar form as in Eq. (4.100) and substituted in Eq. (4.132). This leads to the splitting of the Langevin–Schrödinger–Bohm equations into two coupled equations,

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + \gamma v = -\frac{1}{m}\frac{\partial (V + V_r + Q)}{\partial x} \tag{4.134}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 2\chi\left[\ln \rho - \langle \ln \rho \rangle\right]\rho. \tag{4.135}$$

which rule the time evolutions for the velocity and the probability density, respectively. Equation (4.134) is again an Euler-type equation describing trajectories of a fluid particle, with momentum $p = mv$. The two parameters governing this dynamics, χ and γ, that is, the two basic existing decoherence mechanisms here, are put on equal footing, leading to an intertwining or entanglement among them.

In the Bohmian formalism, Eq. (4.135) describes the evolution of the quantum fluid density ρ with a source/sink term $R(x,t) = 2\chi[\ln\rho - \langle\ln\rho\rangle]\rho$, the continuity equation being no longer valid. This fact has very important consequences when analyzing the relationship between the classical and quantum trajectories and the stability of the stationary solutions. Even more, when the divergence or spatial derivative term is neglected and only the source term is taken into account in Eq. (4.135), the corresponding solution of the probability density is given by [8]

$$\rho(x,t) = \frac{\exp[e^{2\chi t}\ln\rho(x,0)]}{\int_{-\infty}^{+\infty} dx' \exp[e^{2\chi t}\ln\rho(x',0)]} \tag{4.136}$$

which is properly normalized for all times t. For an initial Gaussian distribution given by $\rho(x,0) = (1/\sqrt{2\pi})\exp(-x^2/2)$, Eq. (4.136) becomes

$$\rho(x,t) = \frac{1}{\sqrt{2\pi e^{-2\chi t}}}\exp[-x^2/2e^{-2\chi t}] \tag{4.137}$$

and then

$$R(x,t) = 2\chi\left[\frac{1}{2} - \frac{x^2}{2e^{-2\chi t}}\right]\rho(x,t). \tag{4.138}$$

It is clear from the above equations, and what follows below, that the sign of the χ parameter plays a very important role; the $R(x,t)$-term can be negative (or sink term) or positive (or source term). Furthermore, when $\chi < 0$, the width of the Gaussian function increases with time whereas, when $\chi > 0$, the corresponding width decreases leading to a localization of the wave packet due to the measurement process of the particle position. Thus, Eq. (4.135) provides us the time evolution of the probability density resulting from the corresponding evolution of the density current ρv and the source/sink term, depending on the sign of χ. It should be noted that the normalization of ρ is then conserved globally, not locally, since it is not governed by a continuity equation.

The evaluation of the entropy $\mathcal{S}[\rho]$ and its time evolution is also a useful tool to characterize the degree of localization exhibited by ρ due to the measurement process. From

$$\mathcal{S}[\rho] = -\int \rho\ln\rho \tag{4.139}$$

its time evolution is governed by [8]

$$\begin{aligned}\dot{\mathcal{S}} &= -\int \frac{\partial\rho}{\partial t}\ln\rho\, dx \\ &= \left[\int_{-\infty}^{\infty}\frac{\partial v}{\partial x}\rho\, dx\right] - 2\chi\int_{-\infty}^{\infty}\rho\,(\ln\rho - <\ln\rho>)^2\, dx.\end{aligned} \tag{4.140}$$

where Eq. (4.135) has been used and an integration by parts has been carried out by considering that the probability density goes to zero fast enough in the integration limits.

4.8.1 Stability of Quantum Stochastic Trajectories

Following the same theoretical scheme used in previous chapters, a good starting point to analyze the stability of the solutions to Eqs. (4.134) and (4.135) is by considering the interaction potential $V(x)$ as a Taylor series expansion around the classical trajectory $q(t)$ up to second order

$$V(x) \approx V(q) + V'(q)(x-q) + \frac{1}{2}V''(q)(x-q)^2 + \cdots \tag{4.141}$$

as well as its first derivative,

$$V'(x) \approx V'(q) + V''(q)(x-q) + \cdots \tag{4.142}$$

where primes denote derivatives with respect to position and evaluated at the center of the wave packet which is time-dependent, $q(t)$, and $\omega^2(t) = V''(q)/m$ provides the frequency of the harmonic motion up to second order expansion. Thus, these derivatives are only functions of time through $q(t)$. Within the spatial region where the wave function is appreciably different from zero, this local approximation is assumed to be valid [38].

For a fluid particle, ρ is interpreted as the probability density of a particle being actually present within a specific region. This particle follows a definite space-time trajectory that is determined by the time evolution of the wave function through an equation of motion in accordance with the initial position. As usual assumed in this monograph, a time dependent Gaussian ansatz given by Eq. (4.107) is considered. Then, it can be readily shown that

$$\int_{-\infty}^{+\infty} \left([x-q(t)]^2\right) \rho(x,t)dx = \langle (x-q(t))^2 \rangle = \delta^2(t). \tag{4.143}$$

and the nonlocal character of the dynamical equations is given by the first spatial derivative of the quantum potential Q appearing in Eq. (4.134). For this Gaussian ansatz, this term contributes as

$$-\frac{1}{m}\frac{\partial Q}{\partial x} = -\frac{\hbar^2}{4m^2\delta^4}, \tag{4.144}$$

which is only a time-dependent function.

From Eqs. (4.107) and (4.135), the velocity field is then governed by the time differential equation but in terms now of the parameter characterizing the continuous measurement

$$v(x,t) = \left(\frac{\dot{\delta}}{\delta} + \chi\right)(x-q) + \dot{q}\,. \tag{4.145}$$

Analogously, substitution of Eq. (4.145) into (4.134) yields

$$\left(\ddot{\delta}(t) + (\gamma + 2\chi)\dot{\delta}(t) + (\chi^2 + \chi\gamma)\delta(t) - \frac{\hbar^2}{4m^2\delta^3(t)}\right)(x-q) + \delta(t)\left(\ddot{q} + \gamma\dot{q} + \frac{1}{m}\frac{\partial V_r}{\partial x}\right) = -\frac{\delta(t)}{m}\frac{\partial V}{\partial x}, \tag{4.146}$$

which implies, according to Eqs. (4.141) and (4.142), that

$$\ddot{\delta}(t) + (\gamma + 2\chi)\dot{\delta}(t) + (\chi^2 + \chi\gamma)\delta(t) - \frac{\hbar^2}{4m^2\delta^3(t)} + \frac{\delta(t)}{m}V''(q) = 0 \tag{4.147}$$

and

$$\ddot{q} + \gamma\dot{q} + \frac{1}{m}\frac{\partial V_r}{\partial x} + \frac{1}{m}V'(q) = 0. \tag{4.148}$$

where, as mentioned above, the spatial derivatives are evaluated at the center of the wave packet, $q(t)$. Equation (4.147) gives the time differential equation for the width of the Gaussian wave packet and Eq. (4.148) is the standard Langevin equation fulfilled by the center of the wave packet with $V_r(x,t) = -xF_r(t)$, $F_r(t)$ being the random force or noise. It is worth stressing that both dynamical equations are not coupled each other and their time evolutions are totally independent except that the force field has to be evaluated at the points of the classical trajectory followed by the center of the wave packet. Moreover, the Langevin equation is not affected by the parameter characterizing the continuous measurement. As seen in Chap. 3, when $\chi = 0$, the same partial differential equations for δ and q are recovered.

As clearly showed by Zander et al. [8], Eq. (4.147) can also be reexpressed by assuming the following Gaussian wave function

$$\Psi(x,t) = e^{a(t)x^2 + b(t)x + c(t)} \tag{4.149}$$

where the time dependent functions a, b and c are complex functions. From the resulting six first-order coupled differential equations for the corresponding real and imaginary parts, only the two equations governing the evolution of the complex

function $a(t)$ do not involve the b and c coefficients. In particular, with the initial conditions for the real part of a, $a_R(0)$ and $\dot{a}_R(0)$, we have that

$$a_R(t) = -\frac{1}{4\delta^2} \tag{4.150}$$

$a_R(t)$ being the real part of $a(t)$. Furthermore, Eq. (4.147) can be formally written as [8]

$$\ddot{\delta}(t) = -(2\chi + \gamma)\dot{\delta}(t) - \frac{\partial U}{\partial \delta} \tag{4.151}$$

representing an equation of motion of a particle of unit mass and coordinate δ moving in a one-dimensional effective potential given by

$$U = \frac{1}{2}(\chi^2 + \chi\gamma)\delta^2 + \frac{\hbar^2}{8m^2\delta^2} + \frac{\delta^2}{2m}V''(q), \tag{4.152}$$

the second spatial derivative being evaluated at $x = q$. This is a good starting point to analyze the stability properties of the wave packet width and, therefore, of the corresponding quantum trajectories.

After Eq. (4.145), it is easy to show that quantum trajectories are governed by

$$x(t) = q(t) + (x(0) - q(0))\frac{\delta(t)}{\delta(0)}e^{\chi t}, \tag{4.153}$$

displaying clearly the relationship with classical trajectories, $q(t)$ (dressing scheme). In principle, the gradual decoherence process due to the continuous measurement of the particle position is easily established. At asymptotic times, the exponential term, with negative χ values, is approaching zero and the decoherence should be complete; in other words, the quantum trajectory is approaching the classical one with time. Thus, in this asymptotic regime, the noncrossing rule of quantum trajectories is no longer valid. However, we are going to see that this simply analysis is not always right when studying the stability properties of the solutions due to the source/sink term in Eq. (4.135) which is not, strictly speaking, a continuity equation. Moreover, the velocity field (4.145) is then written as

$$v(t) = \dot{q}(t) + \left(\frac{\dot{\delta}(t)}{\delta(t)} + \chi\right)(x(0) - q(0))\frac{\delta(t)}{\delta(0)}e^{\chi t}, \tag{4.154}$$

showing again that the quantum velocity has clearly two independent contributions, one coming from the velocity of the center of the wave packet and the other one from the velocity of its spreading. The important difference is now the presence of the χ parameter characterizing the continuous measurement process.

4.8.2 Free Gaussian Wave Packet

4.8.2.1 Stationary Solutions

Apart from the discussion of soliton-like solutions seen in Sect. 4.8, a second case worth discussing is when the width of the Gaussian function reaches a stationary value, δ_s, after a certain time. When no interaction potential ($V = 0$) is present, the time differential equations governing such a free motion are issued from Eqs. (4.147) and (4.148) to be

$$\ddot{\delta}(t) + (\gamma + 2\chi)\dot{\delta}(t) + (\chi^2 + \chi\gamma)\delta(t) - \frac{\hbar^2}{4m^2\delta^3(t)} = 0 \tag{4.155}$$

and

$$\ddot{q} + \gamma\dot{q} + \frac{1}{m}\frac{\partial V_r}{\partial x} = 0. \tag{4.156}$$

The stability of this solution can be analyzed from Eqs. (4.151) and (4.152) with the effective potential written as

$$U = \frac{1}{2}(\chi^2 + \chi\gamma)\delta^2 + \frac{\hbar^2}{8m^2\delta^2}. \tag{4.157}$$

In this way, this potential depends on time only through δ. The stability is then obtained when it displays a local minimum, that is, when $U'(\delta_s) = 0$ and $U''(\delta_s) > 0$. Then, a dissipative drag force requires, after Eq. (4.151), that

$$\chi > -\frac{\gamma}{2} \tag{4.158}$$

and the condition for a stationary point is

$$\chi^2 + \chi\gamma - \frac{\hbar^2}{4m^2\delta_s^4} = 0 \tag{4.159}$$

which implies that

$$\delta_s^4 = \frac{\hbar^2}{4m^2(\chi^2 + \chi\gamma)} \tag{4.160}$$

showing the close relationship between the stationary point and the measurement resolution. The second derivative is positive at the stationary point δ_s when

$$\chi(\chi + \gamma) > 0 \tag{4.161}$$

which together with condition (4.158) implies that

$$\chi > 0 \tag{4.162}$$

and, therefore, the stationary point is necessarily a minimum. These facts can be verified by numerically solving Eq. (4.155). Thus, we have that $\chi = \kappa > 0$.

The positive value of χ or κ leads to very interesting properties concerning the behavior of the probability density and entropy, after Eqs. (4.139) and (4.140), as well as the Bohmian trajectories given by Eq. (4.153). As already mentioned when discussing the $R(x,t)$-term, it becomes positive (source) and tends to localize ρ with time whereas the current density has exactly the opposite behavior resulting that the Bohmian trajectories exhibit an exponential deviation from the classical trajectories. Due to the fact the source term is the dominating one, a stable solution or a stationary wave packet is reached. This observation is consistent with a continuous quantum measurement process. As pointed out by Zander et al. [8], this process could be describing the collapse of the wave function (localization). Thus, for the Gaussian ansatz given by Eq. (4.107), the entropy becomes

$$\mathcal{S}(\delta) = \frac{1}{2} + \ln\sqrt{2\pi\delta(t)^2} \tag{4.163}$$

and

$$\dot{\mathcal{S}} = \frac{\dot{\delta}}{\delta} + \kappa - 2\kappa \int \rho \left(\ln\rho - \langle\rho\rangle\right)^2 dx \tag{4.164}$$

and the localization effect contributes to the decreasing of the entropy. The time derivative of the entropy can be seen as a balance between two contributions, one of them being local, $(\dot{\delta}/\delta)+\kappa$, with no definite sign, and the other one being nonlocal and formed by the integral term with a definite sign. A stable solution means that it is an attractor of the probability density, being a more localized solution as time progresses. A characteristic time can then be defined as the time makes $\delta(t)$ to reach the stationary point δ_s. Following the mechanical analogy of Ref. [8], from the mechanical energy defined as $\epsilon(t) = \dot{\delta}^2/2 + U(\delta)$, the stationary state is estimated to be reached at time $\tau = 1/2(\gamma + 2\kappa)$. Finally, the opposite behavior of χ (negative values) makes the solution unstable and can not be considered an acceptable description of such a measurement. In other words, the very appealing property of the Bohmian trajectories approaching the classical ones is lost.

4.8.2.2 Monitoring the Bohmian–Brownian Particle

One of the paradigmatic examples where the interaction potential is negligible or constant (we are going to assume that $V(x) = 0$) is the Brownian motion. The diffusion process of an adsorbate on a flat surface, at a given surface temperature, and interacting with other adparticles, can be carried out under the presence of

a continuous monitoring of the position, the Bohmian–Brownian particle. In Eq. (4.148), the random forces or noises arising from the thermal fluctuations of the surface and the collision among particles are acting on the adparticle. This problem has already been discussed in Chap. 1, Sect. 1.3.2., from a different perspective, that is, within a linear theoretical framework and, therefore, without any continuous quantum measurement. In the previous subsection, emphasis has been only put on the stability of the solutions in terms of the χ parameter because the friction parameter γ is always a positive real number. As discussed in Chap. 3, and along this subsection, when dealing with surface diffusion, we are going to assume a simple model where the interaction of the adparticle with other adparticles is described by a collisional friction, λ, coming from a shot noise. Thus, the total friction is given by $\eta = \gamma + \lambda$ [35, 39]. So far no discussion about the classical solution $q(t)$ has been carried out.

Consider an adparticle of mass m initially placed at a given position on a flat surface. This particle can be represented by a Gaussian wave packet,

$$\Psi(x,0) = (2\pi\delta^2(0))^{-1/4} e^{-(x-q(t))^2/4\delta^2(0)}, \tag{4.165}$$

with initial width, $\delta(0)$. The adparticle is also assumed to be initially in equilibrium with the reservoir or heat bath (surface) at a temperature T, but weakly coupled to the environment, so that dissipation can be neglected. The corresponding standard Langevin equation given by Eq. (4.148) can be conveniently written for Ohmic (constant) friction as

$$\ddot{q}(t) = -\eta\dot{q}(t) + \Delta F_r(t). \tag{4.166}$$

where the mass has been absorbed in the noise or random force term (per mass unit). Two independent noise terms are supposed to well describe this simple stochastic dynamics. Lattice vibrational effects due to the surface temperature are usually represented by a Gaussian (G) white noise and collisions among adsorbates by a shot (S) white noise. These two random forces affect importantly the wave packet dynamics of the adsorbate, $F_r = F_r^G + F_r^S$. It is customarily to write the total noise fluctuations acting on the adparticle as $\Delta F_r(t) = F_r(t) - \langle F_r \rangle$, its autocorrelation function at two different times being described by a Dirac δ-function, that is, $\langle \Delta F_r(t) \Delta F_r(t') \rangle = (2\eta k_B T/m)\delta(t-t')$, k_B being the Boltzmann constant [35, 39]. The solution of Eq. (4.166) is readily shown to be (see Chaps. 2 and 3)

$$q(t) = q(0) + \frac{v(0)}{\eta}\Phi(\eta t) + \frac{1}{\eta}\int_0^t \Phi(\eta t - \eta t')\Delta F_r(t')dt' \tag{4.167}$$

where $\Phi(\eta t) = 1 - \exp(-\eta t)$. Now, after Eq. (4.153), the quantum stochastic trajectories with continuous measurement $\chi = \kappa$ are then given by

$$x(t) = q(0) + \frac{v(0)}{\eta}\Phi(\eta t) + \frac{1}{\eta}\int_0^t \Phi(\eta t - \eta t')\Delta F_r(t')dt' + (x(0) - q(0))\frac{\delta(t)}{\delta(0)}e^{\kappa t}, \tag{4.168}$$

where the requirements to have stable stationary solutions for κ are the same as previously mentioned.

As discussed in Chap. 3, in this diffusion problem, the velocity autocorrelation function $\mathcal{C}_{\Delta\mathbf{K}}(\tau)$, which is defined along with the direction of observation given by $\Delta\mathbf{K}$, provides us information about the diffusion coefficient. It should be recalled that $\Delta\mathbf{K}$ is the parallel momentum transfer of the atoms monitoring the position of the adsorbates. For a flat surface, diffusion is isotropic and, after Eq. (4.154), we have that the corresponding quantum velocity autocorrelation function is

$$\langle v(0)v(t)\rangle = \langle \dot{q}(0)\dot{q}(t)\rangle + \langle (x(0) - q(0))^2\rangle \left(\frac{\dot{\delta}(t)}{\delta(t)} + \kappa\right)\left(\frac{\dot{\delta}(0)}{\delta(0)} + \kappa\right)\frac{\dot{\delta}(t)}{\delta(0)}e^{\kappa t} \tag{4.169}$$

since $\langle \dot{q}(0)(x(0) - q(0))\rangle = 0$ and $\langle (x(0) - q(0))\dot{q}(t)\rangle = 0$, keeping a similar structure than the quantum velocity, that is, a classical contribution given by the classical autocorrelation function and a quantum contribution governed by the time derivative of the Gaussian wave packet width as well as terms involving the κ-parameter. Interestingly enough, when the initial velocity of spreading of the wave packet is zero, the quantum contribution does not disappear due precisely to those terms. In the long time limit, the classical contribution is the same given in Chap. 3. In this limit, the overdamped regime is also established and hence the acceleration term of the differential Eq. (4.155) for this width can again be neglected. However, the corresponding time evolution is marked by its stationary value reached after a certain time.

4.8.3 Linear Potential

As we have studied in previous chapters, the linear potential plays an important role when a gravitational or electric field is present. As in Chap. 2, Sect. 2.12.3, let us assume that $V(x) = -max$ with $a > 0$. In this case, the Taylor expansions given by Eqs. (4.141) and (4.142) are only retained up to first order with $V'(q) = -ma$, which corresponds to a constant force. With this linear potential, the time differential equations governing such a motion are given by Eq. (4.155) and

$$\ddot{q} + \gamma\dot{q} + a + \frac{1}{m}\frac{\partial V_r}{\partial x} = 0. \tag{4.170}$$

The stability of the corresponding stationary solutions can again be analyzed from Eqs. (4.151) and (4.157) since the effective potential has only the dependence on the second spatial derivative of the interaction potential. Therefore, the stability conditions are the same as previously derived for the free particle motion; that is, the effective potential displays a minimum at δ_s when $\chi = \kappa > 0$. Again, these conditions can easily be verified from a numerical evaluation. The stationary state means that the wave packet finally reaches a constant width.

Concerning the analysis of trajectories, we start again from the resulting standard Langevin equation issued from Eq. (4.148) for Ohmic friction

$$\ddot{q}(t) = -\gamma\dot{q}(t) - a + \Delta F_r(t). \tag{4.171}$$

where the mass has been again absorbed in the noise or random force term (per mass unit), which is assumed to be a Gaussian white noise. The solution of Eq. (4.171) is readily shown to be (see Chap. 2, Sect. 2.12.2)

$$q(t) = q(0) + \frac{a}{\gamma}t + \frac{1}{\gamma}\Phi(\gamma t)\left(v(0) - \frac{a}{\gamma}\right) + \frac{1}{m\gamma}\int_0^t \Phi(\gamma t - \gamma t')\Delta F_r(t')dt' \tag{4.172}$$

where $\Phi(\gamma t)$ has been defined above. Again, after Eq. (4.153), the quantum stochastic trajectories with continuous measurement are then given by

$$x(t) = q(t) + (x(0) - q(0))\frac{\delta(t)}{\delta(0)}e^{\kappa t}, \tag{4.173}$$

with $q(t)$ given by Eq. (4.172). It is clear that, as expected, the behavior of the quantum dynamics with time is drastically different from that obtained in Chaps. 2 and 3

4.8.4 *Quadratic Potential*

When a harmonic oscillator of frequency ω is subject to dissipation, noise and continuous measurement, the Taylor expansions given by Eqs. (4.141) and (4.142) are fully considered for the potential $V(x) = m\omega^2/2$ with $V'(q) = m\omega^2 q$ and $V''(q) = m\omega^2$ (as in Chap. 2, Sect. 2.12.4). In this case, the time differential equations governing such a damped harmonic motion are given by Eq. (4.147) rewritten as

$$\ddot{\delta}(t) + (\gamma + 2\chi)\dot{\delta}(t) + (\chi^2 + \chi\gamma + \omega^2)\delta(t) - \frac{\hbar^2}{4m^2\delta^3(t)} = 0 \tag{4.174}$$

and

$$\ddot{q} + \gamma \dot{q} + \frac{1}{m}\frac{\partial V_r}{\partial x} + \omega^2 q = 0. \tag{4.175}$$

The stability of the corresponding stationary solutions can again be analyzed from Eqs. (4.151) and (4.152) where the effective potential includes the dependence on the second spatial derivative of the interaction potential. Therefore, the stability conditions, $U'(\delta_s) = 0$ and $U''(\delta_s) > 0$, are also ruled by such a derivative. The minimum of the effective potential is given by ($\chi = \kappa > 0$)

$$\delta_s^4 = \frac{\hbar^2}{4m^2(\kappa^2 + \kappa\gamma + \omega^2)}. \tag{4.176}$$

provided that

$$\kappa^2 + \kappa\gamma + \omega^2 > 0. \tag{4.177}$$

This inequality is valid whenever κ is a positive real number, which also ensures a stochastic dynamics as well as that the wave packet reaches a constant width δ_s or stationary motion.

If the frequency of the harmonic oscillator is a constant, ω_0, as previously discussed in Chap. 2, three regimes can be established: (i) $\omega_0 > \gamma/2$ (the oscillatory motion is that of underdamped oscillator and the radicand is negative), (ii) $\omega_0 < \gamma/2$ (the overdamped motion is present and the radicand is positive) and (iii) $\omega_0 = \gamma/2$ (the critical damped motion is established). It is clear that in Eq. (4.177) is always fulfilled. As discussed in Chap. 3, this type of motion can be responsible for the so-called T-peak in the dynamical structure factor observed when an adsorbate is oscillating between two potential barriers of a corrugated surface. For simplicity, we are going to focus on the regime where $\omega_0 > \gamma/2$. Concerning the analysis of trajectories, we start again from the resulting standard Langevin equation issued from Eq. (4.148) for Ohmic friction

$$\ddot{q}(t) = -\gamma\dot{q}(t) + \Delta F_r(t) - \omega_0^2 q. \tag{4.178}$$

which is the equation of motion of a damped harmonic oscillator and where the mass has been again absorbed in the noise or random force term (per mass unit). In analogy to Eqs. (3.199) and (3.200), the corresponding quantum trajectories are given by

$$\begin{aligned} x(t) = &\left[q(0)cos(\bar{\omega}t) + \left(\frac{v(0)}{\bar{\omega}} + \frac{\gamma}{2\bar{\omega}}q(0)\right)sin(\bar{\omega}t)\right]e^{-\gamma t/2} \\ &+ \frac{1}{m\bar{\omega}}\int_0^\infty dt' e^{-\gamma t/2} sin(\bar{\omega}t)\Delta F(t') \\ &+ (x(0) - q(0))\frac{\delta(t)}{\delta(0)}e^{\kappa t} \end{aligned} \tag{4.179}$$

where

$$\bar{\omega} = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}} \tag{4.180}$$

is the reduced harmonic frequency. This frequency is obtained from the classical motion as well as from the differential equation governing the time evolution of the width of the wave packet. This is important since the continuous measurement process is able to provide such a reduced frequency. Equation (4.115) describes such a motion resulting from the application of the Schuch–Chung–Hartmann equation obtained when $\kappa = \gamma/2$.

4.8.5 *The Schuch–Chung–Hartmann Equation for Continuous Quantum Measurement*

When dealing with the dissipative harmonic oscillator, the Schuch–Chung–Hartmann equation [40, 41] could be extended to continuous measurement as follows

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2(t)x^2 + i\hbar\left(W_\chi(x,t) + W_\gamma(x,t)\right)\right]\Psi(x,t), \tag{4.181}$$

the dissipative operator being now given by

$$W_\gamma(x,t) = -\gamma\left[\ln\Psi(x,t) - \langle\ln\Psi(x,t)\rangle\right], \tag{4.182}$$

and $W_\chi(x,t)$ by Eq. (4.133). Following the same theoretical procedure as before, the final new Bohmian equations are then

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} - \gamma v + \omega^2(t)x = -\frac{1}{m}\frac{\partial Q}{\partial x} \tag{4.183}$$

and

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) - (2\chi - \gamma)\left[\ln\rho - \langle\ln\rho\rangle\right]\rho = 0. \tag{4.184}$$

Then, by starting from the Gaussian shape for the density given by Eq. (4.107), the differential equations fulfilled by the width and center of the Gaussian wave packet are, respectively,

$$\ddot{\delta}(t) - (2\chi - \gamma)\dot{\delta}(t) + \left(\omega^2(t) + \left(\chi^2 - \frac{\gamma^2}{4}\right)\right)\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)} \quad (4.185)$$

and

$$\ddot{q}(t) - \gamma q + \omega^2(t)q = 0. \quad (4.186)$$

Then, the velocity is written as

$$v(x,t) = \left(\frac{\dot{\delta}}{\delta} + (\chi - \frac{\gamma}{2})\right)(x - q) + \dot{q}\,. \quad (4.187)$$

and the quantum trajectories as

$$x(t) = q(t) + (x_0 - q_0)\frac{\delta(t)}{\delta_0}e^{(\chi-\gamma/2)t} \quad (4.188)$$

with x_0, q_0 and δ_0 being the initial values of the quantum trajectory, the classical trajectory and the width of the Gaussian wave packet.

A similar stability analysis can be carried out for these new dynamical equations.

4.9 Classical and Quantum Lyapunov Exponents

In this Section, we show how the extremely irregular character of classical chaos can be reconciled with the smooth and wavelike nature of phenomena on the atomic scale. It is demonstrated that a wave packet under continuous quantum measurement displays both chaotic and non-chaotic features. The Lyapunov characteristic exponents for the trajectories of classical particle and the quantum wave packet center of mass are calculated and their chaoticities are demonstrated to be about the same. Nonetheless, the width of the wave packet exhibits a non-chaotic behavior and allows for the possibility to beat the standard quantum limit by means of transient, contractive states [42, 43]. In particular, the periodically driven Duffing oscillator, which has become a classic model for analysis of nonlinear phenomena [31, 44, 45], is studied, and its classical chaos is shown to crossover into the quantum regime. The theory presented below deals with some unresolved features posed by chaos and on the correspondence principle which is the main focus of many new experiments with excited atomic and molecular systems. These experiments can directly probe the realm of high quantum numbers or classically chaotic motion.

The question of coupling classical variables to quantum variables is intimately connected to the question of how certain variables become classical in the first place [46]. In reality, there are no fundamentally classical systems, only quantum systems that are effectively classical under certain conditions. One must start from

the underlying quantum theory of the whole composite system and then derive the effective form of the classical theory. The starting point is to think of the classical particle as continuously monitoring the quantum particle position and responding to the measured value. To this end, consider a classical particle of mass M with position X in a nonlinear potential, the periodically driven Duffing oscillator, coupled to a quantum oscillator of frequency ω and mass m

$$M\ddot{X}(t) + BX^3(t) - AX(t) + \lambda q(t) = \Lambda \cos\ (\Omega t)\,, \tag{4.189}$$

where $q(t)$ is associated with the measurement record of the quantum system and Ω is the driving frequency. The evolution of the wave function of the quantum system Ψ can be expressed at first in terms of the path-integral for the unnormalized wave function

$$\Psi(x', t') = \int \mathcal{D}[x(t)] \exp\left[\frac{i}{\hbar}\int_0^{t'} dt\left(\frac{1}{2}m\dot{x}^2(t) - \frac{1}{2}m\omega^2 x^2(t) - \lambda x(t)X(t)\right)\right] \times \exp\left(-\int_0^{t'} dt \frac{[x(t) - q(t)]^2}{4\sigma^2(t)}\right)\Psi(x_0, 0), \tag{4.190}$$

where the path integral is over paths $x(t)$ satisfying $x(0) = x_0$ and $x(t') = x'$. The quantity σ in the equation above represents the resolution of the effective measurement of the particle by the classical system, as indicated by previous works [2, 19, 20]and Sections. However, some differences here are worth mentioning. One is the time dependence of the quantity $\sigma(t)$: most importantly is the novelty that the general resolution of the measurement evolves according to a nonlinear differential equation. Another difference relates to the dimension of the quantity $\sigma(t)$: it should be considered only proportional to the actual position uncertainty in the measurement of the quantum particle. Thus, an explicit connection to a wave packet approach can be established by writing $\sigma^2(t) = \tau\delta^2(t)$, where δ and τ have dimensions of space and time, respectively. This point can be further elucidated by approximating the last term of Eq. (4.190) around an average time $\bar{t}$, i.e., $\sim \exp -[(x(\bar{t}) - q(\bar{t}))^2/4\delta(\bar{t})^2] \exp(-\bar{t}/\tau)$, where $\delta(t)$ clearly stands for the position uncertainty (width of the wave packet) and τ characterizes the time constant (relaxation time) of the measurement.

Now, the squared of the absolute value of Eq. (4.190) yields the probability density for different measurement outputs at different times and, from this equation, the associated Schrödinger equation describing the system undergoing continuous measurement can be written as

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + \left(\frac{1}{2}m\omega^2x^2 + \lambda x X(t)\right)\Psi(x,t) - \frac{i\hbar}{4\tau}\left(\frac{[x-q(t)]^2}{\delta^2(t)} - 1\right)\Psi(x,t). \quad (4.191)$$

Next, a solution to this equation can be found by considering previous works [19, 31] which have shown that continuous position measurement produces and maintains localization in phase space as a necessary result of the information it provides. In addition to localizing the state, a continuous position measurement can also introduce noise in its evolution: the measured value $q(t)$ can be associated with a mean value $< x(t) >$ plus a noise-dependent component $\xi(t)$. Thus, in order to obtain a semiclassical protocol one must be in a regime in which the localization is relatively strong and the noise sufficiently weak. However, a protocol based on a complete hierarchy of stochastic equations associated with the average value of the position $< x(t) >$ makes it difficult to obtain an analytic solution to the problem [19].[5] The details of the variances and resulting noise strength permit only partial solutions based on varying $\hbar$ and steady state regimes. Therefore, a formalism that keeps the measurement record quantity $q(t)$ without dealing with the details of the variances can circumvent this difficult task and give a direct description of the evolution of the quantum system. This rationale entails a wave packet solution around the measurement record $q(t)$ according to Eq. (4.94). As we know, this minimum-uncertainty wave packet solution is further supported by recent, alternative stochastic approaches [31] which have demonstrated that individual quantum trajectories remain minimum-uncertainty localized wave packets for all times: the localization being stronger the smaller $\hbar$ becomes. Similar localization properties hold also for a variety of quantum trajectory methods [49–52] where the mean uncertainty product $M[\Delta x\Delta p]/\hbar$ remains close to 1 almost independent of $\hbar$, thus corroborating the minimum-uncertainty ansatz (4.94).

In the Bohmian framework, and using the standard procedure, the auxiliary functions of time $\delta(t)$ and $q(t)$ of the wave packet fulfill the following equations

$$\ddot{q}(t) + \omega^2 q(t) + \left(\frac{\lambda}{m}\right)X(t) = 0. \quad (4.192)$$

and

$$\ddot{\delta}(t) + \frac{1}{\tau}\dot{\delta}(t) + \left(\omega^2 + \frac{1}{4\tau^2}\right)\delta(t) = \frac{\hbar^2}{4m^2\delta^3(t)} \quad (4.193)$$

[5] If the noise is significant, thermal effects compete with quantum ones. To obtain the average probability solution for this stochastic process, use can be made of Chandrasekhar's convolution lemma: $\langle p(x,t)\rangle = \int_{-\infty}^{+\infty} p(x-\langle x\rangle, t)W(\langle x\rangle, t)d\langle x\rangle$, where $p(x,t) = |\psi(x,t)|^2$ and $W(\langle x\rangle, t)$ is the thermal probability of some value of $\langle x\rangle$ at time t for given initial conditions [47, 48].

Equations (4.192) and (4.193) show that a continuous measurement of a quantum oscillator gives specific features to its evolution: the appearance of distinct classical and quantum elements. This measurement consists of monitoring the position of the quantum system and the result is the measured path $q(t)$ for t within an uncertainty $\delta(t)$.

Equation (4.192) demonstrates the claim that continuous measurement can effectively obtain classical mechanics from quantum mechanics. The Lyapunov exponents that separate different time scales of motion can be established for both classical and quantum solutions as follows

$$\Lambda_{(cl,qu)} = \lim_{\substack{t\to\infty \\ \Delta(0)\to 0}} \left\{ \ln \left[\Delta_{(cl,qu)}(t)/\Delta_{(cl,qu)}(0) \right] / t \right\}, \tag{4.194}$$

where

$$\Delta_{(cl,qu)}(t) = \left\{ [(X^+, q^+) - (X^-, q^-)]^2 + [(\dot{X}^+, \dot{q}^+) - (\dot{X}^-, \dot{q}^-)]^2 \right\}^{1/2} \tag{4.195}$$

represents the renormalized classical, quantum Euclidean distances of the trajectories in phase space, respectively. Equation (4.194) describes explicitly the asymptotic rate of exponential divergence of the classical and quantum trajectories evolving from two initially close initial conditions, respectively. It appears that, at least initially, the logarithmic divergence of trajectories with a very small perturbation in the initial conditions is roughly linear, indicating an exponential relationship. To find the exponent we need to find a line that fits the logarithm of the data. Thus, it is appropriate to use only the data up to the point where the difference is of order one. Although a perturbation causes exponential divergence locally, solutions near this initial condition are attracted to a strange attractor, which is a bounded set with zero area. Since this set is bounded, the divergence can not continue indefinitely. A regression on the data provides us a reasonable exponential function to model the divergence: for the classical case, $8 \times 10^{-7} e^{0.17(1)t}$ and for the quantum case $5 \times 10^{-7} e^{0.16(8)t}$. Thus, the behavior of a quantum wave packet center of mass and the monitoring classical coordinate are equally chaotic and the Lyapunov exponents for both cases is found to be

$$\Lambda_{qu} \simeq \Lambda_{cl} = 0.17. \tag{4.196}$$

On the other hand, Eq. (4.193) shows that the width of the wave packet exhibits a non-chaotic behavior. In this context, a solution to Eq. (4.193) for a free particle ($\omega = 0$) supports qualitatively Yuen's conclusions [42, 43] so far as showing the possibility to beat the standard quantum limit by means of transient, contractive states. Extensive deliberations on how to defend or beat the standard quantum limit for both discrete and continuous measurements of the position of a quantum particle can be found in the literature [53–59]. Accurate measurements of the position of a particle is

of much interest in the context of gravitational-wave detection where questions have arisen as to whether there are fundamental quantum mechanical limits on detection sensitivity. The point here is that discrete or continuous measurements may introduce squeezing that affects subsequent measurements. Besides, the resolution squared $[\sigma^2(t) = \tau\delta^2(t)]$ of the measurement can reach a stationary regime, namely

$$\sigma_0^2 = \frac{\hbar\tau^2/m}{\left(1 + 4\omega^2\tau^2\right)^{1/2}}, \tag{4.197}$$

which indicates that localization can occur on a time scale which might be extremely short compared to the oscillator frequency ω. For the low-frequency limit $\omega\tau \ll 1$ (the free particle limit $\omega = 0$), this result reduces to $\sigma_0^2 = \hbar\tau^2/m$. On the other hand, for the high-frequency limit $\omega\tau \gg 1$, $\sigma_0^2 = \hbar\tau/2m\omega$. These results show that the resolution σ of the effective measurement increases as the characteristic time constant τ (relaxation time) increases.

We have thus established a direct correlation between a classical variable X with the measurement record of the quantum system q. Moreover, it is shown how the extremely irregular character of classical chaos can be reconciled with the smooth and wavelike nature of phenomena by demonstrating that a wave packet under continuous quantum measurement displays both chaotic and non-chaotic features. The Lyapunov characteristic exponents for the trajectories of classical particle and the quantum wave packet center of mass are calculated and their chaoticities are demonstrated to be about the same. On the other hand, the width of the wave packet exhibits a non-chaotic behavior and allows for the possibility to beat the standard quantum limit by means of transient, contractive states.

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Epilogue

Throughout this monograph, our aim has been to introduce the reader to an alternative way to deal with open quantum systems and the continuous quantum measurement within the framework of nonrelativistic Bohmian mechanics. The time evolution of the open quantum system is carried out following the well-known Schrödinger–Langevin equation or Kostin equation and the measuring process treatment is inspired by the so-called restricted path integral due to Mensky. This analysis has been carried out by means of quantum (Bohmian) stochastic trajectories, not to be confused with the same terminology used in different contexts, namely, quantum optics and the stochastic Schrödinger equation. This way of considering the process of measuring as an open quantum process leads us to consider its corresponding dynamics as causal, nonlocal, nonlineal, nonunitary and stochastic and without any collapse of the wave function. Within this theoretical formalism, two contributions of very different character, but considered on equal footing through a given coupling scheme, are present; one coming from the interaction with the measuring device and, the second one, from the interaction with its surroundings. Entanglement among the system, environment and measuring apparatus results in decoherence, leading to the emergence of the classical world. In our opinion, the inflection point in this field is when the measurement problem is no longer considered as a philosophical problem but a quantum process, following the well known rules of quantum mechanics and beyond. When it is established as a process, the corresponding dynamics has somehow to be solved by means of computational/numerical methods.

The measuring process of position has been described in a hydrodynamics-like formulation. When a Gaussian shape for the probability density is assumed, two nonlinear coupled equations for the density and the corresponding flow velocity are obtained. One of the nice features issued from those coupled equations is that the corresponding quantum dynamics can be clearly splitted into two contributions. Thus, following the same dressing scheme obtained in the Bohmian formalism, where a quantum trajectory consists of a classical trajectory dressed by a nonlocal term, a quantum stochastic trajectory is also the result of a classical stochastic trajectory plus a quantum (nonlocal) contribution, consisting of the time evolution of the width of the Gaussian probability density multiplied by a critical exponential function governed

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by the characteristic parameter defining the continuous quantum measurement. For special cases, soliton-like solutions in a dissipative medium, this exponential function decreases with time and, at asymptotic times, the quantum trajectory is approaching the classical one, establishing a natural dividing line (according to Bell's proposal) for decoherence by means of a characteristic time, the so-called Bohmian time. However, in general, when the localization of the particle is settled down due to the measuring process, that is, the width of the Gaussian function reaches its stationary value, this exponential function is not a decaying function of time. In other words, the classical trajectory is no longer an attractor and the decoherence process follows a different route. Several simple examples have been developped to illustrate how this nonlinear and stochastic theory works; in particular, special emphasis has been put on surface diffusion where the Brownian motion is a paradigmatic case.

In our opinion, the increasing development of experimental setups combining weak and strong measurements and continuous measurements can lead to an important advance and use of classical-like objects in all branches of physics, chemistry, and biology. Thus, recent work claiming the direct measurement of the photon transverse wave function or the inference of average trajectories of single photons in a two-slit interferometer open new and exciting perspectives. This is the first step to observing or measuring wave functions and paths or trajectories of massive particles. In the near future, the combination of the measurement process in terms of weak values and stochasticity is going to be of paramount importance for a more complete and deeper understanding of quantum processes in terms of trajectories, beyond the standard meaning of being a purely classical concept. As mentioned in the Preface and illustrated here, it is clear that the enormous effort invested by many researchers in the measurement problem within the standard quantum mechanics outweighs by far that invested in Bohmian mechanics. In our opinion, the only way to overcome such a disparity starts at the universities, when teaching the first courses of quantum mechanics. This mechanics should be seen as an alternative and complementary way to describe the measuring process, at the same level than any other standard picture of quantum mechanics. We sincerely think that this approach will have a long and fruitful life in the future with really unexpected and promising results. As the reader will soon realize, there is plenty left to find out and develop in the near future, this monograph being a small and humble step towards a more general and complete theory of continuous quantum measurement within the Bohmian picture of quantum mechanics. In this regard, if this work has served to foster the use of this picture of quantum mechanics and to make the reader aware of the large variety of potentialities displayed by Bohmian theory for a better understanding of the continuous quantum measurement, all the efforts devoted to this monograph will have been worthwhile.

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