Preface

Trajectory-based formalisms used to describe non-relativistic quantum processes are being continuously developed. Perhaps with increased emphasis in the last 15 years or so, since dealing with "classical" concepts is very appealing owing to the physical insight or intuition one gains into the process under study. The three main theoretical frameworks in use nowadays—apart from classical mechanics—but with significant advances since their initial formulation are, in chronological order, the Jeffreys–Wentzel–Kramers–Brillouin (JWKB) approach (1926), the Feynman path integral approach (1948) based on earlier remarks by Dirac (1935), and the Bohmian approach (1952) with its roots in the pioneering works of Madelung's hydrodynamic formulation of quantum mechanics (1926) and de Broglie's pilot wave theory (1927). Since then, many hybrid methods combining classical and quantum mechanics have been developed, mainly to tackle an accurate description of many–degrees-of-freedom systems.

The semiclassical JWKB approximation is a short-wavelength description of quantum mechanics. The idea behind this approach is to build wave functions from classical trajectories and, in a more pictorial way, to "sew quantum mechanical flesh onto classical bones", quoting Berry and Mount (1972). From a mathematical viewpoint, this treatment is based on asymptotic series. For simple bound systems, quantization schemes are usually based on the JWKB method, the Bohr-Sommerfeld quantization rule, or the multidimensional generalization of the latter, namely the Einstein-Brillouin-Keller quantization rule. Near turning points this approximation breaks down, giving rise to caustics or coalescence of classical trajectories. In order to solve this problem, uniform approximations were developed by linearizing the interaction potential in the vicinity of turning points. Taking into account this theoretical scheme, one of the processes that has been more intensively studied is that of tunneling through a barrier. In classically forbidden regions, trajectories are analytically continued in the complex plane in order to account for a quantum problem (for example, tunneling) that has no classical analog. Furthermore, this approach has also been exploited within semiclassical scattering, starting with Ford and Wheeler (1959), who explained the rainbow effect observed in the gas phase. Nonetheless, from a practical point of

view, it is easier to solve an initial-value problem than a boundary-value one. This is the reason why real-time propagators are usually based on the so-called initial-value representation in phase space. Alternatively, a very powerful and elegant route to the semiclassical approach is Feynman's path integral, which is another formulation of quantum mechanics. In this formulation, the time propagator arising from the integral representation of the Schrödinger equation is written in terms of a path integral—or sum over classical paths—which is dominated by those trajectories extremalizing the action. At present, one of the most important applications of this approach is the calculation of the density matrix for many-body (or many–degrees-of-freedom) systems—actually, the path-integral Monte Carlo method used to deal with particle clusters is based on it.

Bohmian 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 focused on the completeness of the wave function and the quantum theory of measurement. Within Bohmian mechanics, a quantum system is described by 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 that enables us to characterize, interpret and predict quantum processes, standing on equal footing with the standard theory. The central topic of this monograph is Bohmian mechanics. This formulation has also received an important impulse over the last 15 years from different communities, which translates into an impressive and fruitful theoretical development.

At present, there are several books on Bohmian mechanics, which somehow summarize the trends mentioned above. *The Quantum Theory of Motion* (1993) by Holland, *The Undivided Universe: an Ontological Interpretation of Quantum Theory* (1993) by Bohm and Hiley, and *Bohmsche Mechanik als Grundlage der Quantenmechanik* (2001) by Dürr—with its recently published English's version, *Bohmian Mechanics* (2009), in collaboration with Teufel—mainly deal with the conceptual grounds and foundations of this theory as well as epistemological problems. On the other hand, Wyatt's monograph, *Quantum Dynamics with Trajectories* (2005), tackles a more practical side of this theory, dealing with the potential application of quantum trajectories in applied problems and stressing their computational aspect as a means of solving the time-dependent Schrödinger equation. A collection of chapters published very recently in two monographs, *Quantum Trajectories* (2010) edited by Chattaraj and *Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology* (2012) edited by Oriols and Mompart, give an ample overview of Bohmian mechanics in which the corresponding theory has been successfully applied. However, in spite of the wide range of applications within Bohmian mechanics covered by these books, from the foundations to

computation, its interpretational importance is, somehow, lacking. It is missing in the sense that one cannot find many applications and discussions of this trajectory-based viewpoint within the context of realistic quantum phenomena, that are of broad interest to different scientific communities.

Moreover, explaining the dynamics of quantum phenomena in terms of trajectories has always attracted many physicists and chemists. The interpretations arising from Bohmian mechanics are very intuitive, powerful, and simpler than those provided by the standard version of quantum mechanics. Taking this into account, the main purpose of this monograph, and what justifies its publication is to provide and promote the interpretational aspects of Bohmian mechanics as an alternative way of understanding quantum physics and gaining more physical intuition, in particular, with regard to the visualization of the evolution of individual systems (at the same level as Newtonian mechanics with respect to classical statistical mechanics). Furthermore, and from our own longstanding experience in the field, Bohmian mechanics can tackle any quantum problem that standard quantum mechanics does, providing an alternative way of interpreting the phenomenon under analysis. Obviously, the effort invested by many researchers in standard quantum mechanics completely outweighs 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 textbooks at the introductory level (indeed, as John Bell suggested, quantum mechanics should be studied from a Bohmian perspective in order to make clear the most striking and strange features of that theory).

With this goal, and in order to be as self-contained as possible, this monograph has been divided into two volumes. The first volume is focused on the classical and quantum theoretical background, whereas the second volume is devoted to simple and basic quantum processes to provide a new and alternative interpretation in terms of quantum trajectories. The chapters of this first volume, which are intended to be as self-conatined as possible, are organized as follows.

In Chap. 1, a brief survey of classical mechanics is presented ranging from trajectories to ensembles of trajectories, paying attention to the dynamics or time evolution of micro-objects when interacting with other micro-particles or with some external potential function. Newtonian physics is based on the idea of a first cause behind the motion of objects. However, perhaps one of the most elegant ways of rationalizing physical laws arises through the *calculus of variations*, from which such laws emerge as a consequence of the application of a *variational principle* (in this sense, Appendix A reminds the reader of the essentials of the calculus of variations for variables and fields). The three main formulations of classical mechanics, that is, Lagrangian, Hamiltonian, and Hamilton–Jacobi formulations, are briefly set out, since they represent the fundamental building blocks of any dynamical theory in terms of time or energy as primary parameters. Very often a first classical approach to a given quantum problem provides us with a complementary understanding of the corresponding dynamics, which results in a considerable gain in intuition—in particular, if the phase-space formulation is used. When dealing with ensembles of trajectories, we expect a natural transition

from regular to chaotic motion owing to the underlying stochasticity present in dynamical (Hamiltonian) problems with two or higher dimensions. Furthermore, the extension to classical statistical mechanics, where the motion is deterministic but unpredictable, is analyzed in terms of the Liouville equation and a field theory. Several important aspects of continuum mechanics are very briefly commented on owing to its basic importance in quantum fluid dynamics.

In Chap. 2, the dynamics of open classical systems are introduced. Open classical systems are usually defined as those where the system of interest is surrounded by an environment at a certain temperature (heat bath or reservoir), exchanging energy in both directions. 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 mathematics required to understand this dynamics is the theory of probability and stochastic processes. This theory is briefly described in Appendix B since it plays a fundamental role in any classical or quantum dynamics. When a "coarse-grained" description is used, where we focus only on the dynamics of the system of interest, neglecting the details of the time evolution of the environment, two types of mechanics arise naturally: the dissipative and stochastic mechanics. In both types of mechanics, there are three standard routes to introduce dissipation and/or stochasticiy. First, from a phenomenological viewpoint, empirical equations are introduced, such as the standard Langevin equation, where a few parameters are required to describe the system–environment interaction. Second, starting from the Liouville equation, which is satisfied by any dynamical variable in phase space, projection operator techniques are applied until a generalized Langevin equation is finally reached. Third, when the starting point is a conservative many-body problem (system plus environment is an isolated system), dissipative forces can be obtained as well as an external stochasticity owing to the fluctuations or noise of the heat bath. A clear distinction between the two mechanics and some links between these three different approaches are presented and discussed.

In Chap. 3, some elements of quantum mechanics are presented. Time-independent and time-dependent Schrödinger equations are derived from the so-called Hamiltonian analogy through the calculus of variation together with de Broglie's ideas of associating a wavelength with matter particles. Some basic notions of wave mechanics, current densities, ensemble distributions and density matrix in phase space are also reviewed. Special emphasis is placed on some approaches to quantum mechanics in which classical concepts and/or trajectories are the main ingredients such as the path integral formulation, semiclassical mechanics and, the eikonal approach.

Chapter 4 is devoted to wave optics in connection to quantum mechanics. The issues covered in this chapter are almost entirely based on the physics described by the *wave equation*. This allows us to understand and offer an alternative optical perspective of many of the basic elements and concepts found in quantum mechanics within the context of any wave theory, and not as something purely specific to quantum physics. According to Ballentine, quantum phenomena can be illustrated by means of three traits: *discreteness*, *diffraction*, and *coherence*. Thus,

the chapter is organized in such a way that shows how such features and related concepts are already present in wave optics, though in a general way. Thus, starting from the main ingredients of wave optics, namely Maxwell's equations and the wave equation, we will move into the superposition or Huygens–Fresnel principle, very closely connected to the notion of *coherence* and the appearance of interference and diffraction phenomena. Regarding discreteness, it is not necessary to go as far as the photoelectric effect, but we already find it in *optical waveguides*, which are the optical analogs of quantum "bound" systems. In order to cover the full spectrum of phenomena that can be found in quantum mechanics, we also revisit the *Goos–Hänchen effect* or the *Hartman effect*, which are good examples related to *optical tunneling*. Furthermore, a direct link to the language of quantum mechanics can be established through the *hydrodynamical formulation of electromagnetism*, a generalized formulation based on the so-called *Riemann–Silberstein vector*.

The dynamics of open quantum systems is briefly treated in Chap. 5. The system-plus-reservoir model used in the classical context is also followed here in quantum mechanics, and dissipation and stochasticity are easier to tackle and understand. Both system and reservoir are in continuous interaction and the effects—coherence loss or decoherence, population transfer, and/or (system–environment) energy exchange—arising from that interaction will depend to a greater or lesser extent on the coupling strength and its intrinsic nature. The system time-evolution is not unitary and therefore cannot be described in terms of the Schrödinger equation. In these cases, it is then necessary to resort to statistical quantum methods invoking, for example, the density matrix and Langevin formalisms and/or introducing, in general, quantum stochasticity into the time-evolution equations: the Linblad equation, quantum Langevin-type equations, and so on. The energy transfer from the system to the environment is termed quantum *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 time scales, the distinction between quantum relaxation and dissipation is obviously unclear. 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, which 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 depends only 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. In analogy to open classical systems, there are also three main different approaches to dealing with quantum dissipative dynamics: (i) effective time-dependent Hamiltonians, (ii) the nonlinear Schrödinger equation, and (iii) the system-plus-reservoir model within a conservative scenario. In particular, the so-called stochastic Schrödinger equation, written in terms of an Itô differential equation, gives rise to quantum trajectories,

not to be confused with those coming from Bohmian mechanics. Finally, in this chapter as well as in Appendix B the measurement process is also very briefly discussed through the introduction of the so-called weak measurement due to Aharonov, Albert and Vaidman, in distinction to the more standard von Neumann strong measurement, since observing very weak effects is becoming more and more important at present.

Chapter 6 can be considered the main chapter of this monograph; to some extent, the previous chapters have been written for the purpose of providing the reader, as far as possible, with the background necessary to better understand the approach developed by David Bohm, nowadays known as Bohmian mechanics. He essentially based his theory on the assumption that a quantum system consists, at the same time, of a wave and a particle. The wave evolves according to Schrödinger's equation and the particle moves according to a certain guidance condition (quantum trajectories), which makes the particle motion dependent on the wave evolution. Although Bohmian mechanics is usually regarded as a "reinterpretation" or an alternative picture of standard quantum mechanics, it is also common to refer to it as a "theory" in order to stress the conceptual difference between the two approaches to the microscopic world. Bohm's ideas were applied to different prototypical models of quantum mechanics during the late 1970s and, particularly, the 1980s and early 1990s, and the attention paid by the scientific community was not very great. However, in the last ten years or so, Bohmian mechanics has passed from being merely a way to formulate a quantum mechanics "without observers" to become a well-known (and increasingly accepted) theoretical framework used as a source of new quantum computational methods as well as new quantum interpretations. This chapter ends by considering open quantum systems from this point of view.

Finally, Chap. 7 has been organized to take into account a gradual transition from simple (light) rays to hydrodynamic (photon) trajectories/paths, i.e., from geometric optics to what we shall denote as *hydrodynamic optics*. This trajectory-based description is analyzed for the propagation of plane waves and Young-type experiments with polarized light, the latter being intimately related to the so-called Arago–Fresnel laws of diffraction for polarized light. Afterwards, a brief account on the relation between hydrodynamic optics and the formulation based on the Riemann–Silberstein vector is given. The reported diffraction pattern for the two-slit experiment has been very recently inferred and explained in terms of photon paths from experiment. The weak measurement of an observable (position and/or momentum) for a quantum system is preselected in an initial state and postselected by a strong measurement in a final different state. Experiments of this kind have also led to a direct measurement of the photon quantum wave function. In our opinion, Bohmian mechanics can again undergo a new revival thanks to these experiments (where weak measurements are carried out), which can provide information on quantum trajectories of the underlying dynamics of any quantum process.

This monograph is the result of more than 15 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 very active fields 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 abroad and from Spain. In this sense, we would like to acknowledge fruitful discussions and collaborations with J. A. Beswick, J. M. Bofill, F. Borondo, M. Božić, P. Brumer, J. Campos-Martínez, P. K. Chattaraj, C. C. Chou, M. Davidović, D. Dürr, E. R. Floyd, X. Giménez, S. Goldstein, T. González-Lezana, B. J. Hiley, B. K. Kendrick, J. Margalef-Roig, B. Poirier, E. Pollak, O. Roncero, J. S. Sánchez-Gómez, D. J. Tannor, T. Uzer and R. E. Wyatt. Also, we would like to thank all members (past and present) of the *Departamento de Física Atómica, Molecular y de Agregados* of the *Instituto de Física Fundamental* (CSIC) in Madrid, where this work has been carried out from its inception, benefiting support from the projects FIS2007-62006, FIS2010-18132, FIS2010-22082 and FIS2011-29596-C02-01 from the Ministerio de Ciencia e Innovación (Spain), a "Ramón y Cajal" Research Fellowship (A. S. S.), and the COST Action MP1006 "Fundamental Problems in Quantum Physics". Special thanks go to Gerardo Delgado-Barrio and Pablo Villarreal, *founding fathers* of this department, for their continuous support of and enthusiasm for our work. Finally, we thank A. Lahee, our Editor, for her enthusiasm when we proposed the monograph to her, as well as her patience and for extending —several times— the deadline for finishing this project.

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