

Preface

In this second volume of the monograph *A Trajectory Description of Quantum Processes. A Bohmian Perspective*, our main goal is to provide the reader with a series of applications of the theory introduced and widely developed in the first volume. These applications range from simple and basic quantum results, which can be easily worked out, to more complex simulations, which require a more specific technical training. In any case, the emphasis is put on the following objectives. First, to furnish a dynamical perspective of some of the fundamental quantum processes, with special attention paid to the time-evolution of wave packets and the corresponding descriptions in terms of trajectories, in particular Bohmian trajectories. This description has been prepared bearing in mind what is now regarded as the Bohmian analytical approach. Accordingly, one first solves Schrödinger's equation and then, as the wave function is propagated in time, the trajectories are obtained from the so-called guidance equation, which requires knowledge of the phase of the wave function. In this sense, this scheme is complementary to the so-called Bohmian synthetic approach, which operates the other way around. That is, the solution of the two coupled fundamental equations in Bohmian mechanics, namely the continuity equation and the quantum Hamilton–Jacobi equation, are determined from hydrodynamic-type numerical methods, and the wave function or any other related quantity is obtained (synthesized) from the trajectories. In this regard, since our focus has been the analysis and understanding of quantum phenomena, we have always considered the former option; however, we advise the avid reader interested in developing new numerical tools also to consider the latter approach. Second, to keep as close as possible to experiment even if some previous analytical work is not fully developed. And third, to focus on our own longstanding experience of work performed in different areas of quantum mechanics and optics, such as diffraction and interferometry, atomic and molecular bound systems, quantum fractals, tunneling, and atom–surface dynamics, particularly from a Bohmian perspective. In this sense, alternative descriptions and/or interpretations to the conventional quantum ones are always provided throughout this volume in order to show the capabilities and insight gained following this approach.

According to our accumulated experience in the areas mentioned above, but also keeping in mind which concepts could be relevant for a general knowledge of quantum processes in real time, we have organized this second volume as follows. In Chap. 1 a very detailed analysis of single-wave-packet dynamics is carried out, with special emphasis on free-particle physics. The chapter starts from some general aspects of time-propagation and spreading of a single wave packet in real and complex configuration space, as well as the connection between wave-packet propagation and diffraction. Non-locality issues are also discussed before the chapter turns to one of the most fundamental aspects of quantum mechanics, namely the role of the measurement process, which eventually breaks down the usual unitary time-evolution of the system. This analysis is carried out in the context of the so-called quantum Zeno and anti-Zeno effects. In this regard, dissipative and stochastic wave packet dynamics are also discussed, in the latter case paying special attention to the evolution of a wave packet on a flat surface, which leads, in a natural fashion, to the introduction of the concept of quantum stochastic trajectory. These trajectories arise when dealing with quantum potentials depending on friction and temperature; an extension of this idea is proposed within the framework of weak measurements and values.

In Chap. 2 we tackle the issue of the superposition principle and the dynamics associated with interference processes. More specifically, we have considered as a working model the superposition of two wave packets, i.e., what is commonly regarded as a Schrödinger cat state. Though simple, this model yet suffices to provide an interesting and general insight into the problem of quantum interference, which plays a key role in other more sophisticated phenomena, such as matter-wave interferometry (for single particles) or entanglement (for two or more particles). Thus, as in the previous chapter, also here we investigate the corresponding real and complex dynamics, noticing the physical implications of the Bohmian non-crossing rule (which have been inferred from measurements in photon interference experiments). In a chapter devoted to interference it would be unforgivable to leave out the celebrated Young's two-slit experiment, which here is discussed from different viewpoints, including the decoherence action of an environment over the system. Actually, the latter aspect also serves us to introduce dissipation and stochastic dynamics in the context of interference.

Chapter 3 deals with matter-wave diffraction and one of its most immediate and important applications at present, namely matter-wave interferometry. This chapter starts from general considerations of periodic grating diffraction in the near- and far-field regimes. Then a detailed analysis of atomic and molecular Mach-Zehnder interferometry follows, where the so-called Talbot effect, a near-field grating-diffraction effect, and the formation of quantum carpets arise naturally. The starting point is the analysis of a wave-packet dynamics using Bohmian mechanics, which very conveniently sheds some light on real experiments—notice that pictures in terms of the motion of individual particles are always highly desirable, particularly if these particles follow the quantum flow, unlike what usually happens in other alternative classical and semiclassical models. Apart from grating interferometry, this is an also important issue, for example, in surface science experiments, where the illumination of a surface for its study and characterization is limited in extension.

Periodic surfaces are reflection gratings equivalent to (transmission) multiple-slit arrays. Owing to the availability of surface models in the literature, though, they turn out to be more convenient than transmission gratings to analyze short-range, attractive effects near the surface. This attractive interaction has been shown to lead to a slight distortion of the Talbot distance and the corresponding quantum carpets, namely the Talbot–Beeby effect—in surface science the variation of the diffracted beam wavelength due to the presence of attractive wells is known as the Beeby correction. Apart from these treatments, this chapter also includes an analysis of the Fraunhofer, far-field regime, as well as a discussion of the meaning of the classical limit in this context.

In Chap. 4 we study the dynamics associated with bound systems, starting from the “puzzling” non-degenerate eigenstates associated with motionless Bohmian trajectories. The meaning of this rest state is discussed as well as the origin of motion as soon as the wave function acquires a phase that varies locally in either time (eigenstate superpositions) or space (degenerate eigenstates). Owing to the finiteness of the basis of bound states, bound wave functions often display recurrences in time, leading to quantum carpets similar to those described in the previous chapter. Hence the origin of these recurrences and links to the quantum-classical correspondence in bound systems are also introduced. Under some conditions, such recurrences give rise to fractal features and, when dealing with Bohmian trajectories, to quantum fractal trajectories, which are also analyzed. To complete the chapter, we present an analysis of the real and complex dynamics of coherent wave packets, as well as dissipative extensions in the context of the so-called quantum van der Pol equation on the one hand and the Caldirola–Kanai dissipative model on the other.

Quantum tunneling is treated in Chap. 5. This fundamental quantum trait is analyzed from a series of alternative contexts, each one stressing a different aspect of the tunneling dynamics. In this sense, first we show how Bohmian mechanics allows one to determine tunneling conditions, discriminating between sets of initial conditions that lead to tunneling and those that do not. This analysis is extended to time-dependent models, such as strong-field ionization, where one observes how the spectra of interest can be precisely determined from a set of particular Bohmian trajectories. Besides Bohmian applications, the quantum stochastic dynamics of a non-isolated chiral, two-level system is also studied, but using a canonical formalism within the Langevin framework. Apart from its intrinsic interest, this problem has been chosen because it constitutes a nice illustration of quantum and/or classical coherence. Furthermore, within the field of surface science, we analyze the tunneling surface diffusion of hydrogen and deuterium on a platinum (111) surface, this being motivated by the experimental results reported on this paradigmatic system.

Chapter 6 is devoted to atom–surface scattering from periodic surfaces. After a brief survey of the background in the energy domain, developing the elastic close-coupling method, we tackle the problem of the time-dependence in quantum diffraction and a Bohmian trajectory description of the so-called selective adsorption resonances, i.e., the bound motion of scattered light particles along the surface. As is shown, the corresponding quantum trapping picture is radically different from the classical trapping one, as is easily deduced from a Bohmian trajectory analysis. This

chapter also covers a brief theoretical treatment of the classical stochastic (elastic and inelastic) scattering that takes place when heavy particles are used to probe the surface.

In Chap. 7 we consider the case of non-periodic surfaces, i.e., surfaces displaying a breaking of the periodicity caused by the presence of adsorbates. In this regard, we have focused on He-atom diffraction dynamics in the presence of fixed adsorbates. As is shown, this system gives rise to a rich vortical dynamics, with Bohmian trajectories displaying vortices and explaining the motion of the scattered particles across the surface. One of the paradigmatic examples in this context is the scattering of helium atoms with a carbon monoxide molecule on the platinum (111) surface. As an extension, the stochastic dynamics of adsorbates on the surface is also analyzed in order to understand the activated surface diffusion process and how quantum corrections can be taken into account. In this case, the surface is considered as a thermal bath and the interaction with the phonons of the substrate as Gaussian white noise. The interaction among adsorbates is introduced by means of a collisional friction associated with a Poissonian time-distribution among collisions.

In Chap. 8, the problem of many-body (or equivalently many degrees-of-freedom) interactions is tackled from the viewpoint of quantum chemistry and chemical physics. The reason to considering this perspective is because of the important influence that Madelung's quantum hydrodynamics (a pre-Bohmian model dating back to 1926) has had in these fields since the 1970s as a practical working tool, from the development of electronic structure methodologies to the investigation and analysis of chemical processes (some of them already studied in previous chapters), or as inspiration to develop new numerical tools to attack large, complex systems. In this sense, this theoretical approach is so far developed as to be able to attack large-scale problems. The application of the Schrödinger equation to discern electronic structural properties of materials is commonly regarded as quantum chemistry (i.e., electronic structure and its methodology), while the dynamical and statistical part of the theoretical chemistry are the subjects of chemical physics. In this regard, first we introduce the Born–Oppenheimer approximation, used both to devise electronic structure methodologies and to deal with many-degrees-of-freedom systems within the open quantum theory scenario. Then a brief account of density functional theory, both time-independent and time-dependent, is presented, with special emphasis on the quantum hydrodynamic approach. At a different level, but also within this context, we also discuss Hirschfelder's approach to quantum equations of change, an unfortunately missed precedent of the now celebrated weak values. The chapter ends with a general discussion of the possibility of connecting particular sectors of the initial state with individual features of the final state by means of probability tubes defined following the prescriptions of Bohmian mechanics.

This volume closes with an epilogue, where some final remarks and future perspectives on the development of the Bohmian approach and, by extension, the Bohmian thinking are discussed. Nevertheless, for the interested reader, we have also prepared an appendix, where some basic tools are briefly described to design wave-packet propagation schemes from which to compute the corresponding Bohmian trajectories.

Last but not least, we would like to finish this preface by thanking once again our many colleagues and friends from Spain and abroad, the many fruitful and interesting discussions and collaborations with whom have without a doubt contributed importantly to the completion of this work in this form. We mention in particular B.B. Augstein, P. Bargueño, J.A. Beswick, J.M. Bofill, F. Borondo, M. Božić, P. Brumer, M.L. Calvo, J. Campos-Martínez, L. Celotti, P.K. Chattaraj, L. Choque, C.C. Chou, M. Davidović, I. Delgado, A. Dorta-Urra, D. Dürr, C. Efthymiopoulos, C. Figueira de Morisson Faria, E.R. Floyd, X. Giménez, S. Goldstein, T. González-Lezana, A. González-Ureña, I. Gonzalo, G. Grössing, G. Grübl, B. Hiley, B.K. Kendrick, A. Luis, J. Margalef-Roig, R. Martínez-Casado, J. Mompert, A.B. Nassar, T. Norsen, X. Oriols, H. Peñate-Rodríguez, J. Pérez-Ríos, B. Poirier, E. Pollak, M.A. Porras, R. Röhmer, G. Rojas-Lorenzo, O. Roncero, J. Rubayo-Soneira, J.L. Sánchez-Gómez, C. Sanz, D.J. Tannor, T. Uzer, J. Wu, R.E. Wyatt, and N. Zanghì. 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 was carried out from its inception, as well as University College London (AS) for its kind hospitality. Support from projects FIS2011-29596-C02-C01 and FIS2010-22082 from the Ministerio de Economía y Competitividad (Spain), a “Ramón y Cajal” Research Fellowship (AS), and the COST Action MP1006 “Fundamental Problems in Quantum Physics” are also acknowledged. Finally, we thank again A. Lahee, our editor, for her enthusiasm when we proposed this monograph, as well as her patience for extending—several times—the deadline for finishing this project.

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