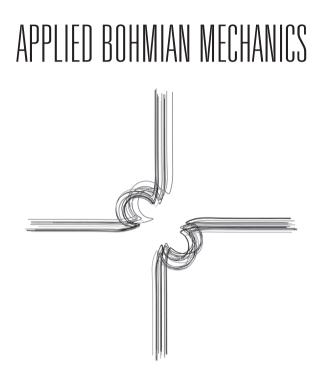
APPLIED BOHMIAN MECHANICS From Nanoscale Systems to Cosmology

^{edited by} Xavier Oriols Jordi Mompart





APPLIED BOHMIAN MECHANICS From Nanoscale Systems to Cosmology

edited by

Xavier Oriols Jordi Mompart

Published by

Pan Stanford Publishing Pte. Ltd. Penthouse Level, Suntec Tower 3 8 Temasek Boulevard Singapore 038988

Email: editorial@panstanford.com Web: www.panstanford.com

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology

Copyright © 2012 Pan Stanford Publishing Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN 978-981-4316-39-2 (Hardcover) ISBN 978-981-4364-10-2 (eBook)

Printed in the USA

Contents

Foreword						
Pr	Preface					
Introduction						
1	Overview of Bohmian Mechanics					
	Xavier Oriols and Jordi Mompart					
	1.1 Historical Development of Bohmian					
	Mechanics					
		1.1.1	Particles and waves	20		
			Origins of the quantum theory	22		
		1.1.3	"Wave or particle?" vs. "wave and particle"	23		
		1.1.4	Louis de Broglie and the fifth Solvay			
	Conference					
		1.1.5	Albert Einstein and locality	28		
	1.1.6 David Bohm and why the "impossibility					
	proofs" were wrong?					
		1.1.7	John Bell and nonlocality	34		
		1.1.8	Quantum hydrodynamics	36		
		1.1.9	Is Bohmian mechanics a useful theory?	37		
	1.2	Bohm	ian Mechanics for a Single Particle	38		
		1.2.1	Preliminary discussions	39		
		1.2.2	Creating a wave equation for classical			
			mechanics	39		
		1.2.3	Trajectories for quantum systems	47		
		1.2.4	Similarities and differences between classical			
			and quantum mechanics	52		
		1.2.5	Feynman paths	56		
		1.2.6	Basic postulates for a single particle	58		

	1.3	Bohm	ian Mechanics for Many-Particle Systems	60	
		1.3.1	Preliminary discussions: The many body		
			problem	60	
		1.3.2	Many-particle quantum trajectories	63	
		1.3.3	Factorizability, entanglement,		
			and correlations	65	
		1.3.4	Spin and identical particles	68	
		1.3.5	Basic postulates for a many-particle system	73	
		1.3.6	The conditional wave function: many-particle		
			Bohmian trajectories without the		
			many-particle wave function	76	
	1.4	Bohm	ian Explanation of the Measurement Process	88	
		1.4.1	Differences between orthodox and Bohmian		
			measurements	89	
		1.4.2	Theory of the Bohmian measurement process	94	
		1.4.3			
			Hermitian operators	101	
	1.5	Concl	uding Remarks	107	
	1.6	Probl	0	108	
	A.1 Appendix: Numerical Algorithms for the Computat				
			hmian Mechanics	119	
		A.1.1	Analytical computation of Bohmian		
			trajectories	122	
		A.1.2	Synthetic computation of Bohmian trajectories	133	
			More elaborated algorithms	139	
2	Hvd	lrogen	Photoionization with Strong Lasers	149	
-	-	-	seny, Antonio Picón, Jordi Mompart, Luis Plaja,		
		Luis Re			
	2.1	Intro	luction	150	
		2.1.1	A brief overview of photoionization	150	
		2.1.2	The computational problem of photoionization	152	
			Photoionization with Bohmian trajectories	154	
	2.2		Dimensional Photoionization of Hydrogen	155	
			The physical model	155	
			Harmonic generation	158	
		2.2.3	Above-threshold ionization	162	
	2.3		ogen Photoionization with Beams Carrying		
		-	al Angular Momentum	168	

168

		2.3.2	Bohmian equations in an electromagnetic field	172		
		2.3.3	Selection rules	173		
		2.3.4	Numerical simulations	174		
	2.4	Concl	usions	182		
3	3 Atomtronics: Coherent Control of Atomic Flow via					
	Adia	abatic	Passage	189		
	Albe	ert Bens	seny, Joan Bagudà, Xavier Oriols, Gerhard Birkl,			
	and	Jordi M	Iompart			
	3.1	Introd	luction	191		
		3.1.1	Atomtronics	191		
		3.1.2	Three-level atom optics	192		
		3.1.3	Adiabatic transport with trajectories	195		
	3.2	-	cal System: Neutral Atoms in Optical			
		Micro	-	198		
			One-dimensional Hamiltonian	200		
	3.3	Adiab	atic Transport of a Single Atom	201		
		3.3.1	I I I I I I I I I I I I I I I I I I I			
			Bohmian trajectories	201		
		3.3.2	Velocities and accelerations of Bohmian			
			trajectories	202		
	3.4		atic Transport of a Single Hole	206		
		3.4.1	, 8 I	206		
		3.4.2	1 5			
			three traps	208		
			Hole transport fidelity	212		
			Bohmian trajectories for the hole transport	213		
			Atomtronics with holes	215		
	3.5		atic Transport of a Bose–Einstein Condensate	219		
		3.5.1	8 , , , , , , , , , , , , , , , , , , ,	222		
			Numerical simulations	223		
	3.6	Concl	usions	227		
4			of Trajectories in Quantum Chemistry and			
			Physics	235		
			nz and Salvador Miret-Artés	_		
	4.1	Introc	luction	236		

2.3.1 The physical system

	4.2	A Con	densed Overview on Quantum Chemistry and					
		Chem	ical Physics	240				
		4.2.1	The Born-Oppenheimer approximation	241				
		4.2.2	Electronic structure	244				
		4.2.3	Chemical dynamics	247				
		4.2.4	Statistical mechanics	249				
	4.3	Quant	tum Trajectories vs. Quantum Streamlines	253				
		4.3.1	Fundamental ingredients	253				
		4.3.2	Aspects of nonlocality	255				
		4.3.3	Quantum mechanical equations of change	257				
	4.4	Appli	cations	260				
		4.4.1	Quantum hydrodynamical approach to					
			time-dependent DFT	260				
		4.4.2	Bound system dynamics: Chemical reactivity	264				
		4.4.3	Dynamics in the continuum: Two-slit					
			diffraction	271				
			Reduced quantum trajectories	275				
		4.4.5	Mixed Bohmian classical mechanics	276				
	4.5	Unify	ing Structure, Dynamics, and Statistics	279				
5	Adaptive Quantum Monte Carlo Approach States for							
		-	ensional Systems	303				
	Eric R. Bittner, Donald J. Kouri, Sean Derrickson,							
	and Jeremy B. Maddox							
	5.1 Introduction							
	5.2	Mixture Modeling Approach						
		5.2.1		307				
		5.2.2	Density estimation	314				
		5.2.3	Computational results	319				
		5.2.4	The ground state of methyl iodide	326				
	5.3	Quant	tum Effects in Atomic Clusters at Finite					
		Temp	erature	330				
	5.4	Quant	tum Structures at Zero and Finite Temperature	331				
		5.4.1	Zero temperature theory	331				
		5.4.2	Finite temperature theory	333				
		5.4.3	Computational studies	340				
	5.5	Overc	oming the Node Problem	353				
		5.5.1	Supersymmetric quantum mechanics	355				

		5.5.2	Implementation of SUSY QM in an adaptive			
			Monte Carlo scheme	357		
			Test case: Tunneling in a double-well potential	358		
			Extension to higher dimensions	362		
	5.6	Sumn	nary	364		
6			tronics: Quantum Electron Transport	375		
	Alfonso Alarcón, Guillem Albareda, Fabio Lorenzo Traversa,					
	and	Xavier	Oriols			
	6.1	Intro	duction: From Electronics to Nanoelectronics	377		
	6.2	Evalu	ation of the Current and Its Fluctuations	379		
		6.2.1	Bohmian measurement of the current as a			
			function of the particle positions	379		
		6.2.2	Practical computation of DC, AC, and transient			
			currents	388		
		6.2.3	Practical computation of current fluctuations			
			and higher moments	390		
	6.3	Solvir	ng Many-Particle Systems with Bohmian			
		Trajeo	ctories	394		
		6.3.1	Coulomb interaction among electrons	395		
		6.3.2	Exchange and Coulomb interactions among			
			electrons	396		
	6.4	The B	BITLLES Simulator	399		
		6.4.1	Overall charge neutrality	400		
			Practical computation of time-dependent			
			current using Ramo-Shockley-Pellegrini			
			theorems	403		
	6.5	Appli	cation to Resonant Tunneling Diodes	407		
	0.0	6.5.1	0	107		
		01011	simulation models	407		
		652	Numerical results with the BITLLES simulator	411		
	6.6		usions	419		
				11		
7	-		e Eikonal Approximation in Classical Optics tum Physics	425		
		-	refice, Raffaele Giovanelli, and Domenico Ditto	140		
			duction	426		
	7.2		holtz Equation and Geometrical Optics	428		
	1.4	nenn	none Equation and deconcerted optics	rru		

	7.3	Beyon	nd the Geometrical Optics Approximation	431
	7.4	The T	ime-Independent Schrödinger Equation	433
	7.5	Hamil	Itonian Description of Quantum Particle Motion	434
	7.6	The U	nique Dimensionless Hamiltonian System	436
	7.7	Wave	-Like Features in Hamiltonian Form	438
	7.8	Discu	ssion and Conclusions	449
	A.1	Apper	ndix: The Paraxial Approach	451
8			ic Quantum Mechanics and Quantum Field	
	The	-		455
		oje Niko		
	8.1		luction	456
	8.2		cal Relativistic Mechanics	458
		8.2.1	Kinematics	458
		8.2.2	5	461
	8.3		vistic Quantum Mechanics	467
		8.3.1	Wave functions and their relativistic	
			probabilistic interpretation	467
		8.3.2	5 1 1	470
		8.3.3	Relativistic wave equations	472
		8.3.4	Bohmian interpretation	481
	8.4	Quant	tum Field Theory	484
		8.4.1	Main ideas of QFT and its Bohmian	
			interpretation	484
		8.4.2	Measurement in QFT as entanglement with the	
			environment	488
		8.4.3	Free scalar QFT in the particle-position picture	490
		8.4.4	Generalization to interacting QFT	495
		8.4.5	Generalization to other types of particles	498
		8.4.6	Probabilistic interpretation	498
		8.4.7	Bohmian interpretation	500
	8.5	Concl	usion	503
~		_		
9		-	um Accelerating Universe	507
			nzález-Díaz and Alberto Rozas-Fernández	500
	9.1		luction	508
	9.2		riginal Subquantum Dark-Energy Model	511
	9.3	Relati	vistic Bohmian Backgrounds	515

	9.3.1	The Klein–Gordon subquantum model	515		
	9.3.2	Quantum theory of special relativity	516		
9.4	Dark l	Energy Without Dark Energy	522		
9.5	Benig	n Phantom Cosmology	531		
	9.5.1	Thermodynamics	531		
	9.5.2	Violation of classical DEC	535		
	9.5.3	Holographic models	537		
	9.5.4	Quantum cosmic models and entanglement			
		entropy	539		
9.6	Gener	alized Cosmic Solutions	540		
9.7	Gravit	Gravitational Waves and Semiclassical Instability			
9.8	On the	e Onset of the Cosmic Accelerating Phase	547		
9.9	Concl	usions and Comments	554		
Index			561		

Foreword

Quantum theory, born at the beginning of the twentieth century, represents one of the biggest revolutions ever performed in science. Reputed physicists, led by Niels Bohr, Werner Heisenberg, and others, devoted their careers both to formulate quantum mechanics in a consistent way, constructing what is known as the Copenhagen or orthodox formulation of quantum mechanics, and to extend it to other realms, such as thermodynamics, solid-state physics, relativity, particle physics, and quantum field theory, to cite only a few. Thus, the orthodox formulation of quantum mechanics became the standard formulation to understand the quantum world. In parallel, Louis de Broglie and David Bohm showed that there is an alternative formulation of quantum mechanics, nowadays named Bohmian mechanics, that addresses the problem from a different perspective and provides exactly the same results as the orthodox formulation. However, Bohmian mechanics has been almost ignored by the scientific community until now.

During the second half of the twentieth century, a significant number of physicists dedicated strong efforts to look for practical applications of quantum mechanics. For example, the development of the laser brought a new scenario for precision experiments with extremely high control on the atomic manipulation. Thus, quantum mechanics evolved from a theory focused only on the fundamental principles of nature into a broad engineering discipline directly involved in the timely needs of our society. One enlightening example in this evolution of the use of quantum mechanics is the emerging field of quantum information science. Can Bohmian mechanics help in *applied* quantum physics?

I have to admit that before reading this book, I only had a vague knowledge of Bohmian mechanics. Now, after having the pleasure of reading it, the persistent question that bothered John S. Bell appears also in my mind: Why has Bohmian mechanics been so ignored among the scientific community when the most *devastating* criticism against it is just that *we are all too busy with our own work to spend time on something that doesn't seem likely to help us make progress with our real problems*? In fact, this book shows that even this criticism is not at all evident. It is mainly a consequence that very few efforts have been made to explore the possible utility of the door opened by de Broglie almost a century ago.

Contrarily to others, one of the most original and attractive features of this book is the description of Bohmian mechanics from an engineering point of view. It is time to convert all the physical and mathematical ideas developed by de Broglie, Bohm, Bell, and many others into *applied* tools for thinking, computing, and understanding quantum phenomena. In my opinion, this is the main message of this book.

In addition, since the progress in scientific and engineering research feeds from unexplored routes, I hope that this book will be very welcomed by the scientific community. Students and researchers have a new open door to pass through (without closing the others) for *playing* with the Schrödinger and continuity equations in terms of waves and particles when addressing their particular quantum problems.

> **Ignacio Cirac** Garching, March 2012

Preface

Most of our collective activities are regulated by other people who decide whether they are well done or not. One has to learn some arbitrary symbols to write understandable messages or to read those from others. Human rules over collective activities govern the evolution of our culture. On the contrary, natural systems, from atoms to galaxies, evolve independently of the human rules. We cannot modify physical laws. We can only try to understand them. Nature itself judges, through experiments, whether a plausible explanation for some natural phenomena is correct or incorrect. Nevertheless, in forefront research where the unknowns start to become understandable, the new knowledge is still unstable, somehow immature. It is supported by unclear experimental evidence, or the evidence is still subjected to different interpretations. Certainly, novel research grows up closely tied to the economical, sociological, or historical circumstances of the involved researchers. A period of time is needed in order to distil new knowledge, separating pure scientific arguments from cultural influences.

The past and the present status of Bohmian mechanics cannot be understood without these cultural considerations. The Bohmian formalism was proposed by Louis de Broglie even before the standard, that is, Copenhagen, explanation of quantum phenomena was established. Bohmian mechanics provides an explanation of quantum phenomena in terms of point particles guided by waves. One object cannot be a wave and a particle simultaneously, but two can, especially if one of the objects is a wave and the other is a particle. Unfortunately, de Broglie himself abandoned these ideas. Later, in the fifties, David Bohm clarified the meaning and applications of this explanation of quantum phenomena. Bohmian mechanics agrees with all quantum experiments done up to now. However, it remains almost ignored by most of the scientific community. In our opinion, there are no scientific arguments to support its marginal status but only cultural reasons. One of the motivations for writing this book is helping in the maturing process that the scientific community needs about Bohmian mechanics.

Certainly, the distilling process of Bohmian mechanics is being quite slow. Anyone interested enough to walk this causal road of quantum mechanics can be easily confused by many misleading signposts that have been raised in the scientific literature, not only by its detractors, but, unfortunately, very often, also by some of its advocates. Nowadays, following opinions from other reputed physicists (we are easily persuaded by those scientists with authority) is far from being a proper scientific strategy to get our own opinion about Bohmian mechanics.

In any case, since the mathematical structure of Bohmian mechanics is quite simple, it can be easily learned by anyone with only a basic knowledge of classical and quantum mechanics who makes the necessary effort to build his or her own scientific opinion based on logical deductions, free from cultural influences. The introductory chapter of this book, including a thorough list of exercises and easily programmable algorithms, provides a reasonable and objective source of information in order to achieve this later goal, even for undergraduate students.

Curiously, the fact that Bohmian mechanics is ignored and remains mainly unexplored is an attractive feature for some adventurous scientists. They know that very often *new cutting-edge ideas come from outside of the main stream* and find in Bohmian mechanics a useful tool in their research activity. On the one hand, it provides an explanation of quantum mechanics, in terms of trajectories, that results to be very useful in explaining the dynamics of quantum systems, being thus also a source of inspiration to look for novel quantum phenomena. On the other hand, since it provides an alternative mathematical formulation, Bohmian mechanics offers new computational tools to explore physical scenarios that presently are computationally inaccessible, such as many-particle solutions of the Schrödinger equation. In addition, Bohmian mechanics sheds light on the limits and extensions of our present understanding of quantum mechanics toward other paradigms such as relativity or cosmology, where the internal structure of Bohmian mechanics in terms of well-defined trajectories is very attractive. With all these previous motivations in mind, this book provides eight chapters with practical examples showing how Bohmian mechanics helps us in our daily research activities.

Obviously, there are other books focused on Bohmian mechanics. However, many of them are devoted to the foundations of guantum mechanics, emphasizing the difficulties or limitations of the Copenhagen interpretation for providing an ontological description of our world. On the contrary, this book is not at all devoted to the foundations of quantum mechanics; it only discusses the practical applications of the ideas of de Broglie and Bohm to understand the quantum world. Several examples of such practical applications written by leading experts in different fields, with an extensive updated bibliography, are provided here. The book, in general, is addressed to students of physics, chemistry, electrical engineering, applied mathematics, and nanotechnology, as well as to both theoretical and experimental researchers who seek new computational and interpretative tools for their everyday research activity. We hope that the newcomers to this causal explanation of quantum mechanics will use Bohmian mechanics in their research activities so that Bohmian mechanics will become more and more popular for the broad scientific community. If so, we expect that, in the near future, Bohmian mechanics will be taught regularly at universities, not as a unique and revolutionary way of understanding quantum phenomena, but as an additional and useful interpretation of all quantum phenomena in terms of quantum trajectories. In fact, Bohmian mechanics has the ability of removing most of the mysteries of the Copenhagen interpretation and, somehow, simplifying quantum mechanics. We will be very glad if this book can contribute to shorten the time needed to achieve all these goals.

Finally, we want to acknowledge many different people who have allowed us to embark on and successfully finish this book project. First of all, we want to thank Alfonso Alarcón and Albert Benseny, who became involved in the book project from the very beginning, as two additional editors. We also want to thank the rest of the authors of the book for accepting our invitation to participate in this project and writing their chapters according to the general spirit of the book. Due to page limitations, only eight examples of practical applications of Bohmian mechanics in forefront research activity are presented in this book. Therefore, we want to apologize to many other researchers who could have certainly been also included in the book. We also want to express our gratitude to Pan Stanford Publishing for accepting our book project and for its kind attention during the publishing process.

> Xavier Oriols Jordi Mompart

Introduction

The beginning of the twentieth century brought surprising nonclassical phenomena. Max Planck's explanation of black-body radiation [1], the work of Albert Einstein on the photoelectric effect [2], and Niels Bohr's model to account for the electron orbits around the nuclei [3] established what is now known as the *old quantum theory*. To describe and explain these effects, phenomenological models and theories were first developed, without any rigorous and global justification. In order to provide a complete explanation for the underlying physics of such new nonclassical phenomena, physicists were forced to abandon classical mechanics to develop novel, abstract, and imaginative formalisms.

In 1924, Louis de Broglie suggested in his doctoral thesis that matter, apart from its intrinsic particle-like behavior, could exhibit also a wave-like one [4]. Three years later he proposed an interpretation of quantum phenomena based on nonclassical trajectories guided by a wave field [5]. This was the origin of the pilot-wave formulation of quantum mechanics that we will refer to as Bohmian mechanics to account for the following work of David Bohm [6, 7]. In the Bohmian formulation, an individual quantum system is formed by a point particle and a guiding wave. Contemporaneously, Max Born and Werner Heisenberg, in the course of their collaboration in Copenhagen with Niels Bohr, provided an original formulation of quantum mechanics without the need for trajectories [8, 9]. This was the origin of the so-called Copenhagen interpretation of quantum phenomena, and since it is the most accepted formulation, it is the only one explained at most universities. Thus, it is also known as the orthodox formulation of quantum mechanics. In the Copenhagen interpretation, an individual quantum system is simultaneously both a wave and a particle and exhibits its wave or its particle nature, depending on the experimental arrangement.

The present status of Bohmian mechanics among the scientific community is quite marginal (the quantum chemistry community is an encouraging exception). Most researchers do not know about it or believe that is not fully correct. There are others who know that quantum phenomena can be interpreted in terms of trajectories, but they think that this formalism cannot be useful in their daily research activity. Finally, there are few researchers, the authors of this book among them, who think that Bohmian mechanics is a useful tool to make progress in frontline research fields involving quantum phenomena.

The main (nonscientific) reason why still many researchers believe that there is something wrong with Bohmian mechanics can be illustrated with Hans Christian Andersen's tale "The Emperor's New Clothes." Two swindlers promise the emperor the finest clothes that, as they tell him, are invisible to anyone who is unfit for their position. The emperor cannot see the (nonexisting) clothes but pretends that he can, for fear of appearing stupid. The rest of the people do the same. Advocates of the Copenhagen interpretation have attempted to produce impossibility proofs in order to demonstrate that Bohmian mechanics is incompatible with quantum phenomena [10]. Most researchers, who are not aware of the incorrectness of such proofs, might conclude that there is some controversy with the Bohmian formulation of quantum mechanics. and they prefer not to support it, for fear of appearing discordant. At the end of the tale, during the course of a procession, a small child cries out "The Emperor is Naked!" In the tale of quantum mechanics, Bohm [6, 7] and John S. Bell [11] were the first to exclaim to the scientific community, "Bohmian mechanics is a correct interpretation of quantum phenomena that exactly reproduces the predictions of the orthodox interpretation!"

How Bohmian Mechanics Helps?

Researchers who have spent the necessary time to analyze the ideas of de Broglie and Bohm with the pertinent scientific rigor accept that there is no scientific argument against them. Bohmian mechanics agrees with all quantum experiments done up to now. However, most of such researchers do also believe that Bohmian mechanics is not a useful tool to do research. In the words of Steven Weinberg, in a private exchange of letters with Sheldon Goldstein [12], "In any case, the basic reason for not paying attention to the Bohm approach is not some sort of ideological rigidity, but much simpler–it is just that we are all too busy with our own work to spend time on something that doesn't seem likely to help us make progress with our real problems."

The history of science seems to give credit to Weinberg's sentence. In spite of the controversies that have always been associated with the Copenhagen interpretation since its birth a century ago, its mathematical and computational machinery has enabled physicists, chemists, and (quantum) engineers to calculate and predict the outcomes of a vast number of experiments, while the contribution of Bohmian mechanics during the same period is much less significative. In our opinion, the differences are due to the fact that Bohmian mechanics remains mainly unexplored.

Contrarily to Weinberg's opinion, we believe that Bohmian mechanics *can help us make progress with our real problems*. There are, at least, three clear reasons why one could be interested in studying quantum problems with Bohmian mechanics:

(1) Bohmian explaining: Even when the Copenhagen mathematical machinery is used to compute observable results, the Bohmian formulation often offers better interpretational tools. We can find descriptions of electron dynamics such as an electron crosses a resonant tunneling barrier and interacts with another electron inside the well. However, an electron crossing a tunneling region is not rigourously supported within orthodox quantum mechanics, but it is within the Bohmian picture. Thus, in contrast to the Copenhagen formulation, the Bohmian formulation allows for easy visualization of quantum phenomena in terms of trajectories that has important demystifying or clarifying consequences. In particular, it provides a single-event description of the experiment, while Copenhagen quantum mechanics accounts for its statistical or ensemble explanation. We will present several examples in chapters 2 and 3, emphasizing all these points.

- (2) **Bohmian** *computing:* Although the predictions of the Bohmian formulation reproduce the ones of the orthodox formulation of quantum mechanics, its mathematical formalism is different. In some systems, Bohmian equations might provide better computational tools than the ones obtained from the orthodox machinery, resulting in a reduction of the computational time, an increase in the number of degrees of freedom directly simulated, etc. We will see examples of these computational issues in quantum chemistry in chapters 4 and 5, as well as in quantum electron transport in chapter 6.
- (3) Bohmian thinking: From a more fundamental point of view, alternative formulations of quantum mechanics can provide alternative routes to look for the limits and possible extensions of quantum theory. As we will discuss later, the work of Bell on nonlocality is a clear example of the unquestionable utility of understanding quantum phenomena with Bohmian mechanics. In particular, chapter 7 presents the route to connect Bohmian mechanics with geometrical optics and beyond. The natural extension of Bohmian mechanics to the relativistic regime and to quantum field theory are presented in chapter 8, while chapter 9 discusses its application to cosmology.

The fact that all measurable results of orthodox quantum mechanics can be exactly reproduced with Bohmian mechanics is the relevant point that completely justifies why Bohmian mechanics can be used for *explaining* or *computing* different quantum phenomena in physics, chemistry, electrical engineering, applied mathematics, nanotechnology, etc. In the scientific literature, the **Bohmian** *computing* technique to find the trajectories (without directly computing the wave function) is also known as a *syntectic* technique, while the **Bohmian** *explaining* technique (where the wave function is directly computed first) is referred to as the *analytic* technique [13]. Furthermore, among others, the fact that Bohmian mechanics provides a picture in terms of single events, which is missing in the orthodox explanation, is an attractive feature for those researchers interested in *thinking* about the limits or extensions of quantum theory.

In order to convince the reader about the practical utility of Bohmian mechanics for *explaining, computing* or, *thinking*, we will not present elaborated mathematical developments or philosophical discussions but provide practical examples. Apart from the first chapter, devoted to an overview of Bohmian mechanics, the book is divided into eight additional chapters with several examples on the practical applications of Bohmian mechanics in different research fields, ranging from atomic systems to cosmology. These examples will clearly show that the previous quotation by Weinberg does not have to be always true.

On the Name "Bohmian Mechanics"

Any possible newcomer to Bohmian mechanics can certainly be quite confused and disoriented by the large list of names and slightly different explanations of the original ideas of de Broglie and Bohm that are present in the scientific literature. Different researchers use different names. Certainly, this is an indication that the theory is still not correctly settled down among the scientific community.

In his original works [4, 5], de Broglie used the term *pilot-wave theory* [14] to emphasize the fact that wave fields guided the motion of point particles. After de Broglie abandoned his theory, Bohm rediscovered it in the seminal papers entitled "A Suggested Interpretation of the Quantum Theory in Terms of Hidden Variables" [6, 7]. The term *hidden variables*,^a referring to the positions of the particles, was perhaps pertinent in 1952, in the context of the *impossibility proofs* [10]. Nowadays, these words might seem inappropriate because they suggest something metaphysical on the trajectories.^b

^aNote that the term *hidden variables* can also refer to other (local and nonlocal) formulations of quantum mechanics.

^bSometimes it is argued that the name *hidden variables* is because Bohmian trajectories cannot be measured directly. However, what is not directly measured in experiments is the (complex) wave function amplitude, while the final positions of particles can be directly measured, for example, by the imprint they leave on a screen. Bell wrote [11] (page 201), "Absurdly, such theories are known as 'hidden variable' theories. Absurdly, for there it is not in the wave function that one finds an image of the visible world, and the results of experiments, but in the complementary 'hidden'(!) variables."

To give credit to both de Broglie and Bohm, some researchers refer to their works as *de Broglie–Bohm theory* [17].^a Some reputed researchers argue that de Broglie and Bohm did not provide the same exact presentation of the theory [14, 18]. While de Broglie presented a first-order development of the quantum trajectories (integrated from the velocity), Bohm himself did a second-order development (integrated from the acceleration) emphasizing the role of the quantum potential. The differences between both approaches appear when one considers initial ensembles of trajectories that are not in quantum equilibrium.^b Except for this issue, which will not be addressed in this book, both approaches are identical.

Many researchers prefer to use the name *Bohmian mechanics* [19]. It is perhaps the most popular name. We know directly from his collaborators who are alive, Basile Hiley and David Peat [20], that this name irritated Bohm and he said about its own work, "It's Bohmian non-mechanics." He argued that the *quantum potential* is a nonlocal potential that depends on the relative shape of the wave function and thus it is completely different from other mechanical (such as gravitational or electrostatic) potentials. See this particular discussion in the last chapters of Bohm and Hiley's book entitled *The Undivided Universe: An Ontological Interpretation of Quantum Theory* [21]. He preferred the names *causal* or *ontological interpretation* of quantum mechanics [17, 21]. The latter names emphasize the foundational aspects of its formulation of quantum mechanics.

Finally, another very common term is *quantum hydrodynamics* [13], which underlines the fact that Bohmian trajectories provide a

^aIn fact, even de Broglie and Bohm were not the original names of the scientists' families. De Broglie's family, which included dukes, princes, ambassadors, and marshals of France, changed its original Italian name Broglia to de Broglie when they established in France in the seventeenth century [15]. Bohm's father, Shmuel Düm, was born in the Hungarian town of Munkács and was sent to America when he was young. Upon landing at Ellis Island, he was told by an immigration official that his name, Düm, would mean "stupid" in English. The official himself decided to change the name to Bohm [16].

^bQuantum equilibrium assumes that the initial positions and velocities of Bohmian trajectories are defined compatible with the initial wave function. Then the trajectories computed from Bohm's or de Broglie's formulations will become identical. However, if the quantum equilibrium hypothesis is not considered, one can select completely arbitrary initial positions from the (first-order) de Broglie explanation and arbitrary initial velocities and positions from the (second-order) Bohm work (see Sec. 1.2.6).

mathematical relationship between the Schrödinger equation and fluid dynamics. In fact, this name is more appropriate when one refers to Madelung's theory [22], which is considered a precursor of de Broglie's and Bohm's work (see Sec. 1.1.8).

From all these different names, we chose *Bohmian mechanics* because it is short and clearly specifies what we are referring to. It has the inconvenience of not giving credit to the initial work of de Broglie. Although it might be argued that Bohm merely reinterpreted the prior work of de Broglie, we think that he was the first person to genuinely understand its significance and implications. As we mentioned, Bohm himself disliked this name. However, as any work of art, the merits and influence of Bohm's 1952 paper evolve independently of the own author opinion.^a The paper becomes part of the scientific heritage. In any case, we understand Bohmian mechanics as a generic name that includes all those works inspired from the original ideas of Bohm and de Broglie. In Figure 1, we plot the numbers of citations per year for Bohm's 1952 seminal papers [6, 7], certifying the exponentially growing influence of these papers, which is not the case for the original work of de Broglie [5].

On the Book Contents

The book contains nine chapters. It can be clearly divided into two different parts. The first part is formed by chapter 1 alone, which provides an accessible introduction to Bohmian mechanics. The second part is composed of the rest of the chapters with practical examples on the applicability of Bohmian mechanics.

Chapter 1 is the longest one, and it is entitled "Overview of Bohmian Mechanics." It is written by Xavier Oriols and Jordi Mompart, the editors of the book, both from Universitat Autònoma de Barcelona, Spain. This chapter is intended to be an introduction to any newcomer interested in Bohmian mechanics. No previous knowledge of Bohmian mechanics is required. Only basic concepts of classical and quantum mechanics are assumed. The chapter is divided into four different sections. First, the historical development

^aFor example, Erwin Schrödinger, talking about quantum theory, wrote, "I don't like it, and I'm sorry I ever had anything to do with it," but his opinion did not influence the great applicability of his famous equation.

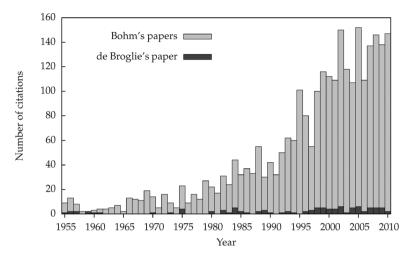


Figure 1. Number of citations per year for (a) the two 1952 Bohm papers entitled "A Suggested Interpretation of the Quantum Theory in Terms of Hidden Variables" [6, 7] and (b) de Broglie's paper "La mécanique ondulatorie et la structure atomique de la matière et du rayonnement" [5]. Data retrieved from ISI Web of Knowledge [23] in December 2010.

of Bohmian mechanics is presented. Then, Bohmian mechanics for single-particle and for many-particle systems (with spin and entanglement explanations) is discussed in Secs. 1.2 and 1.3, respectively. The topic of Bohmian measurement is addressed in Sec. 1.4. The chapter also contains a list of exercises, mathematical demonstrations, and easily implementable algorithms for computation of Bohmian trajectories.

Chapter 2 is entitled "Hydrogen Photoionization with Strong Lasers." It is written by Albert Benseny and Jordi Mompart from Universitat Autònoma de Barcelona, Spain; Antonio Picón from the ANL, the Argonne National Laboratory, Illinois, USA; Luis Plaja from Universidad de Salamanca, Spain; and Luis Roso from the CLPU, the Laser Center for Ultrashort and Ultraintense Pulses, also in Salamanca. They discuss the dynamics of a single hydrogen atom interacting with a strong laser. In particular, the Bohmian trajectories of these electrons represent an interesting, illustrating view of both above-threshold ionization and harmonic generation spectra problems. They do also present a full, three-dimensional

(3D) model to discuss the dynamics of Bohmian trajectories when the light beam and the hydrogen atom exchange both spin and orbital angular momentum. The chapter does also provide a practical example of how Bohmian mechanics is computed, with an analytical (i.e., **Bohmian** *explaining*) procedure, when full (scalar and vector potentials) electromagnetic fields are considered.

The title of **chapter 3** is "Atomtronics: Coherent Control of Atomic Flow via Adiabatic Passage." It is written by Albert Benseny, Joan Bagudà, Xavier Oriols, and Jordi Mompart from Universitat Autònoma de Barcelona, Spain, and Gerhard Birkl from Institut für Angewandte Physik, Technische Universität Darmstadt in Germany. Here, it is discussed an efficient and robust technique to coherently transport a single neutral atom, a single hole, or even a Bose-Einstein condensate between the two extreme traps of the triple-well potential. The dynamical evolution of this system with the direct integration of the Schrödinger equation presents a very counterintuitive effect: by slowing down the total time duration of the transport process it is possible to achieve atomic transport between the two extrem traps with a very small (almost negligible) probability to populate the middle trap. The analytical (i.e., Bohmian explaining) solution of this problem with Bohmian trajectories enlightens the role of the particle conservation law in quantum systems showing that the negligible particle presence is due to a sudden particle acceleration yielding, in fact, ultra-high atomic velocities. The Bohmian contribution opens the discussion about the possible detection of such high kinetic energies or the need for a relativistic formulation to accurately describe such a simple quantum system.

Chapter 4, entitled "The Role of Trajectories in Quantum Chemistry and Chemical Physics," is written by Ángel S. Sanz and Salvador Miret-Artès from Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Spain. Up to very recently, the **Bohmian** *computing* abilities have been explored almost exclusively by the quantum chemistry community. In the words of the authors, "It is interesting to note that Bohmian mechanics is better accepted within the chemistry community than within the physics one, which is often quite reluctant...To some extent, it could be said that the pedagogical advantages that Bell associated with Bohmian Mechanics have been better appreciated by chemists than by physicists." There are many different Bohmian computational techniques developed by the quantum chemistry community, mainly, during the past 10 years. Since it was impossible to dedicate a chapter to each, here, the authors provide a clear summary of the problems and Bohmian solutions.

Chapter 5, whose title is "Adaptive Quantum Monte Carlo Approach States for High-Dimensional Systems," is written by Eric R. Bittner, Donald J. Kouri, and Sean Derrickson from University of Houston and Jeremy B. Maddox from Western Kentucky University, in the United States. They provide one particular example on the success of Bohmian mechanics in the chemistry community. In this chapter, the authors explain their **Bohmian** *computing* development to calculate the *ab initio* quantum mechanical structure, energetic, and thermodynamics of multiatoms systems. They use a variational approach that finds the quantum ground state (or even excited states at finite temperature) using a statistical modeling approach for determining the best estimate of a quantum potential for a multidimensional system.

Chapter 6 is entitled "Nanoelectronics: Quantum Electron Transport." It is written by Alfonso Alarcón, Guillem Albareda, Fabio Lorenzo Traversa, and Xavier Oriols from Universitat Autònoma de Barcelona, Spain. The authors explain the ability of their own manyparticle **Bohmian** *computing* algorithm to understand and model the behavior of nanoscale electron devices. In particular, it is shown that the adaptation of Bohmian mechanics to electron transport in open systems (with interchange of particles and energies) leads to a quantum Monte Carlo algorithm, where randomness appears because of the uncertainties in the number of electrons, their energies, and the initial positions of (Bohmian) trajectories. A general, versatile, and time-dependent 3D electron transport simulator for nanoelectronic devices, named BITLLES (Bohmian Interacting Transport for nonequiLibrium eLEctronic Structures), is presented, showing its ability for a full prediction (direct current [DC] and alternating current [AC] fluctuations) of the electrical characteristics of any nanoelectronic device.

Chapter 7, entitled "Beyond the Eikonal Approximation in Classical Optics and Quantum Physics," is written by Adriano

Orefice, Raffaele Giovanelli, and Domenico Ditto from Università degli Studi di Milano, Italy. It is devoted to discussing how Bohmian *thinking* can also help in optics, exploring the fact that the timeindependent Schrödinger equation is strictly analogous to the Helmholtz equation appearing in classical wave theory. Starting from this equation they obtain, indeed, without any omission or approximation, a Hamiltonian set of ray-tracing equations providing (in stationary media) the exact description in terms of rays of a family of wave phenomena (such as diffraction and interference) much wider than that allowed by standard geometrical optics, which is contained as a simple limiting case. They show in particular that classical ray trajectories are ruled by a wave potential presenting the same mathematical structure and physical role of Bohm's quantum potential and that the same equations of motion obtained for classical rays hold, in suitable dimensionless form, for quantum particle dynamics, leading to analogous trajectories and reducing to classical dynamics in the absence of such a potential.

Chapter 8, entitled "Relativistic Quantum Mechanics and Quantum Field Theory," is written by Hrvoje Nikolić from the Rudjer Bošković Institute, Croatia. This chapter presents a clear example of how a **Bohmian** *thinking* on superluminal velocities and nonlocal interactions helps in extending quantum theory toward relativity and quantum field theory. A relativistic covariant formulation of relativistic quantum mechanics of a fixed number of particles (with or without spin) is presented, depending on many-time wave functions and on an interpretation of probabilities in the space time. These results are used to formulate the Bohmian interpretation of relativistic quantum mechanics in a manifestly relativistic covariant form and are also generalized to quantum field theory. The corresponding Bohmian interpretation of quantum field theory describes an infinite number of particle trajectories. Even though the particle trajectories are continuous, the appearance of creation and destruction of a finite number of particles results from quantum theory of measurements describing entanglement with particle detectors.

Finally, **chapter 9**, whose title is "Subquantum Accelerating Universe," is written by Pedro F. González-Díaz and Alberto Rozas-Fernández from Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Spain. Contrarily to the general belief, quantum mechanics does not only govern microscopic systems, but it has influence also on the cosmological domain. However, the extension of the Copenhagen version of quantum mechanics to cosmology is not free from conceptual difficulties: the probabilistic interpretation of the wave function of the whole universe is somehow misleading because we cannot make statistical "measurements" of different realizations of our universe. This chapter deals with two new cosmological models describing the accelerating universe in the spatially flat case. Also contained in this chapter is a discussion of the quantum cosmic models that result from the existence of a nonzero entropy of entanglement. In such a realm, they obtain new cosmic solutions for any arbitrary number of spatial dimensions, studying the stability of these solutions, as well as the emergence of gravitational waves in the realm of the most general models.

Only eight chapters of practical applications of Bohmian mechanics in forefront research activity, ranging from atomic systems to cosmology, are presented in this book. Many more chapters could have certainly been also included. In any case, we believe that these examples are enough to convince the reader about the practical utility of *explaining*, *computing*, and *thinking* about quantum phenomena within Bohmian mechanics.

References

- 1. M. Planck, On the Law of Distribution of Energy in the Normal Spectrum, Annalen der Physik, **4**, 553 (1901).
- A. Einstein, Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt, Annalen der Physik, 17, 132 (1905).
- 3. N. Bohr, On the Constitution of Atoms and Molecules, Part I; Part II Systems Containing Only a Single Nucleus; Part III Systems Containing Several Nuclei, Philosophical Magazine, **26**, 1, 476, 857 (1913).
- L. de Broglie, *Recherches sur la théorie des quantas*, Annalen de Physique, 3, 22 (1925).

- L. de Broglie, La mécanique ondulatorie et la structure atomique de la matière et du rayonnement, Journal de Physique et du Radium, 8, 225 (1927).
- 6. D. Bohm, A Suggested Interpretation of the Quantum Theory in Terms of *"Hidden" Variables I*, Physical Review, **85**, 166, (1952).
- 7. D. Bohm, A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables II, Physical Review, **85**, 180, (1952).
- 8. M. Born, *Zur Quantenmechanik der Stovorgänge*, Zeitschrift für Physik **37**, 863 (1926).
- W. Heisenberg, Über quantentheoretishe Umdeutung kinematisher und mechanischer Beziehungen, Zeitschrift für Physik, 33, 879 (1925); English translation in Ref. [10]. B. L. van der Waerden, Sources of Quantum Mechanics, (Dover Publications, 1968).
- J. von Neumann, Mathematische Grundlagen der Quantenmechanik, (Springer Verlag, Berlin 1932); English translation by R. T. Beyer, Mathematical Foundations of Quantum Mechanics, (Princeton University Press, Princeton, 1955).
- 11. J. S. Bell, *Speakable and Unspeakable in Quantum Mechanics*, (Cambridge University Press, Cambridge, 1987).
- Private exchange of letters between S. Goldstein and S. Weinberg; see http://www.mathematik.uni-muenchen.de/bohmmech/BohmHome/ weingold.htm
- 13. R. E. Wyatt, Quantum Dynamics with Trajectories: Introduction to Quantum Hydrodynamics, (Springer, 2005).
- 14. A. Valentini, *Pilot-Wave Theory: An Alternative Approach to Modern Physics*, (Cambridge University Press, Cambridge, 2006).
- G. Bacciagaluppi and A. Valentini, *Quantum Theory at the Cross-roads: Reconsidering the 1927 Solvay Conference*, (Cambridge University Press, Cambridge, 2009).
- D. Peat, Infinite Potential: The Life and Times of David Bohm, (Helix Books, Addison-Wesley, 1997).
- P. R. Holland, The Quantum Theory of Motion: An Account of the de Broglie-Bohm Causal Interpretation of Quantum Mechanics, (Cambridge University Press, Cambridge, 1993).
- S. W. Saunders et al., *Everett and His Critics*, (Oxford University Press, 2009); see also the online publication: quant-ph/0811081
- 19. J. T. Cushing, A. Fine and S. Goldstein, *Bohmian Mechanics and Quantum Theory: An Appraisal*, (Kluwer Academic, 1996).

- 20. Private communication with Basile Hiley and David Peat
- D. Bohm and B. J. Hiley, *The Uundivided Universe: An Ontological Intepretation of Quantum Theory*, (Routledge & Kegan Paul, London, 1993).
- 22. E. Madelung, *Quantentheorie in hydrodynamischer Form*, Zeitschrift für Physik, **40**, 322 (1926).
- 23. http://www.isiknowledge.com/