Graduate Texts in Physics

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Rainer Dick

Advanced Quantum Mechanics

Materials and Photons

Second Edition

Springer

Rainer Dick
Department of Physics and Engineering Physics
University of Saskatchewan
Saskatoon, Saskatchewan
Canada

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Preface to the Second Edition

The second edition features 62 additional end of chapter problems and many sections were edited for clarity and improvement of presentation. Furthermore, the chapter on Klein-Gordon and Dirac fields has been expanded and split into Chapter 21 on relativistic quantum fields and Chapter 22 on applications of quantum electrodynamics. This was motivated by the renewed interest in the notions and techniques of relativistic quantum theory due to their increasing relevance for materials research. Of course, relativistic quantum theory has always been an important tool in subatomic physics and in quantum optics since the dynamics of photons or high energy particles is expressed in terms of relativistic quantum fields. Furthermore, relativistic quantum mechanics has also always been important for chemistry and condensed matter physics through the impact of relativistic corrections to the Schrödinger equation, primarily through the Pauli term and through spin-orbit couplings. These terms usually dominate couplings to magnetic fields and relativistic corrections to energy levels in materials, and spin-orbit couplings became even more prominent due to their role in manipulating spins in materials through electric fields. Relativistic quantum mechanics has therefore always played an important foundational role throughout the physical sciences and engineering.

However, we have even seen discussions of fully quasirelativistic wave equations in materials research in recent years. This development is driven by discoveries of materials like Graphene or Dirac semimetals, which exhibit low energy effective Lorentz symmetries in sectors of momentum space. In these cases c and m become effective low energy parameters which parametrize quasirelativistic cones or hyperboloids in regions of $(E, \boldsymbol{k})$ space. As a consequence, materials researchers now do not only deal with Pauli and spin-orbit terms, but with representations of γ matrices and solutions of Dirac equations in various dimensions.

To prepare graduate students in the physical sciences and engineering better for the increasing number of applications of (quasi-)relativistic quantum physics, Section 21.5 on the non-relativistic limit of the Dirac equation now also contains a detailed discussion of the Foldy-Wouthuysen transformation including a derivation of the general spin-orbit coupling term and a discussion of the origin of Rashba terms, and the Section 21.6 on quantization of the Maxwell field in Lorentz gauge has been added. The discussion of applications of quantum electrodynamics now also includes the new Section 22.2 on electron-nucleus scattering. Finally, the new Appendix I discusses the transformation properties of scalars, spinors and gauge fields under parity or time reversal.

Saskatoon, SK, Canada Rainer Dick

Preface to the First Edition

Quantum mechanics was invented in an era of intense and seminal scientific research between 1900 and 1928 (and in many regards continues to be developed and expanded) because neither the properties of atoms and electrons, nor the spectrum of radiation from heat sources could be explained by the classical theories of mechanics, electrodynamics and thermodynamics. It was a major intellectual achievement and a breakthrough of curiosity driven fundamental research which formed quantum theory into one of the pillars of our present understanding of the fundamental laws of nature. The properties and behavior of every elementary particle is governed by the laws of quantum theory. However, the rule of quantum mechanics is not limited to atomic and subatomic scales, but also affects macroscopic systems in a direct and profound manner. The electric and thermal conductivity properties of materials are determined by quantum effects, and the electromagnetic spectrum emitted by a star is primarily determined by the quantum properties of photons. It is therefore not surprising that quantum mechanics permeates all areas of research in advanced modern physics and materials science, and training in quantum mechanics plays a prominent role in the curriculum of every major physics or chemistry department.

The ubiquity of quantum effects in materials implies that quantum mechanics also evolved into a major tool for advanced technological research. The construction of the first nuclear reactor in Chicago in 1942 and the development of nuclear technology could not have happened without a proper understanding of the quantum properties of particles and nuclei. However, the real breakthrough for a wide recognition of the relevance of quantum effects in technology occurred with the invention of the transistor in 1948 and the ensuing rapid development of semiconductor electronics. This proved once and for all the importance of quantum mechanics for the applied sciences and engineering, only 22 years after publication of the Schrödinger equation! Electronic devices like transistors rely heavily on the quantum mechanical emergence of energy bands in materials, which can be considered as a consequence of combination of many atomic orbitals or as a consequence of delocalized electron states probing a lattice structure. Today the rapid developments of spintronics, photonics and nanotechnology provide continuing testimony to the technological relevance of quantum mechanics.

As a consequence, every physicist, chemist and electrical engineer nowadays has to learn aspects of quantum mechanics, and we are witnessing a time when also mechanical and aerospace engineers are advised to take at least a 2nd year course, due to the importance of quantum mechanics for elasticity and stability properties of materials. Furthermore, quantum information appears to become increasingly relevant for computer science and information technology, and a whole new area of quantum technology will likely follow in the wake of this development. Therefore it seems safe to posit that within the next two generations, 2nd and 3rd year quantum mechanics courses will become as abundant and important in the curricula of science and engineering colleges as first and second year calculus courses.

Quantum mechanics continues to play a dominant role in particle physics and atomic physics – after all, the Standard Model of particle physics is a quantum theory, and the spectra and stability of atoms cannot be explained without quantum mechanics. However, most scientists and engineers use quantum mechanics in advanced materials research. Furthermore, the dominant interaction mechanisms in materials (beyond the nuclear level) are electromagnetic, and many experimental techniques in materials science are based on photon probes. The introduction to quantum mechanics in the present book takes this into account by including aspects of condensed matter theory and the theory of photons at earlier stages and to a larger extent than other quantum mechanics texts. Quantum properties of materials provide neat and very interesting illustrations of time-independent and time-dependent perturbation theory, and many students are better motivated to master the concepts of quantum mechanics when they are aware of the direct relevance for modern technology. A focus on the quantum mechanics of photons and materials is also perfectly suited to prepare students for future developments in quantum information technology, where entanglement of photons or spins, decoherence, and time evolution operators will be key concepts.

Other novel features of the discussion of quantum mechanics in this book concern attention to relevant mathematical aspects which otherwise can only be found in journal articles or mathematical monographs. Special appendices include a mathematically rigorous discussion of the completeness of Sturm-Liouville eigenfunctions in one spatial dimension, an evaluation of the Baker-Campbell-Hausdorff formula to higher orders, and a discussion of logarithms of matrices. Quantum mechanics has an extremely rich and beautiful mathematical structure. The growing prominence of quantum mechanics in the applied sciences and engineering has already reinvigorated increased research efforts on its mathematical aspects. Both students who study quantum mechanics for the sake of its numerous applications, as well as mathematically inclined students with a primary interest in the formal structure of the theory should therefore find this book interesting.

This book emerged from a quantum mechanics course which I had introduced at the University of Saskatchewan in 2001. It should be suitable both for advanced undergraduate and introductory graduate courses on the subject. To make advanced quantum mechanics accessible to wider audiences which might not have been exposed to standard second and third year courses on atomic physics, analytical mechanics, and electrodynamics, important aspects of these topics are briefly, but concisely introduced in special chapters and appendices. The success and relevance of quantum mechanics has reached far beyond the realms of physics research, and physicists have a duty to disseminate the knowledge of quantum mechanics as widely as possible.

Saskatoon, SK, Canada Rainer Dick

To the Students

Congratulations! You have reached a stage in your studies where the topics of your inquiry become ever more interesting and more relevant for modern research in basic science and technology.

Together with your professors, I will have the privilege to accompany you along the exciting road of your own discovery of the bizarre and beautiful world of quantum mechanics. I will aspire to share my own excitement that I continue to feel for the subject and for science in general.

You will be introduced to many analytical and technical skills that are used in everyday applications of quantum mechanics. These skills are essential in virtually every aspect of modern research. A proper understanding of a materials science measurement at a synchrotron requires a proper understanding of photons and quantum mechanical scattering, just like manipulation of qubits in quantum information research requires a proper understanding of spin and photons and entangled quantum states. Quantum mechanics is ubiquitous in modern research. It governs the formation of microfractures in materials, the conversion of light into chemical energy in chlorophyll or into electric impulses in our eyes, and the creation of particles at the Large Hadron Collider.

Technical mastery of the subject is of utmost importance for understanding quantum mechanics. Trying to decipher or apply quantum mechanics without knowing how it really works in the calculation of wave functions, energy levels, and cross sections is just idle talk, and always prone for misconceptions. Therefore we will go through a great many technicalities and calculations, because you and I (and your professor!) have a common goal: You should become an expert in quantum mechanics.

However, there is also another message in this book. The apparently exotic world of quantum mechanics is *our* world. Our bodies and all the world around us is built on quantum effects and ruled by quantum mechanics. It is not apparent and only visible to the *cognoscenti*. Therefore we have developed a mode of thought and explanation of the world that is based on classical pictures – mostly waves and particles in mechanical interaction. This mode of thought was amended by the notions of gravitational and electromagnetic forces, thus culminating in a powerful tool called classical physics. However, by 1900 those who were paying attention had caught enough glimpses of the underlying non-classical world to embark on the exciting journey of discovering quantum mechanics. Indeed, every single atom in your body is ruled by the laws of quantum mechanics, and could not even exist as a classical particle. The electrons that provide the light for your long nights of studying generate this light in stochastic quantum leaps from a state of a single electron to a state of an electron and a photon. And maybe the most striking example of all: There is *absolutely nothing classical* in the sunlight that provides the energy for all life on Earth.

Quantum theory is not a young theory any more. The scientific foundations of the subject were developed over half a century between 1900 and 1949, and many of the mathematical foundations were even developed in the 19th century. The steepest ascent in the development of quantum theory appeared between 1924 and 1928, when matrix mechanics, Schrödinger's equation, the Dirac equation and field quantization were invented. I have included numerous references to original papers from this period, not to ask you to read all those papers – after all, the primary purpose of a textbook is to put major achievements into context, provide an introductory overview at an appropriate level, and replace often indirect and circuitous original derivations with simpler explanations – but to honour the people who brought the then nascent theory to maturity. Quantum theory is an extremely well established and developed theory now, which has proven itself on numerous occasions. However, we still continue to improve our collective understanding of the theory and its wide ranging applications, and we test its predictions and its probabilistic interpretation with ever increasing accuracy. The implications and applications of quantum mechanics are limitless, and we are witnessing a time when many technologies have reached their "quantum limit", which is a misnomer for the fact that any methods of classical physics are just useless in trying to describe or predict the behavior of atomic scale devices. It is a "limit" for those who do not want to learn quantum physics. For you, it holds the promise of excitement and opportunity if you are prepared to work hard and if you can understand the calculations.

Quantum mechanics combines power and beauty in a way that even supersedes advanced analytical mechanics and electrodynamics. Quantum mechanics is universal and therefore incredibly versatile, and if you have a sense for mathematical beauty: The structure of quantum mechanics is breathtaking, indeed.

I sincerely hope that reading this book will be an enjoyable and exciting experience for you.

To the Instructor

Dear Colleague,

As professors of quantum mechanics courses, we enjoy the privilege of teaching one of the most exciting subjects in the world. However, we often have to do this with fewer lecture hours than were available for the subject in the past, when at the same time we should include more material to prepare students for research or modern applications of quantum mechanics. Furthermore, students have become more mobile between universities (which is good) and between academic programs (which can have positive and negative implications). Therefore we are facing the task to teach an advanced subject to an increasingly heterogeneous student body with very different levels of preparation. Nowadays the audience in a fourth year undergraduate or beginning graduate course often includes students who have not gone through a course on Lagrangian mechanics, or have not seen the covariant formulation of electrodynamics in their electromagnetism courses. I deal with this problem by including one special lecture on each topic in my quantum mechanics course, and this is what Appendices A and B are for. I have also tried to be as inclusive as possible without sacrificing content or level of understanding by starting at a level that would correspond to an advanced second year Modern Physics or Quantum Chemistry course and then follow a steeply ascending route that takes the students all the way from Planck's law to the photon scattering tensor.

The selection and arrangement of topics in this book is determined by the desire to develop an advanced undergraduate and introductory graduate level course that is useful to as many students as possible, in the sense of giving them a head start into major current research areas or modern applications of quantum mechanics without neglecting the necessary foundational training.

There is a core of knowledge that every student is expected to know by heart after having taken a course in quantum mechanics. Students must know the Schrödinger equation. They must know how to solve the harmonic oscillator and the Coulomb problem, and they must know how to extract information from the wave function. They should also be able to apply basic perturbation theory, and they should understand that a wave function $\langle \boldsymbol{x}|\psi(t)\rangle$ is only one particular representation of a quantum state $|\psi(t)\rangle$.

In a North American physics program, students would traditionally learn all these subjects in a 300-level Quantum Mechanics course. Here these subjects are discussed in Chapters 1–7 and 9. This allows the instructor to use this book also in 300-level courses or introduce those chapters in a 400-level or graduate course if needed. Depending on their specialization, there will be an increasing number of students from many different science and engineering programs who will have to learn these subjects at M.Sc. or beginning Ph.D. level before they can learn about photon scattering or quantum effects in materials, and catering to these students will also become an increasingly important part of the mandate of physics departments. Including chapters 1–7 and 9 with the book is part of the philosophy of being as inclusive as possible to disseminate knowledge in advanced quantum mechanics as widely as possible.

Additional training in quantum mechanics in the past traditionally focused on atomic and nuclear physics applications, and these are still very important topics in fundamental and applied science. However, a vast number of our current students in quantum mechanics will apply the subject in materials science in a broad sense encompassing condensed matter physics, chemistry and engineering. For these students it is beneficial to see Bloch's theorem, Wannier states, and basics of the theory of covalent bonding embedded with their quantum mechanics course. Another important topic for these students is quantization of the Schrödinger field. Indeed, it is also useful for students in nuclear and particle physics to learn quantization of the Schrödinger field because it makes quantization of gauge fields and relativistic matter fields so much easier if they know quantum field theory in the non-relativistic setting.

Furthermore, many of our current students will use or manipulate photon probes in their future graduate and professional work. A proper discussion of photon-matter interactions is therefore also important for a modern quantum mechanics course.

This should include minimal coupling, quantization of the Maxwell field, and applications of time-dependent perturbation theory for photon absorption, emission and scattering.

Students should also know the Klein-Gordon and Dirac equations after completion of their course, not only to understand that Schrödinger's equation is not the final answer in terms of wave equations for matter particles, but to understand the nature of relativistic corrections like the Pauli term or spin-orbit coupling.

The scattering matrix is introduced as early as possible in terms of matrix elements of the time evolution operator on states in the interaction picture, $S_{fi}(t,t') = \langle f|U_D(t,t')|i\rangle$, cf. equation (13.26). This representation of the scattering matrix appears so naturally in ordinary time-dependent perturbation theory that it makes no sense to defer the notion of an S-matrix to the discussion of scattering in quantum field theory with two or more particles in the initial state. It actually mystifies the scattering matrix to defer its discussion until field quantization has been introduced. On the other hand, introducing the scattering matrix even earlier in the framework of scattering off static potentials is counterproductive, because its natural and useful definition as matrix elements of a time evolution operator cannot properly be introduced at that level, and the notion of the scattering matrix does not really help with the calculation of cross sections for scattering off static potentials.

I have also emphasized the discussion of the various roles of transition matrix elements depending on whether the initial or final states are discrete or continuous. It helps students to understand transition probabilities, decay rates, absorption cross sections and scattering cross sections if the discussion of these concepts is integrated in one chapter, cf. Chapter 13. Furthermore, I have put an emphasis on canonical field quantization. Path integrals provide a very elegant description for free-free scattering, but bound states and energy levels, and basic many-particle quantum phenomena like exchange holes are very efficiently described in the canonical formalism. Feynman rules also appear more intuitive in the canonical formalism of explicit particle creation and annihilation.

The core advanced topics in quantum mechanics that an instructor might want to cover in a traditional 400-level or introductory graduate course are included with Chapters 8, 11–13, 15–18, and 21. However, instructors of a more inclusive course for general science and engineering students should include materials from Chapters 1–7 and 9, as appropriate.

The direct integration of training in quantum mechanics with the foundations of condensed matter physics, field quantization, and quantum optics is very important for the advancement of science and technology. I hope that this book will help to achieve that goal. I would greatly appreciate your comments and criticism. Please send them to rainer.dick@usask.ca.

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