ADVANCED QUANTUM MECHANICS

Yuli V. Nazarov and
Jeroen Danon

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Advanced Quantum Mechanics

An accessible introduction to advanced quantum theory, this graduate-level textbook focuses on its practical applications rather than on mathematical technicalities. It treats real-life examples, from topics ranging from quantum transport to nanotechnology, to equip students with a toolbox of theoretical techniques.

Beginning with second quantization, the authors illustrate its use with different condensed matter physics examples. They then explain how to quantize classical fields, with a focus on the electromagnetic field, taking students from Maxwell's equations to photons, coherent states, and absorption and emission of photons. Following this is a unique master-level presentation on dissipative quantum mechanics, before the textbook concludes with a short introduction to relativistic quantum mechanics, covering the Dirac equation and a relativistic second quantization formalism.

The textbook includes 70 end-of-chapter problems. Solutions to some problems are given at the end of the chapter, and full solutions to all problems are available for instructors at www.cambridge.org/9780521761505.

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A practical guide

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Preface

Courses on advanced quantum mechanics have a long tradition. The tradition is in fact so long that the word “advanced” in this context does not usually mean “new” or “up-to-date.” The basic concepts of quantum mechanics were developed in the twenties of the last century, initially to explain experiments in atomic physics. This was then followed by a fast and great *advance* in the thirties and forties, when a quantum theory for large numbers of identical particles was developed. This advance ultimately led to the modern concepts of elementary particles and quantum fields that concern the underlying structure of our Universe. At a less fundamental and more practical level, it has also laid the basis for our present understanding of solid state and condensed matter physics and, at a later stage, for artificially made quantum systems. The basics of this leap forward of quantum theory are what is usually covered by a course on advanced quantum mechanics.

Most courses and textbooks are designed for a fundamentally oriented education: building on basic quantum theory, they provide an introduction for students who wish to learn the advanced quantum theory of elementary particles and quantum fields. In order to do this in a “right” way, there is usually a strong emphasis on technicalities related to relativity and on the underlying mathematics of the theory. Less frequently, a course serves as a brief introduction to advanced topics in advanced solid state or condensed matter.

Such presentation style does not necessarily reflect the taste and interests of the modern student. The last 20 years brought enormous progress in applying quantum mechanics in a very different context. Nanometer-sized quantum devices of different kinds are being manufactured in research centers around the world, aiming at processing quantum information or making elements of nano-electronic circuits. This development resulted in a fascination of the present generation of students with topics like quantum computing and nanotechnology. Many students would like to put this fascination on more solid grounds, and base their understanding of these topics on scientific fundamentals. These are usually people with a practical attitude, who are not immediately interested in brain-teasing concepts of modern string theory or cosmology. They need fundamental knowledge to work with and to apply to “real-life” quantum mechanical problems arising in an unusual context. This book is mainly aimed at this category of students.

The present book is based on the contents of the course Advanced Quantum Mechanics, a part of the master program of the Applied Physics curriculum of the Delft University of Technology. The DUT is a university for practically inclined people, jokingly called “bike-repairmen” by the students of more traditional universities located in nearby cities. While probably meant to be belittling, the joke does capture the essence of the research in Delft. Indeed, the structure of the Universe is not in the center of the physics curriculum in Delft, where both research and education rather concentrate on down-to-earth topics. The DUT is one of the world-leading centers doing research on quantum devices such as semiconductor quantum dots, superconducting qubits, molecular electronics, and many others. The theoretical part of the curriculum is designed to support this research in the most efficient way: after a solid treatment of the basics, the emphasis is quickly shifted to *apply* the theory to understand the essential properties of quantum devices. This book is written with the same philosophy. It presents the fundamentals of advanced quantum theory at an operational level: we have tried to keep the technical and mathematical basis as simple as possible, and as soon as we have enough theoretical tools at hand we move on and give examples how to use them.

The book starts with an introductory chapter on basic quantum mechanics. Since this book is intended for a course on *advanced* quantum mechanics, we assume that the reader is already familiar with all concepts discussed in this chapter. The reason we included it was to make the book more "self-contained," as well as to make sure that we all understand the basics in the same way when we discuss advanced topics. The following two chapters introduce new material: we extend the basic quantum theory to describe many (identical) particles, instead of just one or two, and we show how this description fits conveniently in the framework of second quantization.

We then have all the tools at our disposal to construct simple models for quantum effects in many-particle systems. In the second part of the book (Chapters 4–6), we provide some examples and show how we can understand magnetism, superconductivity, and superfluidity by straightforward use of the theoretical toolbox presented in the previous chapters.

After focusing exclusively on many-*particle* quantum theory in the first parts of the book, we then move on to include *fields* into our theoretical framework. In Chapters 7 and 8, we explain in very general terms how almost any classical field can be "quantized" and how this procedure naturally leads to a very particle-like treatment of the excitations of the fields. We give many examples, but keep an emphasis on the electromagnetic field because of its fundamental importance. In Chapter 9 we then provide the last "missing piece of the puzzle": we explain how to describe the *interaction* between particles and the electromagnetic field. With this knowledge at hand, we construct simple models to describe several phenomena from the field of quantum optics: we discuss the radiative decay of excited atomic states, as well as Cherenkov radiation and Bremsstrahlung, and we give a simplified picture of how a laser works. This third part is concluded with a short introduction on *coherent states*: a very general concept, but in particular very important in the field of quantum optics.

In the fourth part of the book follows a unique master-level introduction to dissipative quantum mechanics. This field developed relatively recently (in the last three decades), and is usually not discussed in textbooks on quantum mechanics. In practice, however, the concept of dissipation is as important in quantum mechanics as it is in classical mechanics. The idea of a quantum system, e.g. a harmonic oscillator, which is brought into a stationary excited eigenstate and will stay there forever, is in reality too idealized: interactions with a (possibly very complicated) environment can dissipate energy from the system and can ultimately bring it to its ground state. Although the problem seems inconceivably hard at first sight (one needs a quantum description of a huge number of degrees of freedom), we show that it can be reduced to a much simpler form, characterizing the environment in terms of its damping coefficient or dynamical susceptibility. After explaining this procedure for the damped oscillator in Chapter 11 and discussing dissipation and fluctuations, in Chapter 12 we extend the picture to a *qubit* (two-level system) in a dissipative environment. We elucidate the role the environment plays in transitions between the two qubit states, and, based on what we find, we provide a very general scheme to classify all possible types of environment.

In the last part (and chapter) of the book, we give a short introduction to relativistic quantum mechanics. We explain how relativity is a fundamental symmetry of our world, and recognize how this leads to the need for a revised "relativistic Schrödinger equation." We follow the search for this equation, which finally leads us to the Dirac equation. Apart from obeying the relativistic symmetry, the Dirac equation predicted revolutionary new concepts, such as the existence of particles and *anti-particles*. Since the existence of anti-particles has been experimentally confirmed, just a few years after Dirac had put forward his theory, we accept their existence and try to include them into our second quantization framework. We then explain how a description of particles, anti-particles, and the electromagnetic field constitutes the basis of *quantum electrodynamics*. We briefly touch on this topic and show how a naive application of perturbation theory in the interaction between radiation and matter leads to divergences of almost all corrections one tries to calculate. The way to handle these divergences is given by the theory of *renormalization*, of which we discuss the basic idea in the last section of the chapter.

The book thus takes examples and applications from many different fields: we discuss the laser, the Cooper pair box, magnetism, positrons, vortices in superfluids, and many more examples. In this way, the book gives a very broad view on advanced quantum theory. It would be very well suited to serve as the principal required text for a master-level course on advanced quantum mechanics which is not exclusively directed toward elementary particle physics. All material in the book could be covered in one or two semesters, depending on the amount of time available per week. The five parts of the book are also relatively self-contained, and could be used separately.

All chapters contain many "control questions," which are meant to slow the pace of the student and make sure that he or she is actively following the thread of the text. These questions could for instance be discussed in class during the lectures. At the end of each chapter there are four to ten larger exercises, some meant to practice technicalities, others presenting more interesting physical problems. We decided to provide in this book the solutions to one or two exercises per chapter, enabling students to independently try to solve a serious problem and check what they may have done wrong. The rest of the solutions are available online for teachers, and the corresponding exercises could be used as homework for the students.

We hope that many students around the world will enjoy this book. We did our absolute best to make sure that no single typo or missing minus sign made it to the printed version, but this is probably an unrealistic endeavor: we apologize beforehand for surviving errors. If you find one, please be so kind to notify us, this would highly improve the quality of a possible next edition of this book.

Finally, we would like to thank our colleagues in the Kavli Institute of Nanoscience at the Delft University of Technology and in the Dahlem Center for Complex Quantum Systems at the Free University of Berlin. Especially in the last few months, our work on this book often interfered severely with our regular tasks, and we very much appreciate the understanding of everyone around us for this. J.D. would like to thank in particular Piet Brouwer and Dganit Meidan: they both were always willing to free some time for very helpful discussions about the content and style of the material in preparation.

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PART I

SECOND QUANTIZATION

1 Elementary quantum mechanics

We assume that the reader is already acquainted with elementary quantum mechanics. An introductory course in quantum mechanics usually addresses most if not all concepts discussed in this chapter. However, there are many ways to teach and learn these subjects. By including this chapter, we can make sure that we understand the basics in the same way. We advise students to read the first six sections (those on classical mechanics, the Schrödinger equation, the Dirac formulation, and perturbation theory) before going on to the advanced subjects of the next chapters, since these concepts will be needed immediately. While the other sections of this chapter address fundamentals of quantum mechanics as well, they do not have to be read right away and are referred to in the corresponding places of the following chapters. The text of this chapter is meant to be concise, so we do not supply rigorous proofs or lengthy explanations. The basics of quantum mechanics should be mastered at an operational level: please also check Table 1.1 and the exercises at the end of the chapter.

1.1 Classical mechanics

Let us start by considering a single particle of mass m, which is moving in a coordinate-dependent potential $V(\mathbf{r})$. In classical physics, the state of this particle at a given moment of time is fully characterized by two vectors, its coordinate $\mathbf{r}(t)$ and its momentum $\mathbf{p}(t)$. Since classical mechanics is a completely deterministic theory, the state of the particle in the future – its position and momentum – can be unambiguously predicted once the initial state of the particle is known. The time evolution of the state is given by Newton's well-known equations

$$\frac{d\mathbf{p}}{dt} = \mathbf{F} = -\frac{\partial V(\mathbf{r})}{\partial \mathbf{r}} \quad \text{and} \quad \frac{d\mathbf{r}}{dt} = \mathbf{v} = \frac{\mathbf{p}}{m}. \tag{1.1}$$

Here the force $\mathbf{F}$ acting on the particle is given by the derivative of the potential $V(\mathbf{r})$, and momentum and velocity are related by $\mathbf{p} = m\mathbf{v}$.

Classical mechanics can be formulated in a variety of equivalent ways. A commonly used alternative to Newton's laws are Hamilton's equations of motion

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{r}} \quad \text{and} \quad \frac{d\mathbf{r}}{dt} = \frac{\partial H}{\partial \mathbf{p}}, \tag{1.2}$$

where the Hamiltonian function $H(\mathbf{r}, \mathbf{p})$ of a particle is defined as the total of its kinetic and potential energy,

$$H = \frac{p^2}{2m} + V(\mathbf{r}). \tag{1.3}$$

One advantage of this formalism is a clear link to the quantum mechanical description of the particle we present below.

An important property of Hamilton's equations of motion is that the Hamiltonian H itself is a constant of motion, i.e. $dH/dt = 0$ in the course of motion.

Control question. Can you prove that $dH/dt = 0$ directly follows from the equations of motion (1.2)?

This is natural since it represents the total energy of the particle, and energy is conserved. This conservation of energy does not hold for Hamiltonians that explicitly depend on time. For instance, an external time-dependent force $\mathbf{F}_{\text{ext}}$ gives an addition $-\mathbf{F}_{\text{ext}} \cdot \mathbf{r}$ to the Hamiltonian. By changing the force, we can manipulate the particle and change its energy.

1.2 Schrödinger equation

The quantum mechanical description of the same particle does not include any new parameters, except for a universal constant $\hbar$. The dynamics of the particle are still determined by its mass m and the external potential $V(\mathbf{r})$. The difference is now that the state of the particle is no longer characterized by just two vectors $\mathbf{r}(t)$ and $\mathbf{p}(t)$, but rather by a continuous function of coordinate $\psi(\mathbf{r}, t)$ which is called the *wave function* of the particle. The interpretation of this wave function is probabilistic: its modulus square $|\psi(\mathbf{r}, t)|^2$ gives the probability density to find the particle at time t at the point $\mathbf{r}$. For this interpretation to make sense, the wave function must obey the normalization condition

$$\int d\mathbf{r}\, |\psi(\mathbf{r}, t)|^2 = 1, \tag{1.4}$$

i.e. the total probability to find the particle anywhere is 1, or in other words, the particle must be *somewhere* at any moment of time.

Since this is a probabilistic description, we never know exactly where the particle is. If the particle is at some time t_0 in a definite state $\psi(\mathbf{r}, t_0)$, then it is generally still impossible to predict at which point in space we will find the particle if we look for it at another time t. However, despite its intrinsically probabilistic nature, quantum mechanics is a deterministic theory. Starting from the state $\psi(\mathbf{r}, t_0)$, the state $\psi(\mathbf{r}, t)$ at any future time t is completely determined by an evolution equation, the time-dependent *Schrödinger equation*

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + V(\mathbf{r}) \right\} \psi. \tag{1.5}$$