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量子力学概论

Introduction to Quantum Mechanics

(美) David J.Griffiths 著

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这套教材出版后，我们将根据各高校的双语教学计划，举办原版教材的教师培训，及时地将其推荐给各高校选用。希望高校师生在使用教材后及时反馈意见和建议，使我们更好地为教学改革服务。

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序

David J.Griffiths 著的《Introduction to Quantum Mechanics》一书是美国许多一流理工科大学，包括麻省理工学院（MIT）和加州大学洛杉矶分校（UCLA），物理系学生的教学用书，在欧美被认为是最合适、最现代的教材之一。清华大学自2003年开始两次在物理系使用该书为教材，得到同学们的一致好评。

该书的特点有：①内容合适，包含了大学量子力学最主要的内容，直接从Schrödinger方程开始。叙述非常“物理”，强调实验基础和基本概念，改变了量子力学难于理解、难于接受的教学状况。②内容现代，在科学研究中有关的部分，在物理学各个分支中常用的部分既有精辟的叙述，又有实际举例。而与原子物理、近代物理中相关的部分，由于在低年级已有讨论，基本上不再重复。③习题分为容易、中等和较难三个层次，可供不同基础的学生选择，且配有大量的思考性习题。根据国内的教学实际，本影印版删去了原书的第12章（后记）和附录。

该书适合作为国内高等院校理工科专业“量子力学”课程教材。

庄鹏飞　于清华大学

2005 年 8 月

PREFACE

Unlike Newton's mechanics, or Maxwell's electrodynamics, or Einstein's relativity, quantum theory was not created—or even definitively packaged—by one individual, and it retains to this day some of the scars of its exhilarating but traumatic youth. There is no general consensus as to what its fundamental principles are, how it should be taught, or what it really "means." Every competent physicist can "do" quantum mechanics, but the stories we tell ourselves about what we are doing are as various as the tales of Scheherazade, and almost as implausible. Niels Bohr said, "If you are not confused by quantum physics then you haven't really understood it"; Richard Feynman remarked, "I think I can safely say that nobody understands quantum mechanics."

The purpose of this book is to teach you how to *do* quantum mechanics. Apart from some essential background in Chapter 1, the deeper quasi-philosophical questions are saved for the end. I do not believe one can intelligently discuss what quantum mechanics *means* until one has a firm sense of what quantum mechanics *does*. But if you absolutely cannot wait, by all means read the Afterword immediately following Chapter 1.

Not only is quantum theory conceptually rich, it is also technically difficult, and exact solutions to all but the most artificial textbook examples are few and far between. It is therefore essential to develop special techniques for attacking more realistic problems. Accordingly, this book is divided into two parts;[1] Part I covers the basic theory, and Part II assembles an arsenal of approximation schemes, with illustrative applications. Although it is important to keep the two parts *logically* separate, it is not necessary to study the material in the order presented here. Some

[1] This structure was inspired by David Park's classic text, *Introduction to the Quantum Theory*, 3rd ed., McGraw-Hill, New York (1992).

instructors, for example, may wish to treat time-independent perturbation theory immediately after Chapter 2.

This book is intended for a one-semester or one-year course at the junior or senior level. A one-semester course will have to concentrate mainly on Part I; a full-year course should have room for supplementary material beyond Part II. The reader must be familiar with the rudiments of linear algebra (as summarized in the Appendix), complex numbers, and calculus up through partial derivatives; some acquaintance with Fourier analysis and the Dirac delta function would help. Elementary classical mechanics is essential, of course, and a little electrodynamics would be useful in places. As always, the more physics and math you know the easier it will be, and the more you will get out of your study. But I would like to emphasize that quantum mechanics is not, in my view, something that flows smoothly and naturally from earlier theories. On the contrary, it represents an abrupt and revolutionary departure from classical ideas, calling forth a wholly new and radically counterintuitive way of thinking about the world. That, indeed, is what makes it such a fascinating subject.

At first glance, this book may strike you as forbiddingly mathematical. We encounter Legendre, Hermite, and Laguerre polynomials, spherical harmonics, Bessel, Neumann, and Hankel functions, Airy functions, and even the Riemann zeta function—not to mention Fourier transforms, Hilbert spaces, hermitian operators, Clebsch-Gordan coefficients, and Lagrange multipliers. Is all this baggage really necessary? Perhaps not, but physics is like carpentry: Using the right tool makes the job *easier*, not more difficult, and teaching quantum mechanics without the appropriate mathematical equipment is like asking the student to dig a foundation with a screwdriver. (On the other hand, it can be tedious and diverting if the instructor feels obliged to give elaborate lessons on the proper use of each tool. My own instinct is to hand the students shovels and tell them to start digging. They may develop blisters at first, but I still think this is the most efficient and exciting way to learn.) At any rate, I can assure you that there is no *deep* mathematics in this book, and if you run into something unfamiliar, and you don't find my explanation adequate, by all means *ask* someone about it, or look it up. There are many good books on mathematical methods—I particularly recommend Mary Boas, *Mathematical Methods in the Physical Sciences*, 2nd ed., Wiley, New York (1983), or George Arfken and Hans-Jurgen Weber, *Mathematical Methods for Physicists*, 5th ed., Academic Press, Orlando (2000). But whatever you do, don't let the mathematics—which, for us, is only a *tool*—interfere with the physics.

Several readers have noted that there are fewer worked examples in this book than is customary, and that some important material is relegated to the problems. This is no accident. I don't believe you can learn quantum mechanics without doing many exercises for yourself. Instructors should of course go over as many problems in class as time allows, but students should be warned that this is not a subject about which *any*one has natural intuitions—you're developing a whole new set of muscles here, and there is simply no substitute for calisthenics. Mark Semon suggested that I offer a "Michelin Guide" to the problems, with varying numbers of stars to indicate the level of difficulty and importance. This seemed like a good idea (though, like the quality of a restaurant, the significance of a problem is partly a matter of taste); I have adopted the following rating scheme:

- $*$ an *essential* problem that every reader should study;
- $**$ a somewhat more difficult or more peripheral problem;
- $***$ an unusually challenging problem, that may take over an hour.

(No stars at all means fast food: OK if you're hungry, but not very nourishing.) Most of the one-star problems appear at the end of the relevant section; most of the three-star problems are at the end of the chapter. A solution manual is available (to instructors only) from the publisher.

In preparing the second edition I have tried to retain as much as possible the spirit of the first. The only wholesale change is Chapter 3, which was much too long and diverting; it has been completely rewritten, with the background material on finite-dimensional vector spaces (a subject with which most students at this level are already comfortable) relegated to the Appendix. I have added some examples in Chapter 2 (and fixed the awkward definition of raising and lowering operators for the harmonic oscillator). In later chapters I have made as few changes as I could, even preserving the numbering of problems and equations, where possible. The treatment is streamlined in places (a better introduction to angular momentum in Chapter 4, for instance, a simpler proof of the adiabatic theorem in Chapter 10, and a new section on partial wave phase shifts in Chapter 11). Inevitably, the second edition is a bit longer than the first, which I regret, but I hope it is cleaner and more accessible.

I have benefited from the comments and advice of many colleagues, who read the original manuscript, pointed out weaknesses (or errors) in the first edition, suggested improvements in the presentation, and supplied interesting problems. I would like to thank in particular P. K. Aravind (Worcester Polytech), Greg Benesh (Baylor), David Boness (Seattle), Burt Brody (Bard), Ash Carter (Drew), Edward Chang (Massachusetts), Peter Collings (Swarthmore), Richard Crandall (Reed), Jeff Dunham (Middlebury), Greg Elliott (Puget Sound), John Essick (Reed), Gregg Franklin (Carnegie Mellon), Henry Greenside (Duke), Paul Haines (Dartmouth), J. R. Huddle (Navy), Larry Hunter (Amherst), David Kaplan (Washington), Alex Kuzmich (Georgia Tech), Peter Leung (Portland State), Tony Liss (Illinois), Jeffry Mallow (Chicago Loyola), James McTavish (Liverpool), James Nearing (Miami), Johnny Powell (Reed), Krishna Rajagopal (MIT), Brian Raue (Florida International), Robert Reynolds (Reed), Keith Riles (Michigan), Mark Semon (Bates), Herschel Snodgrass (Lewis and Clark), John Taylor (Colorado), Stavros Theodorakis (Cyprus), A. S. Tremsin (Berkeley), Dan Velleman (Amherst), Nicholas Wheeler (Reed), Scott Willenbrock (Illinois), William Wootters (Williams), Sam Wurzel (Brown), and Jens Zorn (Michigan).

CONTENTS

PART I THEORY

CHAPTER 1

THE WAVE FUNCTION

1.1 THE SCHRÖDINGER EQUATION

Imagine a particle of mass m, constrained to move along the x-axis, subject to some specified force $F(x, t)$ (Figure 1.1). The program of *classical* mechanics is to determine the position of the particle at any given time: $x(t)$. Once we know that, we can figure out the velocity ($v = dx/dt$), the momentum ($p = mv$), the kinetic energy ($T = (1/2)mv^2$), or any other dynamical variable of interest. And how do we go about determining $x(t)$? We apply Newton's second law: $F = ma$. (For *conservative* systems—the only kind we shall consider, and, fortunately, the only kind that *occur* at the microscopic level—the force can be expressed as the derivative of a potential energy function,[1] $F = -\partial V/\partial x$, and Newton's law reads $m\, d^2x/dt^2 = -\partial V/\partial x$.) This, together with appropriate initial conditions (typically the position and velocity at $t = 0$), determines $x(t)$.

Quantum mechanics approaches this same problem quite differently. In this case what we're looking for is the particle's **wave function**, $\Psi(x, t)$, and we get it by solving the **Schrödinger equation**:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi. \qquad [1.1]$$

[1] Magnetic forces are an exception, but let's not worry about them just yet. By the way, we shall assume throughout this book that the motion is nonrelativistic ($v \ll c$).

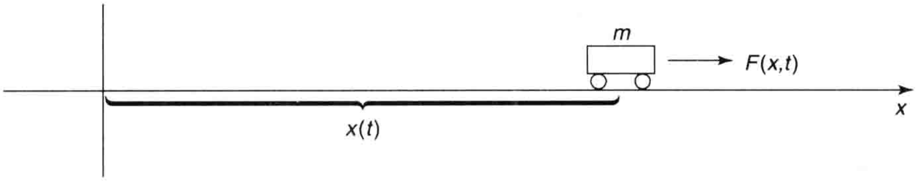

FIGURE 1.1: A "particle" constrained to move in one dimension under the influence of a specified force.

Here i is the square root of -1, and $\hbar$ is Planck's constant—or rather, his *original* constant (h) divided by 2π:

$$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34} \text{J s}. \quad [1.2]$$

The Schrödinger equation plays a role logically analogous to Newton's second law: Given suitable initial conditions (typically, $\Psi(x, 0)$), the Schrödinger equation determines $\Psi(x, t)$ for all future time, just as, in classical mechanics, Newton's law determines $x(t)$ for all future time.[2]

1.2 THE STATISTICAL INTERPRETATION

But what exactly *is* this "wave function," and what does it do for you once you've *got* it? After all, a particle, by its nature, is localized at a point, whereas the wave function (as its name suggests) is spread out in space (it's a function of x, for any given time t). How can such an object represent the state of a *particle*? The answer is provided by Born's **statistical interpretation** of the wave function, which says that $|\Psi(x, t)|^2$ gives the *probability* of finding the particle at point x, at time t—or, more precisely,[3]

$$\int_a^b |\Psi(x, t)|^2 \, dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between } a \text{ and } b, \text{ at time } t. \end{array} \right\} \quad [1.3]$$

Probability is the *area* under the graph of $|\Psi|^2$. For the wave function in Figure 1.2, you would be quite likely to find the particle in the vicinity of point A, where $|\Psi|^2$ is large, and relatively *un*likely to find it near point B.

[2] For a delightful first-hand account of the origins of the Schrödinger equation see the article by Felix Bloch in *Physics Today*, December 1976.

[3] The wave function itself is complex, but $|\Psi|^2 = \Psi^*\Psi$ (where Ψ^* is the complex conjugate of Ψ) is real and nonnegative—as a probability, of course, *must* be.

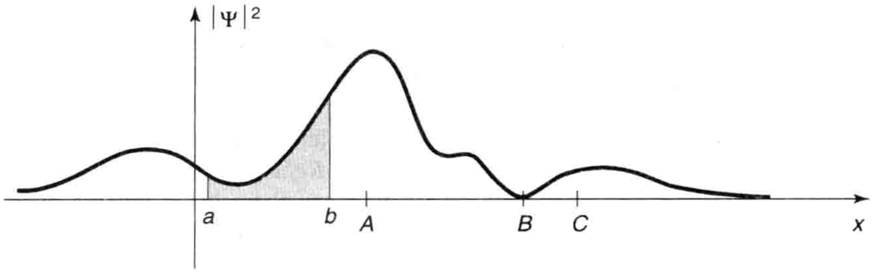

FIGURE 1.2: **A typical wave function. The shaded area represents the probability of finding the particle between *a* and *b*. The particle would be relatively likely to be found near *A*, and unlikely to be found near *B*.**

The statistical interpretation introduces a kind of **indeterminacy** into quantum mechanics, for even if you know everything the theory has to tell you about the particle (to wit: its wave function), still you cannot predict with certainty the outcome of a simple experiment to measure its position—all quantum mechanics has to offer is *statistical* information about the *possible* results. This indeterminacy has been profoundly disturbing to physicists and philosophers alike, and it is natural to wonder whether it is a fact of nature, or a defect in the theory.

Suppose I *do* measure the position of the particle, and I find it to be at point C.[4] *Question:* Where was the particle just *before* I made the measurement? There are three plausible answers to this question, and they serve to characterize the main schools of thought regarding quantum indeterminacy:

1. The **realist** position: *The particle was at C.* This certainly seems like a sensible response, and it is the one Einstein advocated. Note, however, that if this is true then quantum mechanics is an *incomplete* theory, since the particle *really was* at C, and yet quantum mechanics was unable to tell us so. To the realist, indeterminacy is not a fact of nature, but a reflection of our ignorance. As d'Espagnat put it, "the position of the particle was never indeterminate, but was merely unknown to the experimenter."[5] Evidently Ψ is not the whole story—some additional information (known as a **hidden variable**) is needed to provide a complete description of the particle.

2. The **orthodox** position: *The particle wasn't really anywhere.* It was the act of measurement that forced the particle to "take a stand" (though how and why it decided on the point C we dare not ask). Jordan said it most starkly: "Observations not only *disturb* what is to be measured, they *produce* it ... We *compel* (the

[4]Of course, no measuring instrument is perfectly precise; what I *mean* is that the particle was found *in the vicinity* of C, to within the tolerance of the equipment.

[5]Bernard d'Espagnat, "The Quantum Theory and Reality" (Scientific American, November 1979, p. 165).

particle) to assume a definite position."[6] This view (the so-called **Copenhagen interpretation**), is associated with Bohr and his followers. Among physicists it has always been the most widely accepted position. Note, however, that if it is correct there is something very peculiar about the act of measurement—something that over half a century of debate has done precious little to illuminate.

3. The **agnostic** position: *Refuse to answer.* This is not quite as silly as it sounds—after all, what sense can there be in making assertions about the status of a particle *before* a measurement, when the only way of knowing whether you were right is precisely to conduct a measurement, in which case what you get is no longer "before the measurement?" It is metaphysics (in the pejorative sense of the word) to worry about something that cannot, by its nature, be tested. Pauli said: "One should no more rack one's brain about the problem of whether something one cannot know anything about exists all the same, than about the ancient question of how many angels are able to sit on the point of a needle."[7] For decades this was the "fall-back" position of most physicists: They'd try to sell you the orthodox answer, but if you were persistent they'd retreat to the agnostic response, and terminate the conversation.

Until fairly recently, all three positions (realist, orthodox, and agnostic) had their partisans. But in 1964 John Bell astonished the physics community by showing that it makes an *observable* difference whether the particle had a precise (though unknown) position prior to the measurement, or not. Bell's discovery effectively eliminated agnosticism as a viable option, and made it an *experimental* question whether 1 or 2 is the correct choice. I'll return to this story at the end of the book, when you will be in a better position to appreciate Bell's argument; for now, suffice it to say that the experiments have decisively confirmed the orthodox interpretation:[8] A particle simply does not *have* a precise position prior to measurement, any more than the ripples on a pond do; it is the measurement process that insists on one particular number, and thereby in a sense *creates* the specific result, limited only by the statistical weighting imposed by the wave function.

What if I made a *second* measurement, *immediately* after the first? Would I get C again, or does the act of measurement cough up some completely new number each time? On this question everyone is in agreement: A repeated measurement (on the same particle) must return the same value. Indeed, it would be tough to prove that the particle was really found at C in the first instance, if this could not be confirmed by immediate repetition of the measurement. How does the orthodox

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[6] Quoted in a lovely article by N. David Mermin, "Is the moon there when nobody looks?" (Physics Today, April 1985, p. 38).

[7] Quoted by Mermin (footnote 6), p. 40.

[8] This statement is a little too strong: There remain a few theoretical and experimental loopholes, some of which I shall discuss in the Afterword. There exist viable nonlocal hidden variable theories (notably David Bohm's), and other formulations (such as the **many worlds** interpretation) that do not fit cleanly into any of my three categories. But I think it is wise, at least from a pedagogical point of view, to adopt a clear and coherent platform at this stage, and worry about the alternatives later.