Gerald D. Mahan

Quantum Mechanics in a Nutshell

简明量子力学

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Preface

This manuscript is a textbook for a graduate course in quantum mechanics. I have taught this course 15–20 times and gradually developed these notes. Orginally, I used as a text *Quantum Mechanics* by A.S. Davydov. When that fine book went out of print, I wrote these notes following a similar syllabus. It contains much new material not found in older texts.

The beginning chapters follow a traditional syllabus. Topics include solving Schrödingers equation in one, two, and three dimensions. Approximate techniques are introduced such as (1) variational, (2) WKBJ, and (3) perturbation theory. Many examples are taken from the quantum mechanics of atoms and small molecules. Solid-state examples include exchange energy, Landau levels, and the quantum Hall effect. Later chapters discuss scattering theory and relativistic quantum mechanics. The chapter on optical properties includes both linear and nonlinear optical phenomena. Each chapter concludes with numerous homework problems.

Preliminary versions of these lectures have been handed to several generations of graduate students. Their feedback has been invaluable in honing the material.

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1 Introduction

1.1 Introduction

Quantum mechanics is a mathematical description of how elementary particles move and interact in nature. It is based on the wave–particle dual description formulated by Bohr, Einstein, Heisenberg, Schrödinger, and others. The basic units of nature are indeed particles, but the description of their motion involves wave mechanics.

The important parameter in quantum mechanics is Planck's constant $h = 6.626 \times 10^{-34}$ J s. It is common to divide it by 2π, and to put a slash through the symbol: $\hbar = 1.054 \times 10^{-34}$ J s. Classical physics treated electromagnetic radiation as waves. It is particles, called *photons*, whose quantum of energy is $\hbar\omega$ where ω is the classical angular frequency. For particles with a mass, such as an electron, the classical momentum $m\vec{v} = \vec{p} = \hbar\mathbf{k}$, where the wave vector k gives the wavelength $k = 2\pi/\lambda$ of the particle. Every particle is actually a wave, and some waves are actually particles.

The *wave function* $\psi(\mathbf{r}, t)$ is the fundamental function for a single particle. The position of the particle at any time t is described by the function $|\psi(\mathbf{r}, t)|^2$, which is the probability that the particle is at position $\mathbf{r}$ at time t. The probability is normalized to one by integrating over all positions:

$$1 = \int d^3 r |\psi(\mathbf{r}, t)|^2 \tag{1.1}$$

In classical mechanics, it is assumed that one can know exactly where a particle is located. Classical mechanics takes this probability to be

$$|\psi(\mathbf{r}, t)|^2 = \delta^3(\mathbf{r} - \mathbf{v}t) \tag{1.2}$$

The three-dimensional delta-function has an argument that includes the particle velocity $\mathbf{v}$. In quantum mechanics, we never know precisely where to locate a particle. There is always an uncertainty in the position, the momentum, or both. This uncertainty can be summarized by the *Heisenberg uncertainty principle*:

$$\Delta x \Delta p_x \geq \hbar \tag{1.3}$$

Table 1.1 Fundamental Constants and Derived Quantities

Name	Symbol	Value
Electron mass	m	$9.10938215 \times 10^{-31}$ kg
Electron charge	e	$1.602176487 \times 10^{-19}$ C
Planck's constant	h	$6.62606896 \times 10^{-34}$ J s
	$\hbar = h/2\pi$	$1.054571628 \times 10^{-34}$ J s
Boltzmann's constant	k_B	$1.3806504 \times 10^{-23}$ J/K
Light speed	c	299,792,458 m/s
Atomic mass unit	AMU	$1.660538782 \times 10^{-27}$ kg
Bohr magneton	μ_B	$927.400915 \times 10^{-26}$ J/T
Neutron magnetic moment	μ_n	$-0.99623641 \times 10^{-26}$ J/T
Bohr radius	a_0	$0.52917720859 \times 10^{-10}$ m
Rydberg energy	E_{Ry}	13.605691 eV
Fine structure constant	α	$7.2973525376 \times 10^{-3}$
Compton wavelength	λ_c	$2.463102175 \times 10^{-12}$ m
Flux quantum	$\phi_0 = h/e$	$4.13566733 \times 10^{-15}$ T/m^2
Resistance quantum	h/e^2	25,812.808 Ω

Source: Taken from NIST web site http://physics.nist.gov/

where Δx is the uncertainty in position along one axis, Δp_x is the uncertainty in momentum along the same axis, and $\hbar$ is Planck's constant h divided by $2\pi(\hbar = h/2\pi)$, and has the value $\hbar = 1.05 \times 10^{-34}$ joules-second. Table 1.1 lists some fundamental constants.

1.2 Schrödinger's Equation

The exact form of the wave function $\psi(\mathbf{r}, t)$ depends on the kind of particle, and its environment. Schrödinger's equation is the fundamental nonrelativistic equation used in quantum mechanics for describing microscopic particle motions. For a system of particles, Schrödinger's equation is written as

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \tag{1.4}$$

$$H = \sum_j \left[\frac{p_j^2}{2m_j} + U(\mathbf{r}_j, s_j) \right] + \sum_{i>j} V(\mathbf{r}_i - \mathbf{r}_j) \tag{1.5}$$

The particles have positions $\mathbf{r}_i$, momentum $\mathbf{p}_j$, and spin s_j. They interact with a potential $U(\mathbf{r}_j, s_j)$ and with each other through the pair interaction $V(\mathbf{r}_i - \mathbf{r}_j)$. The quantity H is the Hamiltonian, and the wave function for a system of many particles is $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \cdot, \mathbf{r}_N; s_1, s_2, \ldots, s_N)$.

The specific forms for H depends on the particular problem. The relativistic form of the Hamiltonian is different than the nonrelativistic one. The relativistic Hamiltonian is discussed in chapter 11. The Hamiltonian can be used to treat a single particle, a collection of identical particles, or different kinds of elementary particles. Many-particle systems are solved in chapter 9.

No effort is made here to justify the correctness of Schrödinger's equation. It is assumed that the student has had an earlier course in the introduction to modern physics and quantum mechanics. A fundamental equation such as eqn. (1.4) cannot be derived from any postulate-free starting point. The only justification for its correctness is that its predictions agree with experiment. The object of this textbook is to teach the student how to solve Schrödinger's equation and to make these predictions. The students will be able to provide their own comparisons to experiment.

Schrödinger's equation for a single nonrelativistic particle of mass m, in the absence of a magnetic field, is

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \tag{1.6}$$

$$H = \frac{p^2}{2m} + V(\mathbf{r}) \tag{1.7}$$

The potential energy of the particle is $V(\mathbf{r})$. This potential is usually independent of the spin variable for nonrelativistic motions in the absence of a magnetic field. Problems involving spin are treated in later chapters. When spin is unimportant in solving Schrödinger's equation, its presense is usually ignored in the notation: the wave function is written as $\psi(\mathbf{r})$.

In quantum mechanics, the particle momentum is replaced by the derivative operator:

$$\mathbf{p} \rightarrow -i\hbar\vec{\nabla} \tag{1.8}$$

$$H = -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \tag{1.9}$$

Schrödinger's equation (1.4) is a partial differential equation in the variables $(\mathbf{r}, t)$. Solving Schrödinger's equation for a single particle is an exercise in ordinary differential equations. The solutions are not just mathematical exercises, since the initial and boundary conditions are always related to a physical problem.

Schrödinger's equation for a single particle is always an artificial problem. An equation with $V(\mathbf{r})$ does not ever describe an actual physical situation. The potential $V(\mathbf{r})$ must be provided by some other particles or by a collection of particles. According to Newton's third law, there is an equal and opposite force acting on these other particles, which are also reacting to this mutual force. The only situation in which one particle is by itself has $V = 0$, which is a dull example. Any potential must be provided by another particle, so

Schrödinger's equation is always a many-particle problem. Nevertheless, there are two reasons why it is useful to solve the one-particle problem using classical potentials. The first is that one has to learn using simple problems as a stepping stone to solving the more realistic examples. Secondly, there are cases where the one-particle Schrödinger's equation is an accurate solution to a many-particle problem: i.e., it describes the relative motion of a two-particle system.

1.3 Eigenfunctions

In solving the time-dependent behavior, for the one-particle Schrödinger's equation (1.8), an important subsidiary problem is to find the eigenvalues ε_n and eigenfunctions $\phi_n(\mathbf{r})$ of the time-independent Hamiltonian:

$$H\phi_n(\mathbf{r}) = \varepsilon_n \phi_n(\mathbf{r}) \tag{1.10}$$

There is a silly convention of treating "eigenfunction" and "eigenvalue" as single words, while "wave function" is two words. The name wave function is usually reserved for the time-dependent solution, while eigenfunction are the solutions of the time-independent equation. The wave function may be a single eigenfunction or a linear combination of eigenfunctions.

The eigenfunctions have important properties that are a direct result of their being solutions to an operator equation. Here we list some important results from linear algebra: The Hamiltonian operator is always Hermitian: $H^\dagger = H$.

- Eigenvalues of Hermitian operators are always real.
- Eigenfunctions with different eigenvalues are orthogonal:

  $$[\varepsilon_n - \varepsilon_m] \int d^3 r \phi_n^*(\mathbf{r}) \phi_m(\mathbf{r}) = 0 \tag{1.11}$$

  which is usually written as

  $$\int d^3 r \phi_n^*(\mathbf{r}) \phi_m(\mathbf{r}) = \delta_{nm} \tag{1.12}$$

  These two statements are not actually identical. The confusing case is where there are several different states with the same eigenvalue. They do not have to obey eqn. (1.12), but they can be constructed to obey this relation. We assume that is the case.

- The eigenfunctions form a complete set:

  $$\sum_n \phi_n^*(\mathbf{r}) \phi_n(\mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}') \tag{1.13}$$

These properties are used often. Orthogonality is important since it implies that each eigenfunction $\phi_n(\mathbf{r})$ is linearly independent of the others. Completeness is important, since any function $f(\mathbf{r})$ can be uniquely and exactly expanded in terms of these eigenfunctions:

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