

Quantum Mechanics

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1 Introduction

In this course we have been studying mechanics as formulated by Sir Isaac Newton; this is called *classical mechanics*. Although classical mechanics can be applied to a wide range of situations, it was discovered at the beginning of the 20th century that it cannot be applied to very small distance scales—say on the order of the size of an atom or smaller. For these small distance scales, classical mechanics no longer works, and a completely different system of mechanics is needed, called *quantum mechanics*. Here we will present a brief overview of quantum mechanics, so that you can get a sense for what it is all about. For simplicity, we will be working in one dimension, although the equations can be generalized for three dimensions.

2 Newtonian Mechanics

We begin by reviewing Newtonian classical mechanics in one dimension. In this formulation, we begin by writing Newton's second law, which gives the force F required to give an acceleration a to a mass m :

$$F = ma. \tag{1}$$

Generally the force is a function of x . Since the acceleration $a = d^2x/dt^2$, Eq. (1) may be written

$$F(x) = m \frac{d^2x}{dt^2}. \tag{2}$$

This is a second-order ordinary differential equation, which we solve for $x(t)$ to find the position x at any time t . Solving a problem in Newtonian mechanics then consists of these steps:

1. Write down Newton's second law (Eq. 2);
2. Substitute for $F(x)$ the specific force present in the problem;
3. Solve the resulting differential equation for $x(t)$.

3 Quantum Mechanics

The quantum world at very small distance scales (atomic sizes and smaller) is very alien and strange, and completely beyond our everyday experience. Here are a few of the key concepts in quantum mechanics:

1. In quantum mechanics, it generally makes no sense to talk about the the exact position x of a particle at a time t . Instead, a particle is thought of as being in many different places at the same time. Only when we go *measure* the position of the particle does it appear at a precise location. When we're not measuring its position, it is, in a sense, in many places at once.
2. The concept of the position x of a particle is replaced by the concept of a *wave function* $\psi(x, t)$. The physical interpretation of the wave function is that its square, $|\psi(x, t)|^2$, gives the *probability* that when we measure the particle's position at time t , it will appear at position x . This idea of probability is a central concept of quantum mechanics: when we go to measure the position of a particle, it is fundamentally impossible to predict where it will appear, no matter how much information we have. It is only possible to predict the probability that it will be found at a given location.
3. This idea of a wave function is closely connected the the idea of *wave-particle duality*: matter fundamentally behaves like both a wave and a particle at the same time. For example, both photons (particles of light) and electrons show both particle-like behavior and wave-like behavior.
4. It is fundamentally impossible to know both a particle's exact position and its velocity at the same time. (This is in contrast to Newtonian mechanics, where a particle's position and velocity can both be measured to arbitrary accuracy.) This idea is called the *Heisenberg uncertainty principle*, and is described in more detail below.
5. In bound systems, we generally find that a particle cannot have just *any* value of energy. Instead, we find that the particle can have only certain *discrete* values of energy; we thus say that the energy is *quantized*. The particle cannot have an energy that lies in between the allowed discrete values. We also often find that quantities like position and angular momentum are also quantized. For example, an electron in orbit around an atom has its orbital position quantized: it can only be at certain allowed positions with respect to the nucleus, and other positions are now allowed.

You may wonder: how can it be that a particle is in many places at once, or that the place where it appears is completely unpredictable, or that it is in an unknown state unless we're measuring it, or that it can be both a particle and a wave at the same time? The truth is that *nobody* really understands how it can be this way—it just *is*. We can write down the equations to describe it, and predict the outcomes of experiments to high accuracy, but nobody has a good intuitive picture of how things can possibly be this way. Nature is far stranger than we can imagine.

Now for a mathematical description of quantum mechanics. Recall how we work with Newtonian mechanics: we write down Newton's Second Law, substitute a specific force for $F(x)$, and solve the resulting differential equation for $x(t)$. Quantum mechanics does not use the concept of a force; rather, everything is formulated in terms of energy. In place of Newton's Second Law, we use the *time-dependent Schrödinger equation*, which is a partial differential equation:

$$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U(x)\psi(x, t) = i\hbar \frac{\partial \psi}{\partial t}} \quad (3)$$

where m is the mass of the particle, $U(x)$ is the potential energy function, and $\psi(x, t)$ is the wave function we wish to solve for. The constant \hbar (pronounced "h-bar") is an abbreviation for Planck's constant h divided by 2π , and has the value $\hbar \equiv h/2\pi = 1.054571628 \times 10^{-34}$ J s. Notice the presence of the factor $i = \sqrt{-1}$ on the right-hand side: in general, quantum mechanical wave functions are *complex*, but the physically meaningful quantity is the *square* of the wave function, which is real.

In the Schrödinger equation, we substitute for $U(x)$ the specific potential energy function that is present in the problem, then solve the resulting differential equation for the wave function $\psi(x, t)$. It turns out that it is possible to separate the solution into the product of two parts: a part that depends only on x and a part that

depends only on t . The solution is $\psi(x, t) = \varphi(x)e^{-iEt/\hbar}$, where $\varphi(x)$ is the solution to the *time-independent Schrödinger equation*:

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\varphi}{dx^2} + U(x)\varphi(x) = E\varphi(x)} \quad (4)$$

and where E is the total energy of the particle. So to solve the *time-dependent* Schrödinger equation for $\psi(x, t)$, we first solve the *time-independent* Schrödinger equation for $\varphi(x)$, then multiply that solution by $e^{-iEt/\hbar}$.

4 Example: Simple Harmonic Oscillator

As an example of the use of the Schrödinger equation, consider a one-dimensional simple harmonic oscillator. We wish to find the wave function $\psi(x, t)$ of the oscillator at any position x and time t .

The potential energy U of a simple harmonic oscillator is given by

$$U(x) = \frac{1}{2}kx^2, \quad (5)$$

where k is the spring constant. With this potential energy function, the time-independent Schrödinger equation (Eq. 4) becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\varphi}{dx^2} + \frac{1}{2}kx^2\varphi(x) = E\varphi(x) \quad (6)$$

This is a second-order differential equation whose solution can be worked out using the theory of differential equations. The solution turns out to be

$$\varphi_n(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}2^n n!}} H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2} \quad (n = 0, 1, 2, 3, \dots) \quad (7)$$

Here α is defined by $\alpha^4 \equiv mk/\hbar^2$ and the H_n are special functions called *Hermite polynomials*, the first few of which are shown in Table 1. Notice that the solution is *quantized*: only certain discrete solutions are allowed, which we find by substituting the integers 0, 1, 2, 3, ... for n .

The solutions to the time-dependent Schrödinger equation are then found by multiplying Eq. (7) by $e^{-iEt/\hbar}$:

$$\psi_n(x, t) = \sqrt{\frac{\alpha}{\sqrt{\pi}2^n n!}} H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2} e^{-iE_n t/\hbar} \quad (n = 0, 1, 2, 3, \dots) \quad (8)$$

The physical significance of the wave function is that its square, $|\psi|^2 = \psi^* \psi$, gives the probability of finding the particle at position x .¹ Squaring Eq. (8), we find this probability function for the harmonic oscillator is

$$|\psi_n(x)|^2 = \frac{\alpha}{\sqrt{\pi}2^n n!} [H_n(\alpha x)]^2 e^{-\alpha^2 x^2} \quad (n = 0, 1, 2, 3, \dots) \quad (9)$$

It turns out that the energy, like the wave function, is also quantized; the allowed values of E are

$$E_n = (n + \frac{1}{2})\hbar\omega \quad (n = 0, 1, 2, 3, \dots) \quad (10)$$

where $\omega = \sqrt{k/m}$ is the angular frequency of a classical simple harmonic oscillator. This is in contrast to the *classical* harmonic oscillator, which can have *any* value of energy, $E = kA^2/2$.

¹Technically, it's the probability of finding the particle between positions x and $x + dx$.

Table 1. Hermite polynomials.

$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_3(x) = 8x^3 - 12x$
$H_4(x) = 16x^4 - 48x^2 + 12$
$H_5(x) = 32x^5 - 160x^3 + 120x$
$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120$

Notice that the quantum simple harmonic oscillator has a minimum energy, called the *zero-point energy*, when $n = 0$: $E_0 = \hbar\omega/2$. The classical harmonic oscillator can have zero energy, but the not quantum harmonic oscillator—in quantum mechanics, there is always a minimum non-zero energy that the particle must have. The same is true of the atom: an electron can be in the lowest-energy K shell of the atom, but cannot have any lower energy. This is fortunate: if the electron energy were not quantized, it would have no minimum energy, and could spiral all the way in to the nucleus. Quantization of energy is what keeps the atom from collapsing.

5 The Heisenberg Uncertainty Principle

The *Heisenberg uncertainty principle* states that it is fundamentally impossible to simultaneously measure, to arbitrary accuracy, certain pairs of variables. No matter how good the experiment, the fundamental randomness of Nature restricts the accuracy to which it is possible to make these measurements.

The Heisenberg uncertainty principle can be stated mathematically by the following relations:

$$\Delta x \Delta p > \hbar \tag{11}$$

$$\Delta \phi \Delta L > \hbar \tag{12}$$

$$\Delta t \Delta E > \hbar \tag{13}$$

Eq. (11) states that we cannot simultaneously measure the position x of a particle and its momentum p to arbitrary accuracy; the product of the uncertainties cannot be less than \hbar . The more accurately you measure the position, the less accurately you know the momentum. Similarly, Eq. (12) states that you cannot simultaneously measure a particle's angular position ϕ and its angular momentum L to arbitrary accuracy. Eq. (13) relates the uncertainty in measuring a particle's energy E and the uncertainty in time t required to make that measurement.

Notice that each of these Heisenberg relations involves the product of the uncertainties in a *conserved* quantity and its so-called *conjugate variable*.

6 References

There doesn't seem to be any one standard quantum mechanics text, but the ones listed below are some popular choices for undergraduate and graduate school courses in quantum mechanics.

- *Quantum Mechanics* (3rd ed.) by Leonard I. Schiff. McGraw-Hill, New York, 1968.
- *Quantum Mechanics* (2 vol.) by Cohen-Tannoudii, Diu, and Laloe. Wiley, New York, 1977.
- *Principles of Quantum Mechanics* (2nd ed.) by R. Shankar. Springer, New York, 1994.