Lecture XXVI

Free Particle and Harmonic Oscillator

The Free Particle

The simplest time-independent Schrodinger equation is the one for the case: $V(x)$ = const. A particle moving under the influence of such a potential is a free particle since $F = -\mathrm{d}V(x)/\mathrm{d}x = 0$.

A trivial choice would be $V = 0$.

Addition of a constant V_0 to the potential energy doesn't change anything in classical mechanics, but in quantum mechanics, the wave function picks up a time-dependent phase factor:

$$\exp(-iV_0t/\hbar).$$

We know that in classical mechanics a free particle may be either at rest or moving with constant momentum p. In either case its total energy E is a constant. To find the behavior predicted by quantum mechanics for a free particle, we solve the time-independent Schrodinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$\psi(x) = e^{ikx}$ where $k = \dfrac{\sqrt{2mE}}{\hbar}$ free particle eigenfunction corresponding to the eigenvalue E.

The solutions are the eigenfunctions $\psi(x)$, and the wave functions $\Psi(x,t)$

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ represents a traveling wave in the direction of increasing x.

Also $\psi(x) = e^{-ikx}$ is a solution to the same time-independent Schrodinger equation with $V(x)$ =0 (representing a wave traveling in the direction of decreasing x) for the same value of E. $\Psi(x,t) = e^{i(-kx-\omega t)}$

Physical interpretation to the free particle eigenfunctions and wave functions:

Consider first $\Psi(x,t) = \mathrm{A}\ e^{ikx}\ e^{-iEt/\hbar}$, expectation value of momentum becomes

$$\bar{p} = \int_{-\infty}^{\infty} \Psi^* p_{\mathrm{op}} \Psi\, dx = +\sqrt{2mE} \int_{-\infty}^{\infty} \Psi^* \Psi\, dx$$
$$= +\sqrt{2mE}$$

This is exactly the momentum that we would expect for a particle moving in the direction of increasing x with total energy E in a region of zero potential energy.

• The eigenfunctions and wave functions just considered represent the idealized situations of a particle moving, in one direction or the other, in a beam of infinite length. A physical example approximating the idealized situation represented by these wave functions would be a proton moving in a highly mono-energetic beam emerging from a cyclotron.

• The probability densities $\Psi^*\Psi = A^*A$ are constants independent of x. Thus the particle is equally likely to be found anywhere, and the uncertainty in its position is $\Delta x = \infty$.

The uncertainty principle states that in these situations we may know the value of the momentum p of the particle with complete precision, since $\Delta p \Delta x \geq \hbar/2$ implies that $\Delta p = 0$, perfectly precise values of p can be known.

A difficulty in Normalization

In order to have, $$\int_{-\infty}^{\infty} \Psi^*\Psi\, dx = \int_{-\infty}^{\infty} A^*A\, dx = A^*A \int_{-\infty}^{\infty} dx = 1$$

the amplitude A must be zero as $\int_{-\infty}^{\infty} dx$ has an infinite value. The difficulty arises from the unrealistic statement made by the wave function that the particle can be found with equal probability anywhere in a beam of infinite length. This is never really true since real beams are always of finite length. The proton beam is limited on one end by the cyclotron and on the other end by a laboratory wall.

• This suggests that normalization can be obtained by setting $\Psi = 0$ outside of the range $-L/2 < x < +L/2$, or else by restricting x to be within that range. In either way we obtain a more realistic description of the actual physical situation, and we can also normalize the wave function with a non-vanishing amplitude ***A***. The procedure is called **box normalization**. Despite the fact that the value of A obtained depends on the length L of the box, it always turns out that the final result of calculation of a measurable quantity is independent of the actual value of L used.

A linear combination

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

in which A and B are arbitrary constants, is also a valid solution to the time-independent Schrodinger equation.

Degeneracy:

We note that the energy eigenvalue equation has two independent solutions,

$$\psi(x) = e^{-ikx} \qquad \text{and} \qquad \psi(x) = e^{ikx}$$

having the same energy associated with them. This is an example which we will find frequently in many other potential problems in quantum mechanics:

•There may be more than one independent eigenfunction that corresponds to the same eigenvalue of a hermitian operator. When this happens, we have a **degeneracy**.

What distinguishes the two degenerate eigenfunctions? For the set (e^{-ikx}, e^{ikx}), the difference is that they are eigenfunctions of the momentum operator

$$p_{\text{op}} e^{\pm ikx} = \frac{\hbar}{i}\frac{d}{dx} e^{\pm ikx} = \pm \hbar k e^{\pm ikx}$$

The two degenerate energy eigenfunctions are distinguished by the fact that they are simultaneously eigenfunctions of the momentum operator, with eigenvalues $\pm p$.

Note: In one-dimensional problems, the energy spectrum of the bound states is always non-degenerate.

1d Infinite square well: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$. $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2\hbar^2 n^2}{2ma^2}$ $n = 1, 2, 3, 4, 5, \ldots$

2d Infinite square well: $\psi_{n_x n_y}(x,y) = \frac{2}{a}\sin\left(\frac{n_x \pi x}{a}\right)\sin\left(\frac{n_y \pi y}{a}\right)$, with $E_{n_x n_y} = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2\right)$

Ground state is non-degenerate but the 1st excited state is doubly degenerate, ψ_{12} and ψ_{21}

3d Hydrogen atom: $\psi_{nlm}(r,\theta,\phi)$ $E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}$

$n = 1, 2, 3, \ldots$

$l = 0, 1, 2, \ldots, n-1$

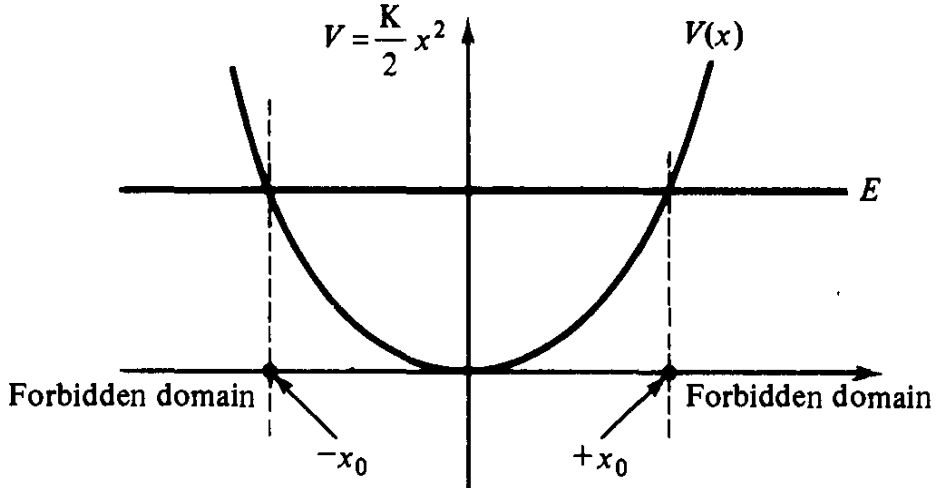
$m_l = -l, -l+1, \ldots, 0, \ldots, +l-1, l$

n^2 degenerate.

THE HARMONIC OSCILLATOR

The simple harmonic oscillator is of tremendous importance in physics, and all fields based on physics, because it is the prototype for any system involving oscillations. For instance, it is used in the study of: the vibration of atoms in diatomic molecules, the thermal properties of solids which arise from atomic vibrations. Generally speaking, the simple harmonic oscillator can be used to describe almost any system in which an entity is executing *small vibrations about a* point of *stable equilibrium.*

Classical picture



The quantum problem is to solve the Schrodinger equation for the potential $V(x) = \frac{1}{2}m\omega^2 x^2$

The time-independent Schrodinger equation for the above potential is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi.$$

• We could re-write the S. Equation into the form: $\frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi.$

where $p \equiv (\hbar/i)d/dx$ is, of course, the momentum operator.

• The basic idea is to factor out the Hamiltonian: $H = \frac{1}{2m}[p^2 + (m\omega x)^2]$

Let us introduce, $\boxed{a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)}$ The factor in front is a conventional choice

But a_+ and a_- are operators, and operators do not, in general, commute, then $a_- a_+$?

$$a_- a_+ = \frac{1}{2\hbar m\omega}(ip + m\omega x)(-ip + m\omega x)$$

$$= \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2 - im\omega(xp - px)]$$, we already know that $\boxed{[x, p] = i\hbar.}$

Therefore, $a_- a_+ = \frac{1}{\hbar\omega}H + \frac{1}{2}$ or $H = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)$

The Hamiltonian does not factor out nicely! Note that we also have, $a_+ a_- = \frac{1}{\hbar\omega}H - \frac{1}{2}$

$$a_- a_+ = \frac{1}{\hbar\omega} H + \frac{1}{2} \quad , \quad a_+ a_- = \frac{1}{\hbar\omega} H - \frac{1}{2} \qquad \text{implying} \qquad [a_-, a_+] = 1.$$

So the Hamiltonian can also be written as, $H = \hbar\omega \left(a_+ a_- + \frac{1}{2} \right)$

• The Schrodinger equation becomes, $\hbar\omega \left(a_\pm a_\mp \pm \frac{1}{2} \right) \psi = E\psi$

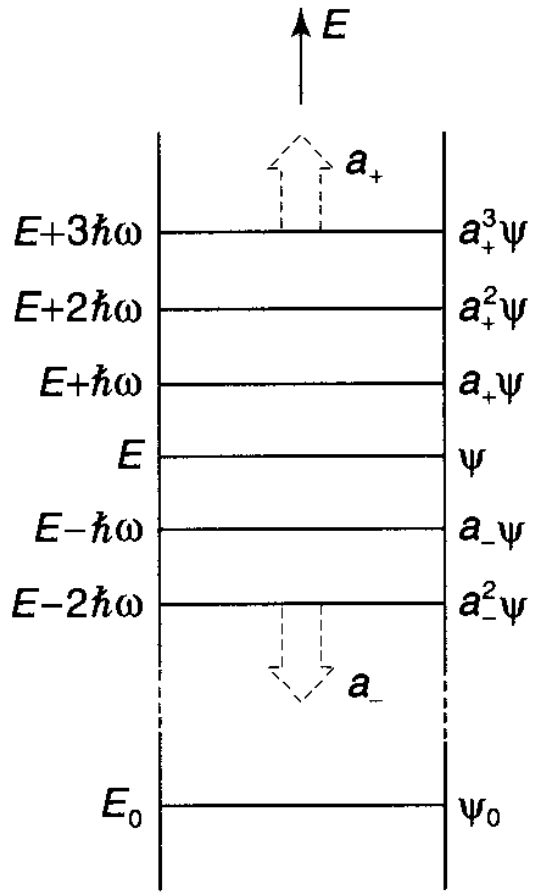
• Show that if Ψ satisfies the Schrodinger equation, with energy E, then $a_+ \Psi$ satisfies the Schrodinger equation with energy $(E + \hbar\omega)$.

$$\begin{aligned} H(a_+\psi) &= \hbar\omega \left(a_+ a_- + \frac{1}{2} \right) (a_+\psi) = \hbar\omega \left(a_+ a_- a_+ + \frac{1}{2} a_+ \right) \psi \\ &= \hbar\omega a_+ \left(a_- a_+ + \frac{1}{2} \right) \psi = a_+ \left[\hbar\omega \left(a_+ a_- + 1 + \frac{1}{2} \right) \psi \right] \\ &= a_+ (H + \hbar\omega)\psi = a_+ (E + \hbar\omega)\psi = (E + \hbar\omega)(a_+\psi). \end{aligned}$$

By the same token, $a_-\Psi$ is a solution with energy $(E - \hbar\omega)$:

$$\begin{aligned} H(a_-\psi) &= \hbar\omega \left(a_- a_+ - \frac{1}{2} \right) (a_-\psi) = \hbar\omega a_- \left(a_+ a_- - \frac{1}{2} \right) \psi \\ &= a_- \left[\hbar\omega \left(a_- a_+ - 1 - \frac{1}{2} \right) \psi \right] = a_- (H - \hbar\omega)\psi = a_- (E - \hbar\omega)\psi \\ &= (E - \hbar\omega)(a_-\psi). \end{aligned}$$

We have got an interesting tool for finding out new solutions, with higher and lower energies--if we can just find one solution, to get started! $\mathbf{a}_+$ is called the **raising operator**, and **a_** the **lowering operator.**



What if we apply the lowering operator repeatedly?

Should we reach a state with energy less than zero? Not allowed!

We should end up having, $a_-\psi_0 = 0$ for a state $\psi_0(x)$

- We can now determine this lowest state (ground state) ψ_0

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0, \qquad \frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0.$$

$$\int \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}\int x\,dx \quad \Rightarrow \quad \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + \text{constant}, \qquad \psi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2}.$$

Normalization: $$1 = |A|^2\int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar}\,dx = |A|^2\sqrt{\frac{\pi\hbar}{m\omega}}.$$

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}.}$$

- Determine the energy of the state $\psi_0(x)$ (the ground state of the quantum harmonic oscillator)

$$H\psi_0 = E_0\psi_0 \qquad \hbar\omega(a_+a_- + 1/2)\psi_0 = E_0\psi_0 \qquad a_-\psi_0 = 0: \qquad E_0 = \frac{1}{2}\hbar\omega.$$

- We simply apply the raising operator repeatedly to generate the excited states:

$$\psi_n(x) = A_n(a_+)^n\psi_0(x), \quad \text{with } E_n = \left(n + \frac{1}{2}\right)\hbar\omega,$$