The Schrodinger Equation: Quantum Tunneling and the Harmonic Oscillator

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1 Introduction

Welcome back to 'Iolani Physics Club. Today, we discuss some quantum mechanics.

2 Schrodinger Equation

2.1 Time-dependent

Newton's second law is $F = m\ddot{x}$. We're looking to solve a differential equation for $x(t)$, which gives us the evolution of position. In quantum mechanics, we're looking for the particle's wavefunction, $\psi(x,t)$, by solving the Schrodinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$

The wavefunction lies in an infinite-dimensional Hilbert space, as we discussed in previous lectures. The probability of finding the particle at point x at time t between points a and b is

$$\int_a^b |\psi(x,t)|^2 dx$$

2.2 Time-independent

In the case that $V = V(x)$ (i.e. the potential is time-independent), we can factor our wavefunction into a purely spatial part and a purely temporal part:

$$\psi(x,t) = \psi(x)T(t)$$

Plugging in to the time-dependent Schrodinger equation,

$$i\hbar\psi(x)\frac{dT}{dt} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x)T(t)$$

Separating variables,

$$i\hbar\frac{1}{T(t)}\frac{dT}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi}{\partial x^2} + V(x)$$

The only way a function of time can remain identically equal to a function of position for all x, t is if both are equal to the same constant, which, actually, turns out to be the energy:

$$i\hbar \frac{1}{T(t)} \frac{dT}{dt} = E$$

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi}{\partial x^2} + V(x) = E$$

The time part gives us

$$\frac{dT}{dt} = -\frac{iE}{\hbar} T \quad \Rightarrow \quad T(t) = Ae^{-iEt/\hbar}$$

The second part is the time-*independent* Schrodinger equation, customarily written as

$$\hat{H}\psi(x) = E\psi(x), \quad \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

where we have defined the Hamiltonian operator $\hat{H}$, similar to the Hamiltonian from classical mechanics. Note that we cannot just "divide" the $\psi(x)$ and conclude that $\hat{H} = E$, because the Hamiltonian is an *operator* and E is an *object.* Really, it's more mathematically telling to say

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

which reminds you that the wavefunction is actually a vector–you can't divide vectors, of course! In the language of linear algebra, then, the admissible "energy levels" are the *eigenvalues* of the Hamiltonian operator. As an example,

$$\begin{bmatrix} 4 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 10 \\ 5 \end{bmatrix} = 5 \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

But obviously, the matrix $\begin{pmatrix} 4 & 2 \\ 1 & 3 \end{pmatrix}$ is not the same thing as 5.

3 Harmonic Oscillator

Consider an arbitrary potential $V(x)$ with a minimum at the origin.The Taylor expansion is

$$V(x) = V(0) + xV'(0) + \frac{1}{2}x^2V''(0) + \mathcal{O}(x^3)$$

Since there's a minimum at $x = 0$, $V'(0) = 0$. Therefore the potential is approximately quadratic:

$$V(x) \approx V(0) + \frac{1}{2}V''(0)x^2$$

The constant term $V(0)$ doesn't really do anything to the dynamics because it's the same everywhere. You might notice this looks a little bit like spring potential energy, $V(x) = \frac{1}{2}kx^2$. In such a system, we often write $\omega = \sqrt{\frac{k}{m}}$. From this we can write the classical oscillator energy

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$$

We have motivated the need to find a quantum-mechanical analogue because any arbitrary potential "looks" like a harmonic oscillator when Taylor-expanded about its minimum. This is a classical problem in quantum mechanics. Our Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

A result from our previous discussions is that the momentum operator is *defined* to be

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

so the time-independent Schrodinger equation is

$$\hat{H}\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\hat{x}^2\right]\psi(x) = E\psi(x)$$

To solve this differential equation for admissible energy levels and the wavefunction, we will introduced the substitution variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x, \quad \epsilon = \frac{2E}{\hbar\omega}$$

and write $\psi(x) = \psi(\xi)$, That then gives us

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - \epsilon)\psi$$

For large values of ξ the term ξ^2 dominates so that $d^2\psi/d\xi^2 \approx \xi^2\psi$. The two asymptotic solutions are $e^{\pm\xi^2/2}$. We previously stated that the probability of a particle being found within some interval is $\int_a^b |\psi(x,t)|^2 dx$; *normalization* requires that the probability of finding the particle *anywhere* (i.e. in $(-\infty, \infty)$) is 1. By consequence, only the decaying solution to our differential equation makes physical sense. Our solution should then be

$$\psi(\xi) = e^{-\xi^2/2}u(\xi)$$

which we insert into the differential equation again to obtain

$$u'' - 2\xi u' + (\epsilon - 1)u = 0$$

Expanding $u(\xi)$ as a polynomial $\sum_{k=0}^{\infty} a_k\xi^k$,

$$\sum_{k=0}^{\infty}(k+2)(k+1)a_{k+2}\xi^k - 2\sum_{k=0}^{\infty}(k+1)a_{k+1}\xi^k + (\epsilon - 1)\sum_{k=0}^{\infty}\xi^k = 0$$

Matching the coefficients,

$$a_{k+2} = \frac{2k+1-\epsilon}{(k+1)(k+2)}a_k$$

The way to preserve normalizability is to terminate the series, meaning that k has a finite maximum value. The series terminates only when $2k_{max} + 1 - \epsilon = 0$, which means that $\epsilon = 2n+1$ $(n = 0, 1, 2, \cdots)$ whith $n = k_{max}$. But then

$$E_n = \frac{\hbar\omega}{2} = \hbar\omega\left(n + \frac{1}{2}\right)$$

This is a *very* important result, because it tells us that the energy levels of the harmonic oscillator are quantized! As for the wavefunction, the solution $u(\xi)$ is the Hermite polynomial $H_n(\xi)$, which is a special type of polynomial that satisfies the Hermite differential equation

$$u'' - 2xu' = -2\lambda u$$

When we make the appropriate substitution and normalize the eigenfunctions we get

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{-m\omega x^2/(2\hbar)}$$

4 Quantum tunneling

The Dirac delta "function" is an infinitely high, narrow spike at the origin whose area is 1:

$$\delta(x) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases} \quad \text{with} \quad \int_{-\infty}^{\infty} \delta(x) dx = 1$$

A property of this function is

$$\int_a^c f(x)\delta(x-b)dx = f(b)$$

for $a < b < c$. Consider a potential of the form

$$V(x) = \alpha x$$

for some positive constant α. The time-independent Schrodinger equation reads

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

The solutions with $E < 0$[1] are called *bound states* because ψ dies away to zero for large distance, meaning that the particle is, with high probability, guaranteed to be in a confined region. But the potential is repulsive, so there should not be any bound states. That would only happen if the potential could "trap" the particle. Solutions with $E > 0$ are a little more interesting. They're called scattering states, because they represent particles that have a high probability to be arbitrarily far away; physically, they are useful when describing particles that start far away, approach the scattering center, and end up far away again. For the scattering states, for $x < 0$ the Schrodinger equation gives us

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

The general solution is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ikx} + De^{-ikx} & x > 0 \end{cases}$$

[1]Note that I'm using 0 because our potential dies off at infinity; really, the condition for bound states is $E < V(\pm\infty)$

A boundary condition for the wavefunction is that it must always be continuous. Continuity at $x = 0$ requires that

$$C + D = A + B$$

There is another boundary condition across the discontinuity in the derivative. We integrate the Schrodinger equation from $-\epsilon$ to ϵ in the limit $\epsilon \to 0$:

$$\int_{-\epsilon}^{\epsilon} \left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha\delta(x)\psi(x) \right) dx = \int_{-\epsilon}^{\epsilon} E\psi(x)dx$$

The second derivative term gives us a discontinuity at the first derivative:

$$-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\right]_{-\epsilon}^{\epsilon} = -\frac{\hbar^2}{2m}\Delta\left(\frac{d\psi}{dx}\right)$$

The delta function term picks out a value at 0, $\alpha\psi(0)$, and the right side tends to zero as $\epsilon \to 0$ since ψ is infinite, so we get the boundary condition

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2m\alpha}{\hbar^2}\psi(0)$$

Differentiating ψ at 0, we get

$$\left.\frac{d\psi}{dx}\right|_{x=0} = \begin{cases} ik(A - B) & x < 0 \\ ik(C - D) & x > 0 \end{cases}$$

So our boundary condition is

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta)$$

where we defined $\beta = -\frac{m\alpha}{\hbar^2 k}$. Note the physical significance of the terms. e^{ikx} gives rise to a wave function propagating to the right, and e^{-ikx} leads to a wave propagating to the left. Consider an experiment where particles are fired towards this infinite dimensional spike in potential from the left. Then, A is the amplitude of the wave coming in from the left, B is the amplitude of the reflected wave, and F is the amplitude of a wave on the other side of the barrier moving to the right (the transmitted wave)). For scattering from the left, then, G should be 0. Since the probability of finding a particle at a specified location is given by $|\psi|^2$, the relative probability that an incident particle will be reflected back is the reflection coefficient

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2}$$

Similarly, the transmission coefficient is

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}$$

Of course, $R + T$ should equal 1. Hence

$$R = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)}, \quad \frac{1}{1 + (m\alpha^2/2\hbar^2 E)}$$

Note the fascinating implication: there is a nonzero probability that an incident wave with finite energy an actually pass the infinite barrier. This is quantum tunneling.