Elementary Solutions to the Schrodinger Equation

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1 The Time Independent Schrodinger Equation

The Schrodinger equation is

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

If we write our solution as

$$\Psi(x,t) = \psi(x)\rho(t),$$

then we get the time independent Schrodinger equation:

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dt^2} + V\psi = E\psi,$$

and the time dependent part

$$\rho(t) = e^{-iEt/\hbar}.$$

There are three nice advantages to using separable solutions:

1. They are **stationary states**. That is, the probability density $|\Psi(x,t)|^2$ does not depend on time.

2. They are states of definite total energy.

3. The general solution is a linear combination of the separable solutions with weighted probabilities:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar}.$$

Note that $\sum_n |c_n|^2 = 1$.

2 The Infinite Square Well

The potential is given as

$$V(x) = \begin{cases} 0, & 0 \le x \le a, \\ \infty, & otherwise \end{cases}.$$

Then the TISE becomes

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dt^2} = E\psi \Rightarrow \frac{d^2\psi}{dt^2} = -k^2\psi,$$

where $k \equiv \frac{\sqrt{2mE}}{\hbar}$. This is solved by the general solution

$$\psi(x) = A\sin(kx) + B\cos(kx).$$

The continuity of the wavefunction requires that $\psi(0) = \psi(a) = 0$. Thus $B = 0$ and

$$\psi(a) = A\sin(ka) = 0 \Rightarrow k_n = \frac{n\pi}{a}, \quad (n = 1, 2, 3, ...)$$

Now we can use k_n to solve for the allowed energies:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2}.$$

And the normalized wavefunction is:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$$

3 The Harmonic Oscillator

The Hamiltonian is given by

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

We define the raising and lowing operators as

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right).$$

They have the commutation relation

$$[a, a^\dagger] = 1.$$

We can also see that if we define the operator $N = aa^\dagger$, then the Hamiltonian can be written as

$$H = \hbar\omega(N + \frac{1}{2}).$$

If we denote an energy eigenket of N by

$$N\left|n\right\rangle = n\left|n\right\rangle,$$

then the energy eigenvalues are given by

$$H\left|n\right\rangle = (n + \frac{1}{2})\hbar\omega.$$

We can note the operation of the raising and lowering operators on the state $\left|n\right\rangle$ as

$$a\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle, \quad a^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle.$$

By successively applying the raising operator to the ground state, we can see that

$$\left|n\right\rangle = \left[\frac{(a^\dagger)^n}{\sqrt{n!}}\right]\left|0\right\rangle.$$

It can also be useful to express the position and momentum operators in terms of the raising and lowering operators:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad p = i\sqrt{\frac{m\omega\hbar}{2}}(-a + a^\dagger).$$

The ground state wavefunction for the simple harmonic oscillator is given by the Gaussian function:

$$\langle x'|0\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{x_0}}\right) exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right],$$

where

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

4 Free Particles (V=0)

The eigenfunction for a free particle is a plane-wave, given by

$$\psi_{\mathbf{k}}(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega t},$$

where

$$\mathbf{k} = \mathbf{p}/\hbar, \quad \omega = \frac{E}{\hbar} = \frac{\mathbf{p}^2}{2m\hbar} = \frac{\hbar \mathbf{k}^2}{2m},$$

and normalization given by

$$\int \psi^*_{\mathbf{k}'} \psi_{\mathbf{k}} d^3k = \delta^{(3)}(\mathbf{k} - \mathbf{k}').$$

The superposition of plane waves leads to the wave-packet description. In 1D,

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk A(k) e^{i(kx - \omega t)}, \quad \left(\omega = \frac{\hbar k^2}{2m}\right).$$

5 The Delta Function Potential

Consider a potential of the form

$$V(x) = -\alpha \delta(x), \quad \alpha > 0.$$

Then the TISE is

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

has both bound ($E < 0$) and scattering ($E > 0$) states.

5.1 Bound States of the Delta Function Potential ($E < 0$)

In the region $x < 0$, we have $V = 0$, so

$$\frac{d^2\psi}{dt^2} = \kappa^2\psi, \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.$$

Note that since E is negative, κ is real and positive. The general solution to the above differential equation is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}.$$

Its clear that as $x \to -\infty$ the first term blows up, so we'll choose $A = 0$. Then

$$\psi(x < 0) = Be^{\kappa x}.$$

Similarly, for the region $x > 0$,

$$\psi(x > 0) = Fe^{-\kappa x}.$$

Now we apply the boundary conditions at the origin:

1. ψ is always continuous.

2. $d\psi/dt$ is continuous except at points where the potential is infinite.

The first boundary condition tells us that $F = B$. One can follow Griffiths QM book page 72 to find that

$$\kappa = \frac{m\alpha}{\hbar^2} \Rightarrow E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

and

$$B = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar}.$$

This involves integrating the Schrodinger equation from $-\epsilon$ to ϵ and then taking the limit as $\epsilon \to 0$ to find the discontinuity in the derivative. So we see that for the delta function potential, we get only one bound state, no matter the "strength" of the potential:

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2}; \quad E = -\frac{m\alpha^2}{2\hbar^2}.$$

6 The Finite Square Well

Consider the finite square well potential ($V_0 > 0$):

$$V(x) = \begin{cases} -V_0, & -a \le x \le a, \\ 0, & |x| > a \end{cases}.$$

The wavefunction in the three regions is (for even parity. For odd parity the cos becomes a sin.)

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & x > a, \\ D\cos(lx), & -a < x < a, \\ \psi(-x), & x < -a \end{cases},$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}, \quad l \equiv \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

Note that the energy $E > -V_0$, so κ and l are both real and positive. Using the continuity conditions of ψ and its derivative at $x = a$, we find that

$$Fe^{-\kappa a} = D\cos(la), \quad -\kappa Fe^{-\kappa a} = -lD\sin(la).$$

Dividing the second equation by the first gives

$$\kappa = l\tan(la).$$

This gives us a formula for the allowed energies, since both κ and l depend on E. Note that if we wanted the odd parity solution, the relation would be

$$\kappa = -l\cot(la).$$

We can also note that κ and l are related by

$$\frac{2mV_0a^2}{\hbar^2} = (\kappa^2 + l^2)a^2.$$