3.3 more on the general solution of Schroedinger equation

The fact that wavefunctions are orthogonal means any shape can be written as a sum over the wavefunctions - think of Fourier series, where any function could be written as a sum of sinusoids of different frequency. So we can have any arbitrary shaped wavefunction, and break it up into a sum of the eigenfunctions

$$\Psi(x, t = 0) = \psi(x) = c_1\psi_1 + c_2\psi_2 + \dots$$

subject to the normalisation condition that $|c_1|^2 + |c_2|^2 + \dots = 1$
The mean value of energy which we measure is then

$$< E >= \int \psi^* \hat{H} \psi = \int (\sum_{n'}(c_{n'}\psi_{n'})^* \sum_{n} E_n c_n \psi_n dx$$

$$= \sum_{n'} \sum_{n} \int c_{n'}^* \psi_{n'}^* E_n c_n \psi_n dx$$

but wavefunctions are orthogonal so

$$= \sum_{n'} \sum_{n} c_{n'}^* E_n c_n \delta_{n'n}$$

$$= \sum_{n} c_n^* E_n c_n = \sum_{n} |c_n|^2 E_n$$

so the answer is the weighted sum of each indivudual eigenvalue energy, where the weight is given by the square of the individual eigenvector normalisation. But we also know that we can only measure a value of the energy which is one of the allowed states - so we can only measure a value E_n. in which case, the only way to get the average value of $< E >$ derived above is if the probability of finding the system in state n is given by $|c_n|^2$.

4 The linear harmonic oscillator

This has a potential $V(x) = \frac{1}{2}\kappa x^2$. This can be used to approximately describe any arbitrary continuuos potential $W(x)$ in the vicinity of a stable

equilibrium position (minimum in $V(x)$). We can see this explicitly by expaning $W(x)$ as a taylor series about its minimum at $x = a$

$$W(x) \approx W(a) + (x - a)\frac{dW}{dx} + \frac{1}{2}(x - a)^2\frac{d^2W}{dx^2} + ...$$

since W has a minimum at $x = a$ then $dW/dx = 0$ at $x = a$ so this

$$W(x) \approx W(a) + \frac{1}{2}(x - a)^2\frac{d^2W}{dx^2}$$

so now choose $x = a$ as the origin of the coordinates, and $W(a)$ as the origin of the energy scale and we get a first approximation

$$W(x) = \frac{1}{2}\kappa x^2 \qquad \kappa = \frac{d^2W}{dx^2}$$

so the schroedinger equation is

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

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

$$\frac{d^2\psi}{dx^2} + (\frac{2mE}{\hbar^2} - \frac{m}{\hbar^2}\kappa x^2)\psi = 0$$

let $\zeta = \alpha x$ ie let $x = \zeta/\alpha$. in other words we want to used a scaled variable instead of x

$$\frac{d^2\psi}{d\zeta^2}\left(\frac{d\zeta}{dx}\right)^2 + (\frac{2mE}{\hbar^2} - \frac{m\kappa}{\hbar^2\alpha^2}\zeta^2)\psi$$

$$\frac{d^2\psi}{d\zeta^2} + (\frac{2mE}{\hbar^2\alpha^2} - \frac{m\kappa}{\hbar^2\alpha^4}\zeta^2)\psi$$

let $\alpha^4 = \frac{m\kappa}{\hbar^2}$ then

$$\frac{d^2\psi}{d\zeta^2} + (\frac{2E}{\hbar}\sqrt{\frac{m}{\kappa}} - \zeta^2)\psi$$

but for classical oscillators $\omega = \sqrt{\kappa/m}$ so

$$\frac{d^2\psi}{d\zeta^2} + \left(\frac{2E}{\hbar\omega} - \zeta^2\right)\psi$$

2

let $\lambda = \frac{2E}{\hbar\omega}$ and then we have the much neater looking equation

$$\frac{d^2\psi}{d\zeta^2} + (\lambda - \zeta^2)\psi = 0$$

Its still not in any way easy to solve, but we can bludgeon it into submission! its separable as $\psi_\lambda(\zeta) = H_n(\zeta)e^{-\zeta^2/2}$ where $H_n(\zeta)$ are a set of special functions called Hermite polynomials which satisfy the differential equation

$$\frac{d^2 H_n}{d\zeta^2} - 2\zeta\frac{dH_n}{d\zeta} + 2nH_n = 0$$

called Hermites equation which are given by

$$H_n(\zeta) = (-1)^n e^{\zeta^2} \frac{d^n e^{-\zeta^2}}{d\zeta^n} \text{and } \lambda = 2n+1$$

so

$$H_0(\zeta) = (-1)^0 1 e^{\zeta^2} e^{-\zeta^2} = 1$$

$$H_1(\zeta) = (-1)e^{\zeta^2}\frac{de^{-\zeta^2}}{d\zeta} = -1.e^{\zeta^2}. - 2\zeta e^{-\zeta^2} = 2\zeta$$

well, that was tedious enough, and it only gets worse with higher orders but there is a simpler way to generate these terms as they also satisfy the recursion relation

$$H_{n+2}(\zeta) - 2\zeta H_{n+1}(\zeta) + 2(n+1)H_n(\zeta) = 0$$

so then we have

$$H_2(\zeta) = ... = 4\zeta^2 - 2$$

$$H_3(\zeta) = ... = 8\zeta^3 - 12\zeta$$

$$H_4(\zeta) = ... = 16\zeta^4 - 48\zeta^3 + 12$$

So now all we need to do is normalise them and we are good to go.

$$\int \psi^*(\zeta)\psi(\zeta)d\zeta = \int e^{-\zeta^2/2}H_n(\zeta)e^{-\zeta^2/2}H_n(\zeta)d\zeta = \int e^{-\zeta^2}H_n^2(\zeta)d\zeta = 2^n n!\sqrt{\pi}$$

where we just looked up the final result. so our normalised wavefunction is

$$\psi(\zeta) = \Big(\frac{1}{\sqrt{\pi}2^n n!}\Big)^{1/2} e^{-\zeta^2/2}H_n(\zeta)$$

3

and transforming back to our original variables where $\zeta = \alpha x$ so $d\zeta = \alpha dx$
we have (at last!)

$$\int \psi^*(\zeta)\psi(\zeta)d\zeta = 1 = \int \psi^*(x)\psi(x)\alpha dx$$

so we (finally!) get

$$\psi_n(x) = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2} e^{-\alpha^2 x^2/2} H_n(\alpha x) \ \ \text{where } \alpha^2 = \frac{m\omega}{\hbar} \ \text{ and } \lambda = \frac{2E}{\hbar\omega} = 2n+1 \text{ and } \omega^2 = \frac{\kappa}{m}$$

so now we can plot them and understand their properties.
1) n runs from 0 rather than 1. This is the lowest energy state. The system
has a zero point energy which is NOT zero due to the Jeisenburg uncertainty
principle $\Delta x \Delta p \geq \hbar/2$. The system cannot sit motionless at the bottom of its
potential well, for then its position and momentum would both be completely
determined to arbitrarily great precision. Therefore, the lowest-energy state
(the ground state) of the system must have a distribution in position and
momentum that satisfies the uncertainty principle, which implies its energy
must be greater than the minimum of the potential well
2) Even n gives symmetric wavefunctions (like odd n in the square well)
3) Odd n gives antisymmetric wavefunctions (like even n in the square well)
they are quite similar in shape to the finite square well potential wavefunc-
tions

4