

4.3 The linear harmonic oscillator

This has a potential $V(x) = \frac{1}{2}kx^2$, and classically it oscillates with frequency $\omega = \sqrt{k/m}$ so $V(x) = \frac{1}{2}m\omega^2x^2$ - this can be used to approximately describe any arbitrary continuous potential $W(x)$ in the vicinity of a stable equilibrium position (minimum in $V(x)$) so its very important as its of very general use.

The time independent Schroedinger equation is

$$\left(\frac{p^2}{2m} + V\right)\psi = E\psi$$

$$\frac{1}{2m}(\hat{p}^2 + m^2\omega^2x^2)\psi = E\psi$$

4.3.1 ladder operators

but this is easy to solve if we were dealing with numbers rather than operators = we know that $(a^2 + b^2) = (a + ib)(a - ib)$ BUT these are OPERATORS, and worse, the operators involved are x and p ...

$$a_+ = N(p + im\omega x) = Ni(p/i + m\omega x) = Ni(-ip + m\omega x)$$

similarly

$$a_- = M(p - im\omega x) = Mi(p/i - m\omega x) = Mi(-ip - m\omega x) = -iM(ip + m\omega x)$$

I'm going to choose $iN = -iM = \frac{1}{\sqrt{2\hbar m\omega}}$ as it makes everything look very pretty later on

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

$$\begin{aligned} a_+a_- &= \frac{1}{2\hbar m\omega}(-ip+m\omega x)(ip+m\omega x) = \frac{1}{2\hbar m\omega}(-ipip-ipm\omega x+m\omega x.ip+m^2\omega^2x^2) \\ &= \frac{1}{2\hbar m\omega}(p^2-im\omega px+im\omega xp+m^2\omega^2x^2) = \frac{1}{2\hbar m\omega}(p^2+im\omega(xp-px)+m^2\omega^2x^2) \\ &= \frac{1}{2\hbar m\omega}(p^2+im\omega i\hbar+m^2\omega^2x^2) = \frac{1}{2\hbar m\omega}(p^2-m\omega\hbar+m^2\omega^2x^2) = \left(\frac{1}{\hbar\omega}H - \frac{1}{2}\right) \end{aligned}$$

so $H = \hbar\omega(a_+a_- + 1/2)$

similarly $a_-a_+ = (\frac{1}{\hbar\omega}H + \frac{1}{2})$ so $H = \hbar\omega(a_-a_+ - 1/2)$

so the hamiltonian does not quite factor perfectly and we have

$$\hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi = E\psi$$

alternatively

$$\hbar\omega\left(a_-a_+ - \frac{1}{2}\right)\psi = E\psi$$

suppose I could find a solution, ψ_n , with associated energy E_n . Then if I operate on it by a_+ I get $a_+\psi_n$. This is also a solution!

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

so if ψ_n satisfies the Schroedinger equation with energy E then $a_+\psi_n$ satisfies it with energy $E + \hbar\omega$

similarly, $H(a_-\psi_n) = (E - \hbar\omega)a_-\psi_n$

so a_{\pm} are *ladder* operators. We have one solution, and we can find all the rest by moving up and down the ladder in energies!

so all we need is ONE solution to get started. There must be a bottom rung, with wavfunction ψ_b at which if we tried to go lower we can't!! so $a_-\psi_b = 0$.

$$\begin{aligned} a_-\psi_b &= \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_b = 0 \\ \frac{d\psi_b}{dx} &= -\frac{m\omega}{\hbar}x\psi_b \\ \ln \psi_b &= -\frac{m\omega}{2\hbar}x^2 + c \end{aligned}$$

where c is a constant. so $\psi_b = Ne^{-m\omega x^2/2\hbar}$ normalise this and we get

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

which is the wavefunction we used in the first couple of lectures with $a = m\omega/\hbar$

The energy associated with this is also easy to find from $H\psi = \hbar\omega(a_+a_- + 1/2)\psi = E\psi$. We know $a_-\psi_b = 0$ so $1/2\hbar\omega\psi_b = E_b\psi_b$ so $E_b = \hbar\omega/2$. I'm going to call this $n = 0$ state as all the rest are $\psi_n = A_n a_+^n \psi_0$ and have energies $E_n = (n + 1/2)\hbar\omega$.

4.3.2 brute force (and ignorance)

if we hadn't been smart, we would just have looked to the mathematicians to have solved this for us. and they have.

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

change variables to $\zeta = \sqrt{\frac{m\omega}{\hbar}}x$ and then we have

$$\frac{d^2\psi}{d\zeta^2} = (\zeta^2 - K)\psi$$

where $K = 2E/\hbar\omega$.

Its still not in any way easy to solve, but we can bludgeon it into submission! In fact it turns out to be related to a set of special functions called Hermite polynomials $H_n(\zeta)$ where n denotes the highest power of ζ present so H_0 is constant, $H_1 = ax + b$ etc.. and this n is also the quantization condition on $K = 2n + 1$ so $(2n + 1)\hbar\omega/2 = E_n$ or $E_n = (n + 1/2)\hbar\omega$ (as before). Then

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

where

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

so

$$H_0(\zeta) = 1$$

$$H_1(\zeta) = 2\zeta$$

etc - and it is very tedious, 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 which is a bit easier to work with

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

so then we have

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

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

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

so now all we do is turn it back from ζ to x

4.4 Properties of harmonic potential

So now lets look at these wavefunctions as a series - infinite well centered at 0, finite well centered on 0 and harmonic potential - and we see how they are showing the same sort of thing each time. Trap an electron and energy levels are quantised.

1) $E_n = (n + 1/2)\hbar\omega$ and n runs from 0 rather than 1. The lowest energy state is $E_0 = \hbar\omega/2$ - the system has a zero point energy which is NOT zero due to the Heisenburg 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 (zero)

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 wavefunctions, but the nice thing here is that the potential doesn't have those unphysical discontinuities. and here we have the turning points from polynomials rather than sin/cos functions which is a general property of a potential which depends on x as a power law rather than being a constant.