Lecture #21

Harmonic oscillator

Consider a particle of mass m moving in 1D potential created by a restoring force $F = -kx$, where k is a force constant.

Hooke's law

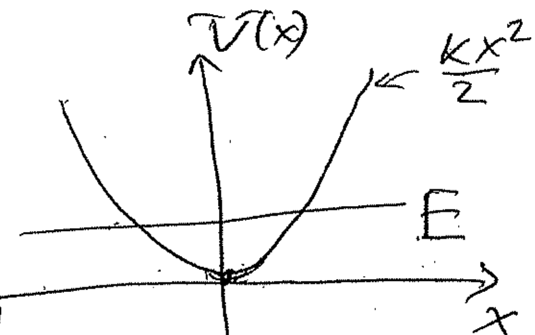
$\Downarrow$

$$V(x) = \frac{1}{2} k x^2$$

In the coordinate representation, the Schrödinger equation is: $-\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}kx^2\psi = E\psi$

$\Downarrow$

$$\psi'' = \frac{2m}{\hbar^2}\left(\frac{kx^2}{2} - E\right)\psi$$



Recall Lecture #19

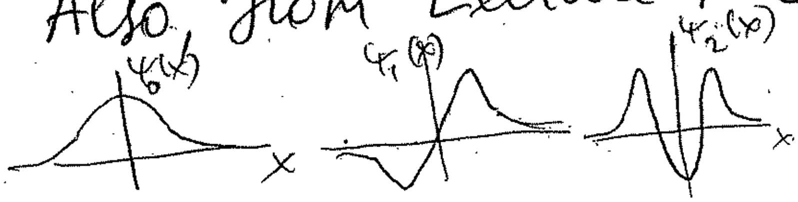
$\Downarrow$

$E < 0 \Rightarrow$ no physical solutions

$E > 0 \Rightarrow$ bound states $\Rightarrow$ discrete energy spectrum

Also from Lecture #20 $\Rightarrow$ since $V(x) = V(-x)$

$\Downarrow$



expect even and odd solutions

Recall from undergrad ⇒ how do we find Ψ_n, E_n?

1) Introduce dimensionless parameters

$$\lambda = \frac{2E}{\hbar\omega}, \quad \text{where } \omega = \sqrt{\frac{K}{m}} \quad ; \quad \xi = \alpha x$$

dimensionless energy; angular frequency; varia...; $\alpha = \sqrt{\frac{m\omega}{\hbar}}$

Then, the Schrödinger equation is:

$$\frac{d^2\Psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\Psi(\xi) = 0 \qquad (22.1)$$

2) First consider asymptotic behavior ⇒

$|\xi| \to \infty$ ⇒ need $\Psi(\xi) \to 0$

⇓

$\xi^2 \gg \lambda$ ⇒ (22.1) reduces to

$$\left(\frac{d^2}{d\xi^2} - \xi^2\right)\Psi(\xi) = 0$$

$$\Psi(\xi) \underset{|\xi|\to\infty}{=} \xi^p e^{\pm \xi^2/2} \qquad (p \text{ is a finite parameter})$$

physically acceptable: $\Psi(\xi) \underset{|\xi|\to\infty}{=} \xi^p e^{-\xi^2/2}$

3) Back to (22.1) ⇒ look for solutions in the form $\Psi(\xi) = e^{-\xi^2/2} H(\xi)$

function not affecting asymptotic behavior

⇓ Hermite equation

$$\boxed{\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\lambda - 1)H = 0} \qquad (22.2)$$

• Even states

$$\Psi(-\xi) = \Psi(\xi) \Rightarrow H(-\xi) = H(\xi)$$

Expand $H(\xi)$ in the power series $\Rightarrow$

$$H(\xi) = \sum_{k=0}^{\infty} C_k \xi^{2k}, \quad C_0 \neq 0 \qquad \text{(only } \underline{\underline{\text{even}}} \text{ powers of } \xi\text{)}$$

$\Downarrow$

substitute into (2.2)

$\Downarrow$

$$\sum_{k=0}^{\infty} \left[\underbrace{2k(2k-1) C_k \xi^{2(k-1)}} + (\lambda - 1 - 4k) \xi^{2k} C_k \right] = 0$$

$\uparrow$

$k-1 \Rightarrow k$

$C_k \Rightarrow C_{k+1}$

$k \Rightarrow k+1$

$$\sum_{k=0}^{\infty} \left[2(k+1)(2k+1) C_{k+1} + (\lambda - 1 - 4k) C_k \right] \xi^{2k} = 0$$

$\Downarrow$

recursion relation $\Rightarrow$ $\underline{C_{k+1} = \dfrac{4k+1-\lambda}{2(k+1)(2k+1)} C_k}$

For large $k \Rightarrow$ $\dfrac{C_{k+1}}{C_k} \sim \dfrac{1}{k}$ $\leftarrow$ Same! $\rightarrow$ larger

Consider $e^{\xi^2} = \sum_{n=0}^{\infty} \dfrac{\xi^{2n}}{n!} \Rightarrow$ $\dfrac{C_{n+1}}{C_n} = \dfrac{n!}{(n+1)!} = \dfrac{1}{n}$

So, if we don't terminate the series $\Rightarrow$ our $H(\xi) \sim e^{\xi^2}$

unphysical!

$\Rightarrow$ Require that at a certain $k = N$, $c_N \neq 0$, but at $k = N+1 \Rightarrow c_{N+1} = 0 \Rightarrow$

$$4N + 1 - \lambda = 0 \Rightarrow \lambda = 4N+1 \quad (N = 0, 1, 2, \ldots)$$

In this case, for each N there is an even function $H(\xi)$, which is a polynomial of the order $2N$ in ξ.

- Odd states

$$\psi(-\xi) = -\psi(\xi); \quad H(-\xi) = -H(\xi)$$

$$H(\xi) = \sum_{k=0}^{\infty} d_k \, \xi^{2k+1}, \quad d_0 \neq 0$$

odd powers only!

Similarly to even states $\Rightarrow$ get a recursion relation $\Rightarrow$

$$d_{k+1} = \frac{4k+3-\lambda}{2(k+1)(2k+3)} d_k, \quad \text{terminate the series}$$

by

$$\lambda = 4N+3, \quad N = 0, 1, 2, \ldots$$

For each N there is an odd function $H(\xi)$ which is a polynomial of order $2N+1$ in ξ.

Combine $\lambda = 4N+1$ and $\lambda = 4N+3$:

$N=0$	1	3
1	5	7

$\Rightarrow \lambda = 2n+1, \quad n = 0, 1, 2, \ldots$

$$\lambda = \frac{2E}{\hbar\omega}$$

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

energy spectrum

So, $\Psi_n(\xi) = e^{-\xi^2/2} H_n(\xi)$

n-th order polynomials (with definite parity)

$$\underbrace{\frac{d^2 H_n}{d\xi^2} - 2\xi \frac{dH_n}{d\xi} + 2n H_n = 0}_{}$$

(22.3)

equation for Hermite polynomials

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

$H_0(\xi) = 1$

$H_1(\xi) = 2\xi$

$H_2(\xi) = 4\xi^2 - 2$

$\vdots$

Another way of defining H_n

use a generating function $\Rightarrow$

$$G(\xi, s) = e^{-s^2 + 2s\xi} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n \quad (22.4)$$

$$H_n(\xi) = \left. \frac{\partial^n}{\partial s^n} G(\xi, s) \right|_{s=0}$$

From (22.3) using (22.4) $\Rightarrow$

$$\frac{\partial G(\xi, s)}{\partial \xi} = 2s \underbrace{G(\xi, s)}_{= \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n} = \sum_{n=0}^{\infty} \frac{dH_n(\xi)}{d\xi \, n!} s^n \Rightarrow$$

$$2\underbrace{\sum_{n=0}^{\infty}\frac{H_n(\xi)}{n!}s^{n+1}}_{\substack{\uparrow\\ n+1 \Rightarrow n}}=\sum_{n=0}^{\infty}\frac{dH_n(\xi)}{d\xi}\frac{s^n}{n!}$$

$$\Downarrow$$

$$\sum_{n=1}^{\infty}\frac{H_{n-1}(\xi)}{(n-1)!}s^n \Rightarrow \frac{2}{(n-1)!}H_{n-1}=\frac{dH_n}{d\xi}\cdot\frac{1}{n!}$$

$$\Downarrow$$

$$\underline{\frac{dH_n}{d\xi}=2nH_{n-1}}$$

Similarly,

$$\underline{\frac{d^2H_n}{d\xi^2}=2n\frac{dH_{n-1}}{d\xi}=2n\left[2\xi H_{n-1}-H_n\right]}$$

Then, the recursion relation is

$$\underline{H_{n+1}(\xi)-2\xi H_n(\xi)+2nH_{n-1}(\xi)=0}$$

Substitude into (22.3)

Altogether, $\Psi_n(x)=N_n e^{-\alpha^2x^2/2}H_n(\alpha x)$, $\alpha = \sqrt{\frac{m\omega}{\hbar}}$

Normalization: $\int_{-\infty}^{+\infty}|\Psi_n(x)|^2dx=1=$

$$=\frac{|N_n|^2}{\alpha}\underbrace{\int_{-\infty}^{+\infty}e^{-\xi^2}H_n^2(\xi)d\xi}_{=\,?}$$

Consider $\int_{-\infty}^{+\infty} e^{-\xi^2} G(\xi,s)\, G(\xi,t)\, d\xi =$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n!\, m!} \int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_m(\xi)\, d\xi \quad (22.5)$$

LHS: $\int_{-\infty}^{+\infty} e^{-\xi^2} e^{-s^2+2s\xi} e^{-t^2+2t\xi}\, d\xi =$

$$\underset{\substack{\uparrow \\ \text{complete} \\ \text{the square}}}{=} e^{2st} \underbrace{\int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2}\, d(\xi-s-t)}_{=\sqrt{\pi}} =$$

$$= \sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!} \quad (22.6)$$

Compare (22.5) and (22.6) $\Rightarrow$

if $n \neq m \Rightarrow \int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_m(\xi)\, d\xi = 0$

if $n = m \Rightarrow \int_{-\infty}^{+\infty} e^{-\xi^2} H_n^2(\xi)\, d\xi = \sqrt{\pi}\, 2^n n!$

orthonormality of Hermite polynomials

So, $$\Psi_n(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}\, 2^n n!}}\, e^{-\alpha^2 x^2/2} H_n(\alpha x)$$

What is the expectation value of x? $\Rightarrow$

$$\langle n | x | n \rangle = \int_{-\infty}^{+\infty} \Psi_n^*(x)\, x\, \Psi_n(x)\, dx =$$

$$= \int_{-\infty}^{\infty} \underbrace{|\Psi_n(x)|^2}\, x\, dx = 0$$

$\Psi_n(x)$ is of definite parity

$\Downarrow$

$|\Psi_n(x)|^2$ is always even

$\Downarrow$

$x\,|\Psi_n(x)|^2$ is always odd

$\Downarrow$

$\int_{-\infty}^{+\infty}$ vanishes!

What about $X_{mn} = \langle m | x | n \rangle$?

$\Downarrow$

homework!