Physics 371 Lecture 19

The simple harmonic oscillator (see Goswami, Ch. 7)

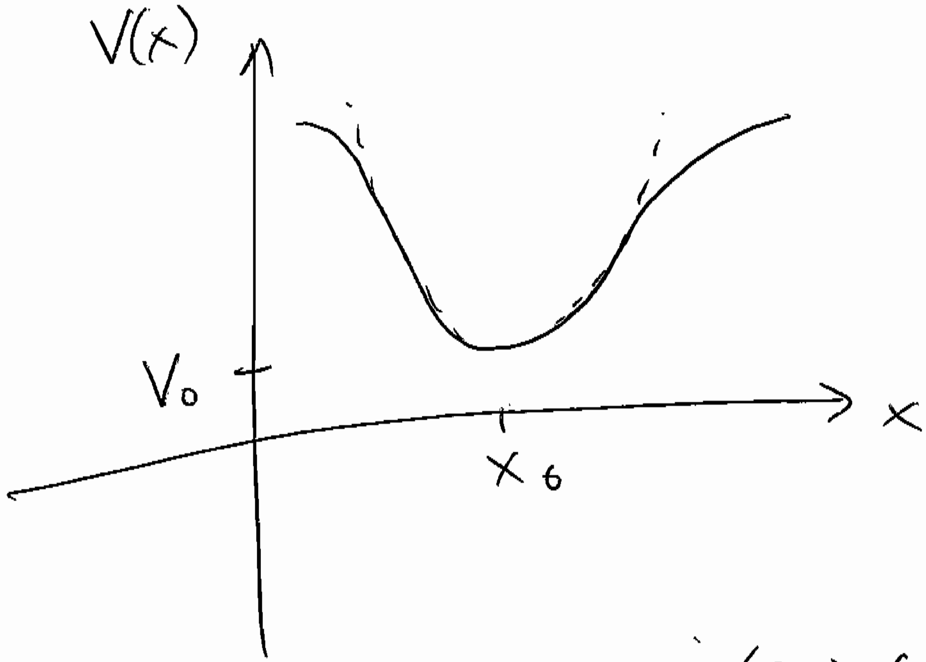
$$H = \frac{p_x^2}{2m} + \frac{1}{2} k x^2$$

Classically, oscillating solutions

$$x(t) = A\cos(\omega t + \delta), \quad \omega = \sqrt{k/m}$$

$$\Rightarrow H = \frac{p_x^2}{2m} + \frac{m\omega^2 x^2}{2}$$

Any potential can be approximated as a harmonic oscillator about its minimum:



$$V(x) = V(x_0) + \underbrace{V'(x_0)}_{0}(x - x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \cdots$$

$$\Rightarrow \quad k = \left.\frac{d^2V}{dx^2}\right|_{x_0}$$

<u>Many</u> systems described by (coupled) harmonic oscillators: photons, phonons, vibrations of molecules, nuclei, etc.

Schrödinger equation

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

Dimensionless variables

Let $\epsilon = \dfrac{2E}{\hbar\omega}$, $\xi = \sqrt{\dfrac{m\omega}{\hbar}}\,x$

$$\Rightarrow \boxed{\frac{d^2\psi}{d\xi^2} + (\epsilon - \xi^2)\psi = 0}$$

Asymptotic behavior

For large $|\xi|$ $(\xi^2 \gg |\epsilon|)$,

$$\frac{d^2\psi}{d\xi^2} - \xi^2\psi \simeq 0.$$

not normalizable

Solutions :

$$\psi \sim A e^{\xi^2/2} + B e^{-\xi^2/2}$$

Insert into Sch. equation :

$$\frac{d^2\psi}{d\xi^2} = \xi^2 \psi + \psi \simeq \xi^2 \psi$$

Thus $\psi(\xi) \underset{|\xi| \to \infty}{\sim} e^{-\xi^2/2}$.

Factoring out the asymptotic behavior,

let $\psi(\xi) = e^{-\xi^2/2} h(\xi)$.

$$\Rightarrow \boxed{\frac{d^2 h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (\epsilon - 1) h(\xi) = 0}$$

Hermite's equation

Power series solution

$$h(\xi) = \sum_{k=0}^{\infty} a_k \xi^k = a_0 + a_1 \xi + a_2 \xi^2 + \cdots$$

$$h'(\xi) = a_1 + 2a_2 \xi + 3a_3 \xi^2 + \cdots$$

$$h''(\xi) = 2a_2 + 2\cdot 3\, a_3 \xi + 3\cdot 4\, a_4 \xi^2 + \cdots$$

Coefficient of each power of ξ must vanish:

1) $2a_2 + (\epsilon - 1) a_0 = 0$

2) $2\cdot 3\, a_3 + (\epsilon - 1 - 2) a_1 = 0$

3) $3\cdot 4\, a_4 + (\epsilon - 1 - 4) a_2 = 0$

$\vdots$

In general,

$$(k+1)(k+2)\, a_{k+2} + (\epsilon - 1 - 2k)\, a_k = 0$$

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

recursion relation

The recursion relation relates all even coefficients to a_0 and all odd coefficients to a_1. The even and odd coefficients are independent of one another.

This reflects the fact that the potential is symmetric in x:

$$V(-x) = V(x).$$

Thus, the energy eigenstates must be either even or odd functions of x (eigenstates of parity).

For the even eigenstates, we can choose $a_0 = 1$ and $a_1 = 0$. For the odd eigenstates, we can choose

$a_0 = 0$ and $a_1 = 1$.

Given ϵ, and the parity of the state (even or odd), the remaining terms in the power series follow from the recursion relation.

For large k, one has

$$\frac{a_{k+2}}{a_k} \sim \frac{2}{k}.$$

Notice that

$$e^{\xi^2} = 1 + \xi^2 + \frac{\xi^4}{2!} + \frac{\xi^6}{3!} + \cdots$$

That is, the coefficient of ξ^k in the expansion of e^{ξ^2} is $b_k = \frac{1}{(k/2)!}$.

$$\frac{b_{k+2}}{b_k} = \frac{(k/2)!}{(k/2+1)!} = \frac{1}{\frac{k}{2}+1} \underset{k\to\infty}{\sim} \frac{2}{k}.$$

Thus $h(\xi) \underset{\xi\to\infty}{\sim} e^{\xi^2}$ if the power series continues for $k \to \infty$.

But then

$$\Psi(\xi) = e^{-\xi^2/2} h(\xi) \sim e^{\xi^2/2} \underset{\xi\to\infty}{\longrightarrow} \infty.$$

This just resurrects the discarded, non-normalizable term.

According to the postulates (1 of QM, ψ must be normalizable. The only way for this to happen is if the polynomial $h(\xi)$ terminates at some finite order n. This will happen if

$$\epsilon - 1 - 2n = 0$$

$$\boxed{E = \frac{\hbar\omega}{2}\epsilon = \hbar\omega\left(n + \frac{1}{2}\right) \qquad n = 0, 1, 2, \ldots, \infty}$$

allowed energy levels