The Harmonic Oscillator (HO)

Suppose a potential $V(x)$ has a minimum at the point x_0 as shown in Fig 2.4. We can expand $V(x)$ around x_0 in a Taylor series as

$$V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{V''(x_0)}{2}(x-x_0)^2$$

$$+ \cdots\cdots$$

where we denote $\left.\frac{dV(x)}{dx}\right|_{x=x_0} = V'(x_0)$

and so on for $V''(x_0)$. Since $V(x_0)$ is a minimum $V'(x_0) = 0$. For x in the vicinity of x_0 we can approximate

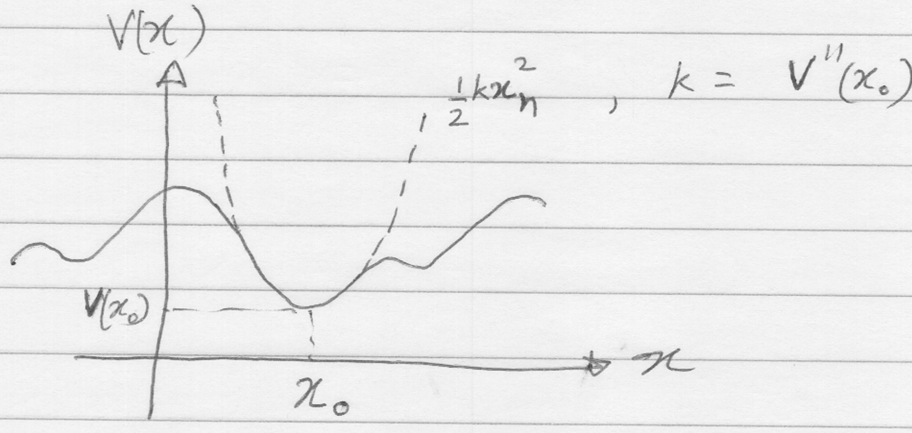
$$V(x) \approx V(x_0) + \left[\frac{V''(x_0)}{2}\right](x-x_0)^2$$

~~Pu~~ Furthermore we can shift the origin to x_0 by choosing $x_n = x - x_0$ and define $V(x_0) = 0$

$$\Rightarrow \quad V(x_n) = \frac{1}{2}\left[\frac{d^2V(x_n)}{dx_n^2}\right]_{x_n=0} x_n^2$$

This is the HO potential. We define a new constant

$$\omega \equiv \left[\left[V''(x_n)\Big|_{x_n=0}\right] \Big/ m\right]^{1/2}$$



Harmonic approximation $\frac{1}{2}kx_n^2$
to $V(x)$ around $x = x_0$
where $x_n \equiv x - x_0$.

Now we drop the subscript n and we get

$$V(x) = \frac{m\omega^2 x^2}{2}$$

$$\Rightarrow \hat{H} = \frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}\hat{X}^2$$

A commutator of two operators $\hat{\Omega}_1$ and $\hat{\Omega}_2$ is defined as

$$[\hat{\Omega}_1, \hat{\Omega}_2] \equiv \hat{\Omega}_1\hat{\Omega}_2 - \hat{\Omega}_2\hat{\Omega}_1$$

As an example let $\hat{\Omega}_1 = \hat{X} = x$ and
$\hat{\Omega}_2 = \hat{P} = -i\hbar\frac{d}{dx}$

Let $f(x)$ be some arbitrary function of x.

$$\Rightarrow [\hat{X}, \hat{P}]f = \left[x, -i\hbar\frac{d}{dx}\right]f(x) = (x)\left(-i\hbar\frac{d}{dx}\right)f(x) - \left(-i\hbar\frac{d}{dx}\right)x f(x)$$

$$= -i\hbar x\frac{d}{dx}f(x) + i\hbar x\frac{d}{dx}f(x) + i\hbar f(x)$$

$$= i\hbar f(x)$$

$$\Rightarrow [\hat{X}, \hat{P}]f(x) = i\hbar f(x) \quad , \forall f(x)$$

$$\Rightarrow [\hat{X}, \hat{P}] = i\hbar \longrightarrow (2.51)$$

Now define

$$\hat{a}_\pm = \frac{1}{\sqrt{2m\hbar\omega}}\left[m\omega x \mp i\hat{P}\right]$$ 3

$$\Rightarrow \hat{a}_+\hat{a}_- = \frac{1}{2m\hbar\omega}\left[m^2\omega^2x^2 + \hat{P}^2 + im\omega\left[x\hat{P} - \hat{P}x\right]\right]$$

$$= \frac{1}{\hbar\omega}\left[\frac{m\omega^2x^2}{2} + \frac{\hat{P}^2}{2m} + \frac{i\omega}{2}\left[\hat{x},\hat{P}\right]\right]$$

$$= \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} - 1 = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$$

Similarly we can show

$$\hat{a}_-\hat{a}_+ = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2}$$

$$\Rightarrow \hat{H} = \hbar\omega\left[\hat{a}_+\hat{a}_- + \frac{1}{2}\right] = \hbar\omega\left[\hat{a}_-\hat{a}_+ - \frac{1}{2}\right]$$

$$= \hbar\omega\left[\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2}\right]$$

Also we get $(\hat{a}_+)^\dagger = \hat{a}_-$ and $\hat{a}_-^\dagger = \hat{a}_+$.

We can also see that

$$\hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+ = \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right) - \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right)$$

$$\left.\begin{array}{l}\Rightarrow \left[\hat{a}_+,\hat{a}_-\right] = -1 \\ \qquad\qquad \Rightarrow \left[\hat{a}_-,\hat{a}_+\right] = 1\end{array}\right\} \rightarrow 2.55$$

We want to solve $\hat{H}\psi_E(x) = E\psi_E(x)$

$$\Rightarrow \left(\hat{a}_+ \hat{a}_- + \frac{1}{2}\right)\hbar\omega\, \psi_E(x) = E\,\psi_E(x)$$

Consider now

$$\hat{H}\left[\hat{a}_-\psi(x)\right] = \hbar\omega\left[\hat{a}_+\hat{a}_-\hat{a}_- + \frac{\hat{a}_-}{2}\right]\psi_E(x)$$

$$= \hbar\omega\left[\frac{\hat{a}_-}{2} + \left(\hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+ + \hat{a}_-\hat{a}_+\right)\hat{a}_-\right]\psi_E(x)$$

$$= \hbar\omega\left[\frac{\hat{a}_-}{2} + \left[\left[\hat{a}_+, \hat{a}_-\right] + \hat{a}_-\hat{a}_+\right]\hat{a}_-\right]\psi_E(x)$$

$$= \hbar\omega\left[\frac{\hat{a}_-}{2} + \hat{a}_-\left[-1 + \hat{a}_+\hat{a}_-\right]\right]\psi_E(x)$$

$$= \hbar\omega\,\hat{a}_-\left[\hat{a}_+\hat{a}_- + \frac{1}{2} - 1\right]\psi_E(x)$$

$$= \hat{a}_-\left[\hat{H} - \hbar\omega\right]\psi_E(x) = (E - \hbar\omega)\,\hat{a}_-\psi_E(x)$$

$$\Rightarrow \hat{H}\left[\hat{a}_-\psi_E(x)\right] = \left[E - \hbar\omega\right]\left[\hat{a}_-\psi_E(x)\right]$$

$\Rightarrow$ if $\psi_E(x)$ solves TISE with energy E then
$\hat{a}_-\psi_E(x)$ " " " " $E - \hbar\omega$
and $(\hat{a}_-)^n\psi_E(x)$ " " " " $E - n\hbar\omega$
$\forall n \in N$,

$N = \{1, 2, 3, \ldots\}$. This process has to stop at some point otherwise $\exists$ a state $\psi_E(x) \ni E < 0$.

This is impossible because $V(x)\Big|_{\text{min.}} = 0$

$\Rightarrow E > 0$

Let us then demand that $\exists$ $\psi_0(x) \ni$

$$\hat{a}_- \psi_0(x) = 0$$ $\boxed{5}$

$$\Rightarrow \frac{1}{\sqrt{2m\hbar\omega}}\left[\hbar \frac{d}{dx} + m\omega x\right]\psi_0(x) = 0$$

$$\Rightarrow \frac{d\psi_0(x)}{dx} = -\frac{m\omega x}{\hbar}\psi_0(x)$$

$$\Rightarrow \int \frac{d\psi_0}{\psi_0} = \frac{-m\omega}{\hbar}\int x\,dx$$

$$\Rightarrow \psi_0(x) = A e^{\frac{-m\omega x^2}{2\hbar}}$$

Normalization gives $A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$

Now $\hat{H}\psi_0(x) = \hbar\omega\left[\hat{a}_+\hat{a}_- + \frac{1}{2}\right]\psi_0(x)$

$$= \frac{\hbar\omega}{2}\psi_0(x)$$

$\Rightarrow E_0 = \frac{\hbar\omega}{2}$ = ground state energy.

$\psi_n(x) = A_n (a_+)^n \psi_0(x)$, $n = 1, 2, 3, \ldots$

$\hat{H}\psi_n(x) = E_n \psi_n(x)$ where $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

$\Psi_n(x)$ $(n>0)$ ~~are~~ is called the n^{TH} excited state of the HO potential.

We want all Ψ_n to be normalized. So

$\Psi_1 = A_1(\hat{a}_+ \Psi_0)$ should be normalized.

In general then we need $\int_{-\infty}^{\infty} |\Psi_n|^2 dx = 1, \forall n$

$$\Psi_n = A_n \hat{a}_+^n \Psi_0 \ , \ \Psi_{n+1} = A_{n+1} \hat{a}_+^{n+1} \Psi_0$$

$$\Rightarrow \Psi_{n+1} = \frac{A_{n+1}}{A_n}(\hat{a}_+ \Psi_n) \longrightarrow \text{2-645}$$

Also $\hat{H}\Psi_n = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)\Psi_n = \left(n+\frac{1}{2}\right)\Psi_n \hbar\omega$

$$\Rightarrow \hat{a}_-\hat{a}_+\Psi_n = (n+1)\Psi_n$$

$$\Rightarrow \int_{-\infty}^{\infty} \Psi_n^* \hat{a}_-\hat{a}_+\Psi_n dx = (n+1)\int_{-\infty}^{\infty} |\Psi_n|^2 dx$$

$$\Rightarrow \int_{-\infty}^{\infty} |(\hat{a}_+\Psi_n)|^2 dx = (n+1)\int_{-\infty}^{\infty} |\Psi_n|^2 dx$$

$\Rightarrow$ using Eq. 2·645 that

$$\left|\frac{A_{n+1}}{A_n}\right|^{-2} \int_{-\infty}^{\infty} |\Psi_{n+1}|^2 dx = (n+1)\int_{-\infty}^{\infty} |\Psi_n|^2 dx$$

If $n=0 \Rightarrow \left|\frac{A_1}{A_0}\right|^2 = 1$

Note $A_0 = 1$, $\Rightarrow A_1 = 1$

$$n=2 \Rightarrow \left(\frac{A_2}{A_1}\right)^{-2} = 2$$

$$\Rightarrow A_2 = 1/\sqrt{2}$$

In general we get $A_n = 1/\sqrt{n!}$

$$\Rightarrow \psi_n(x) = \frac{\hat{a}_+^n}{\sqrt{n!}} \psi_0(x)$$

$$\Rightarrow \psi_{n+1}(x) = (n+1)^{1/2} \hat{a}_+ \psi_n(x).$$

Doing similar work with $\hat{a}_-$ we get

$$\psi_{n-1}(x) = \frac{1}{\sqrt{n}} \hat{a}_- \psi_n(x).$$

The set of ψ_n s is now orthonormal

$$\Rightarrow \int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x)\,dx = \delta_{m,n}.$$

Prove as an excercise.

Find $\hat{P}$ and $\hat{x}$ as linear expressions in $\hat{a}_+$ and $\hat{a}_-$.