One Dimensional Harmonic Oscillator

$$H = \frac{p^2}{2m} + V(x)$$

Suppose $V(x)$ has a stable minimum at $x = x_0$

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

Introduce new coordinate $x \to x - x_0$

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

$$\omega^2 = \frac{V''(x_0)}{m}$$

Classical Solution:

Hamiltons

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x$$

$$m\ddot{x} + m\omega^2 x = 0$$

$$\ddot{x} + \omega^2 x = 0$$

$$x(t) = A\cos\omega t + B\sin\omega t = x_0 \cos(\omega t + \phi)$$

$$A = x_0 \cos\phi \, , \; B = -x_0 \sin\phi$$

Conserved energy

$$E = T + V = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2$$

$$= \frac{1}{2} m x_0^2 \omega^2$$

$$\dot{x} = x_0 \omega \sin(\omega t + \phi)$$

$$= x_0 \omega \sqrt{1 - \cos^2(\omega t + \phi)}$$

$$= \sqrt{x_0^2 \omega^2 - x_0^2 \omega^2 \cos^2(\omega t + \phi)} = \left(\frac{2E}{m} - \omega^2 x^2\right)^{1/2}$$

$$= \omega (x_0^2 - x^2)^{1/2}$$

Particle at rest at turning points $x = \pm x_0$

<u>Quantization in Coordinate Basis</u>

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle$$

$$H = H(x \to X, p \to P) = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2$$

Eigenvalues of H cannot be negative

For any $|\psi\rangle$

$$\langle H \rangle = \frac{1}{2m} \langle \psi^2 | P^2 | \psi \rangle + \frac{1}{2} m \omega^2 \langle \psi | X^2 | \psi \rangle$$

$$= \frac{1}{2m} \langle P\psi | P\psi \rangle + \frac{1}{2} m \omega^2 \langle X\psi | X\psi \rangle$$

$$\geq 0$$

For eigenstate $|\psi\rangle$ $\quad \langle H \rangle = E$, energy eigenvalue

Eigenvalue eq for Hamiltonian

$$\left(\frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2\right) |E\rangle = E |E\rangle$$

Go to coordinate basis

$$X \to x$$
$$P \to -i\hbar \frac{d}{dx}$$
$$|E\rangle \to \psi_E(x)$$

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2} m\omega^2 x^2\right)\psi = 0$$

Try to remove some dimensionful quantities by rescaling

$$x = by$$

$$\frac{d^2\psi}{dy^2} + \frac{2mb^2E}{\hbar^2}\psi - \frac{m^2\omega^2 b^4}{\hbar^2} y^2\psi = 0$$

$$b = \left(\frac{\hbar}{m\omega}\right)^{1/2}, \quad \varepsilon = \frac{mEb^2}{\hbar^2}$$

$$\frac{d^2\psi}{dy^2} + (2\varepsilon - y^2)\psi = 0$$

Nature of solution for limiting values

In limit $y \to \infty$

$$\psi'' - y^2\psi = 0$$

Soln has $\quad$ as $y \to \infty$

$$\psi = A y^m e^{\pm y^2/2}$$

Since $\quad \psi' = A\left(m y^{m-1} \pm y^{m+1}\right) e^{\pm y^2/2}$

$$\psi'' = A\left(m(m-1) y^{m-2} \pm (m+1) y^m \pm m y^m + y^{m+2}\right) e^{\pm y^2/2}$$

$$= A\left(\frac{m(m-1)}{y^4} \pm \frac{(2m+1)}{y^2} + 1\right) y^2 y^m e^{\pm y^2/2}$$

$$\xrightarrow[y\to\infty]{} A y^2 y^m e^{\pm y^2/2} = y^2 \psi$$

Note only keep $A y^m e^{-y^2/2}$ since this normalizable. Next consider limit $y \to 0$

$$\psi'' + 2\epsilon\psi = 0$$

$$\psi = A\cos[\sqrt{2\epsilon}\, y] + B\sin[\sqrt{2\epsilon}\, y]$$

$$\xrightarrow[y\to 0]{} A + cy + O(y^2) \qquad c = B\sqrt{2\epsilon}$$

So $\quad \psi = u(y)\, e^{-y^2/2}$

$u(y) \xrightarrow[y\to 0]{} A + cy \quad$ and $u(y) \to y^m$ as $y \to \infty$

Plug this back into

$$\frac{d\psi}{dy} = \left[u'(y) - y\,u(y)\right] e^{-y^2/2}$$

$$\frac{d^2\psi}{dy^2} = \left[u''(y) - y\,u'(y) - u(y) - y\,u'(y) + y^2 u(y)\right] e^{-y^2/2}$$

$$u''(y) - 2y\,u'(y) + (2\epsilon - 1)\,u(y) = 0$$

Seek series soln

$$u(y) = \sum_{n=0}^{\infty} C_n y^n$$

Know behavior at $y=0$ from previous work

$$\sum_{n=0}^{\infty} C_n \left[n(n-1) y^{n-2} - 2n\,y^n + (2\epsilon - 1) y^n \right] = 0$$

$$\sum_{n=0}^{\infty} n(n-1) C_n y^{n-2} = \sum_{n=2}^{\infty} C_n\, n(n-1) y^{n-2}$$

$$= \sum_{n=0}^{\infty} C_{n+2} (n+2)(n+1)\, y^n$$

$$\sum_{n=0}^{\infty} y^n \left[(n+2)(n+1) C_{n+2} + (2\epsilon - 1 - 2n) \right] = 0$$

$$C_{n+2} = \frac{(2\epsilon + 1 + 2n)\, C_n}{(n+2)(n+1)}$$

For any C_0, C_1 series generates $C_2, C_4, C_6 \ldots,\; C_3, C_5, C_7 \ldots$

Appears energy is arbitrary. Now we have seen asy

$$\psi(y) \to y^m e^{\pm y^2/2}$$

We wrote $\psi(y) = u(y)\, e^{-y^2/2}$

So $u(y) \to y^m$ or $y^m e^{y^2}$

Clearly if series does not terminate its second case. In fact

$$\frac{C_{n+2}}{C_n} \xrightarrow[n\to\infty]{} \frac{2}{n}$$

$$y^m e^{y^2} = \sum_{k=0}^{\infty} \frac{y^{2k+m}}{k!}$$

$2k+m=n$

$k! = \left(\frac{n-m}{2}\right)!$

$$\frac{C_{n+2}}{C_n} \sim \frac{\left[\frac{n-m}{2}\right]!}{\left[\frac{n-m}{2}+1\right]!} \sim \to \frac{1}{\frac{n}{2}} \sim \frac{2}{n}$$

Series must terminate. So need

$$\mathcal{E} = \mathcal{E}_n = \frac{2n+1}{2} \implies C_{n+2} = 0$$

an n'th order polynomial

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

$$E_n = \frac{\hbar\omega}{2}(2n+1) = \hbar\omega(n+1/2) \quad n=0,1,2,\ldots$$

Solutions are called Hermite polynomials

$H_0(y) = 1$

$H_1(y) = 2y$

$H_2(y) = -2(1-2y^2)$

$\vdots$

$$\psi_E(x) = \psi_{(n+\frac{1}{2})\hbar\omega}(x) \equiv \psi_n(x)$$

$$= \left(\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right)^{1/4} \exp\left(-\frac{m\omega}{\hbar 2}x^2\right) H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right]$$

normalization constant $= A_n$

Hermite polynomials satisfy recursion relation

$$H_n'(y) = 2n H_{n-1}$$

$$H_{n+1}(y) = 2y H_n - 2n H_{n-1}$$

and the normalization integral

$$\int_{-\infty}^{\infty} dy\, H_n(y) H_{n'}(y) e^{-y^2} = \delta_{nn'} \left(\pi^{1/2} 2^n n!\right)$$

Propagator

$$U(x,t\,;x',t') = \sum_{n=0}^{\infty} \psi_n^*(x)\psi_n(x') e^{-\frac{iE_n}{\hbar}(t-t')}$$

$$= \sum_{n=0}^{\infty} A_n^2 \exp\left(-\frac{m\omega}{2\hbar}(x^2+x'^2)\right) H_n(x) H_n(x')$$

$$\exp\left[-i(n+\tfrac{1}{2})\omega(t-t')\right]$$

Now discuss eigenvalues & eigenfunctions

(1) Energy quantized but $\Delta E = \hbar\omega$, tiny for macroscopic particles + energies look continuous (ω = 1 rad/sec ! $\Delta E \sim 10^{-27}$ erg.)

(2) Levels of energy are spaced evenly. Pretend associated with oscillator of frequency ω there equal fellows particles called quanta of energy $\hbar\omega$. Energy level n has n such quanta.

(3) Lowest possible energy is $\hbar\omega/2$ not zero.

(4) Oscillator solutions contain even or odd power of x dependent on whether n is even or odd

$$\psi_n(-x) = \psi_n(x) \qquad n \text{ even}$$
$$\psi_n(-x) = -\psi_n(x) \qquad n\text{-odd}$$

(5) Wf does not vanish beyond classical turning points but dies off exponentially

Oscillator in the Energy Basis

Recall we solve $\left(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\right)|E\rangle = E|E\rangle$

and solved in coordinate basis. But a neat trick due to Dirac lets us sidestep this. All we need to use is

$$[X, P] = i\hbar I = i\hbar$$

Introduce

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} p$$

$$a^{\dagger} = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} p$$

They satisfy

$$[a, a^{\dagger}] = \frac{-2i}{2\hbar}[X, P] = 1$$

Also note

$$a^{\dagger}a = \left(\frac{m\omega}{2\hbar}\right) X^2 + \frac{1}{2m\omega\hbar} P^2 + \frac{i}{2\hbar}[X, P]$$

$$= \frac{m\omega}{2\hbar} X^2 + \frac{1}{2m\omega\hbar} P^2 - \frac{1}{2}$$

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

$$H = \hbar\omega\left(a^{\dagger}a + \frac{1}{2}\right)$$

now for

$$\hat{H} = \frac{H}{\hbar\omega} = a^{\dagger}a + \frac{1}{2}$$

$$\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle$$ need to solve eigenvalue problem

Now

$$[a, \hat{H}] = [a, a^\dagger a] = [a, a^\dagger] a = a$$

$$[a^\dagger, \hat{H}] = [\hat{H}, a]^\dagger = -a^\dagger$$

Given an eigenstate of $\hat{H}$ the operators $a, a^\dagger$ generate other

$$\hat{H}\, a|\varepsilon\rangle = (a\hat{H} - [a, \hat{H}])|\epsilon\rangle$$

$$= (\epsilon - 1)\, a|\epsilon\rangle$$

So $a|\epsilon\rangle$ is an eigenstate with energy $\epsilon - 1$

$$a|\epsilon\rangle = C_\epsilon |\epsilon - 1\rangle$$

Similarly

$$\hat{H} a^\dagger|\epsilon\rangle = (a^\dagger \hat{H} - [a^\dagger, \hat{H}])|\epsilon\rangle$$

$$= (\epsilon + 1)\, a^\dagger|\epsilon\rangle$$

$$a^\dagger|\epsilon\rangle = C_{\epsilon+1} |\epsilon + 1\rangle$$

So, if energy eigenvalue of $\hat{H}$ so a $\epsilon+1, \epsilon+2, \ldots \epsilon+\infty$ and $\epsilon-1, \epsilon-2, \ldots \epsilon-\infty$. But latter contradicts conclusion that energy eigenvalues non negative so there must be a ground state $|\epsilon_0\rangle$ such that

$$a|\epsilon_0\rangle = 0 \qquad |\varepsilon_0\rangle = |0\rangle$$

Operating with $a^\dagger$ on $\quad a^\dagger a|\epsilon_0\rangle = 0$

$$(\hat{H} - \tfrac{1}{2})|\epsilon_0\rangle = 0\,, \quad \hat{H}|\epsilon_0\rangle = \tfrac{1}{2}|\epsilon_0\rangle$$

$\epsilon_0 = 1/2$. Then raise energy with a^+ acting to get $|n\rangle$'s.

$$\epsilon_n = (n+1/2)$$

$$E_n = (n+1/2)\hbar\omega$$

If another series it would also have state

$$a^+|\epsilon_0'\rangle = 0$$

$$a^+a|\epsilon_0'\rangle = 0$$

$$\hat{H}|\epsilon_0'\rangle = \tfrac{1}{2}|\epsilon_0'\rangle$$

But no degeneracy in 1-dim so $|\epsilon_0'\rangle = |\epsilon_0\rangle$

Next lets get the constant

$$a|n\rangle = C_n|n-1\rangle$$

$$\langle n|a^+ = \langle n-1|C_n^*$$

$$\langle n|a^+a|n\rangle = \langle n-1|n-1\rangle C_n^*C_n = C_n^*C_n$$

States chosen normalized so

$$\langle n|\hat{H}-\tfrac{1}{2}|n\rangle = C_n^*C_n$$

$$\therefore n = |C_n|^2$$

$$C_n = \sqrt{n}\,\underbrace{e^{i\phi}}_{\text{arbitrary}} \quad \text{choose } \phi = 0$$

$$a|n\rangle = n^{1/2}|n-1\rangle$$

Similarly

$$a^+|n\rangle = (n+1)^{1/2}|n+1\rangle$$

Since that

$$a^+a|n\rangle = n^{1/2}a^+|n-1\rangle = n|n\rangle$$

Operator

$$N = a^+a$$

called number operator

$$\hat{H} = N + 1/2$$

Now for the a^+, a and eigenstates

$$\langle n'|a|n\rangle = n^{1/2}\langle n'|n-1\rangle = n^{1/2}\delta_{n',n-1}$$

$$\langle n'|a^+|n\rangle = (n+1)^{1/2}\langle n'|n+1\rangle = (n+1)^{1/2}\delta_{n',n+1}$$

There let us find matrix elements of X, P in eigenstates

$$X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^+)$$

$$P = i\left(\frac{m\omega\hbar}{2}\right)(a^+-a)$$

Two basic quantities in energy basis are matrix elem of a^+ + a

$\langle n | a^+ | m \rangle$

$\downarrow$ row   colum

$$
= \begin{array}{c|c}
 & \begin{array}{ccccc} m=0 & m=1 & m=2 & , & \ldots \end{array} \\
\begin{array}{c} n=0 \\ n=1 \\ \vdots \\ \vdots \\ \\ \\ \end{array} &
\begin{bmatrix}
0 & 0 & 0 \\
1^{1/2} & 0 & 0 \\
0 & 2^{1/2} & 0 \\
0 & 0 & 3^{1/2} \\
\vdots & & \\
\vdots & &
\end{bmatrix}
\end{array}
$$

just below diagonal

$\langle n | a | m \rangle$

row $\hookleftarrow$ $\hookrightarrow$ colum

$$
\begin{array}{c|c}
 & \begin{array}{cccccc} m=0 & m=1 & m=2 & m=3 & , & \ldots \end{array} \\
n=0 &
\begin{bmatrix}
0 & 1^{1/2} & 0 & 0 \\
0 & 0 & 2^{1/2} & 0 \\
0 & 0 & 0 & 3^{1/2} \\
0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots
\end{bmatrix}
\end{array}
$$

just above diagonal

$\langle n | x | m \rangle =$

$$
\left(\frac{\hbar}{2m\omega}\right)^{1/2}
\begin{bmatrix}
0 & 1^{1/2} & 0 & 0 & - - \\
1^{1/2} & 0 & 2^{1/2} & 0 & - - \\
0 & 2^{1/2} & 0 & 3^{1/2} & - \\
0 & 0 & 3^{1/2} & 0 & \\
\vdots & & & &
\end{bmatrix}
$$

$\langle n|p|m\rangle$

$$= i\left(\frac{m\hbar\omega}{2}\right)^{1/2}\begin{bmatrix} 0 & -1^{1/2} & 0 & 0 & \cdots \\ 1^{1/2} & 0 & -2^{1/2} & 0 & \cdots \\ 0 & 2^{1/2} & 0 & -3^{1/2} & \cdots \\ 0 & 0 & 3^{1/2} & 0 & \\ 0 & \vdots & 0 & & \\ 0 & \vdots & \vdots & & \end{bmatrix}$$

$$H = \hbar\omega\begin{bmatrix} 1/2 & & & \\ & 3/2 & & 0 \\ & 0 & 5/2 & \\ & & & \ddots \end{bmatrix}$$

$$|n\rangle = \frac{a^+}{\sqrt{n}}|n-1\rangle$$

$$= \frac{a^+}{\sqrt{n}}\frac{a^+}{\sqrt{n-1}}|n-2\rangle$$

$$= \ldots \frac{(a^+)^n}{(n!)^{1/2}}|0\rangle$$

Note can now compute very easily various matrix elements