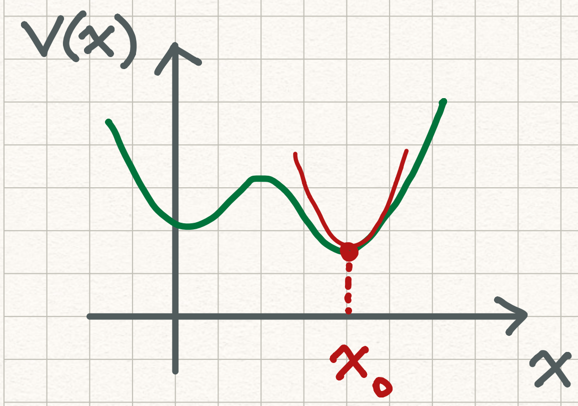
Simple Harmonic Oscillator



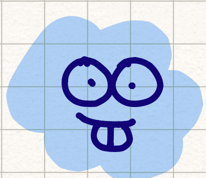
Consider a particle around a stable equilibrium @ $x = x_0$. The potential energy can be approximated as below:

$$V(x) \approx V(x_0) + \frac{1}{2}k(x-x_0)^2$$

Setting the equilibrium point as the origin, the Hamiltonian for the particle is

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

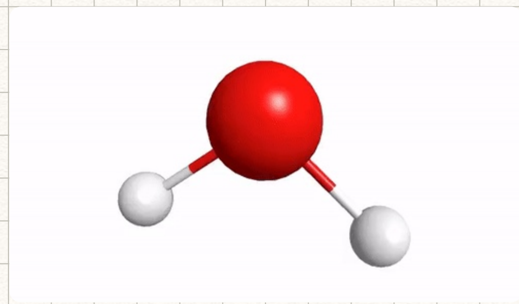
By imposing the commutator $[x, p] = i\hbar$, the quantum SHO is described by exactly the same Hamiltonian.



As the quantization of $\vec{L}$ is dictated by the commutators, quantization of SHO can also be derived from $[x, p] = i\hbar$.

SHO everywhere

How water molecule vibrates differently...



The molecular vibrations can be described by diff. SHOs (normal modes)

The Hamiltonian takes the following form

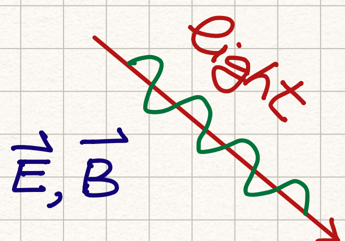
$$H = \sum_{\alpha} \omega_{\alpha} A_{\alpha}^{+} A_{\alpha} \longrightarrow E_{\alpha} = \hbar\omega_{\alpha} \left(n_{\alpha} + \frac{1}{2}\right)$$

normal modes

phonon energy

# of phonons

The EM wave in the free space follows similar dynamics with the quardratic H:



$$H = \int d^3r \, \frac{1}{2}\epsilon_0 E^2 + \frac{1}{2\mu_0} B^2$$

The $\vec{E}$ & $\vec{B}$ fields can be viewed as conjugate variables with similar commutator. $\longrightarrow$ the energy in quantized in the same way

$$E_{\alpha} = \hbar\omega_{\alpha} \left(n_{\alpha} + \frac{1}{2}\right)$$

photon energy

# of photons

Ladder Operators

Introduce a pair of ladder operators $A, A^\dagger$,

$$\boxed{\begin{aligned} A &= \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\, x + i \frac{1}{\sqrt{m\omega}} p\right) \\ A^\dagger &= \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\, x - i \frac{1}{\sqrt{m\omega}} p\right) \end{aligned}}$$

Here $A, A^\dagger$ are Hermitian conjugate to each other.

Consider their products in diff. order ~

$$A^\dagger A = \frac{1}{2} m\omega x^2 + \frac{1}{2m\omega} p^2 + \frac{i}{2} \underbrace{(xp - px)}_{[x,p] = i\hbar}$$

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

$$A A^\dagger = \frac{1}{2} m\omega x^2 + \frac{1}{2m\omega} p^2 - \frac{i}{2} \underbrace{(xp - px)}_{[x,p] = i\hbar}$$

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

Combine the above products together:

$$[A, A^\dagger] = AA^\dagger - A^\dagger A = \hbar$$

$$H = \frac{\omega}{2}\left(A^\dagger A + AA^\dagger\right)$$

One can compute the commutators between H and the ladder operators $A, A^\dagger$

$$[H, A] = [\tfrac{1}{2}\omega(A^\dagger A + AA^\dagger), A]$$

$$= \tfrac{1}{2}\omega\,[A^\dagger A, A] + \tfrac{1}{2}\omega\,[AA^\dagger, A]$$

$$= \tfrac{1}{2}\omega\,\underbrace{[A^\dagger, A]}_{-\hbar}\,A + \tfrac{1}{2}\omega\,A\,\underbrace{[A^\dagger, A]}_{-\hbar}$$

$$\rightarrow \quad [H, A] = -\hbar\omega A \quad \text{or} \quad HA = A(H - \hbar\omega)$$

Taking Hermitian conjugate of the above,

$$(HA - AH)^\dagger = -\hbar\omega A^\dagger$$

$$A^\dagger H - HA^\dagger = -\hbar\omega A^\dagger$$

$$\rightarrow \quad [H, A^\dagger] = \hbar\omega A^\dagger \quad \text{or} \quad HA^\dagger = A^\dagger(H + \hbar\omega)$$

These commutators will help us find out the energy spectrum of SHOs.

Positive Semi-Definite Operators

We would like to prove a simple theorem:

If O is a Hermitian operator, for any $|\psi\rangle$, the expectation value $\langle\psi|O^2|\psi\rangle \geq 0$

Introduce a complete orthonormal basis $|n\rangle$

$$\rightarrow \quad \sum_n |n\rangle\langle n| = \mathbb{1}.$$

$$\langle\psi|O^2|\psi\rangle = \langle\psi|O\cdot\mathbb{1}\cdot O|\psi\rangle$$

$$= \sum_n \langle\psi|O|n\rangle\langle n|O|\psi\rangle$$

note that $\langle\psi|O|n\rangle^* = \langle n|O^\dagger|\psi\rangle = \langle n|O|\psi\rangle$

$$\rightarrow \quad \langle\psi|O^2|\psi\rangle = \sum_n |\langle\psi|O|n\rangle|^2 \geq 0$$

Q.E.D.

The Hamiltonian of a SHO is quadratic,

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

Both p^2 and x^2 are positive semi-definite,

so, $\langle\psi|H|\psi\rangle \geq 0$

Energy Spectrum

Start with the eigen equation for SHO

$$H|n\rangle = \underbrace{E_n}_{\text{eigenvalue}}\underbrace{|n\rangle}_{\text{eigenstate}} \quad \text{and} \quad \langle n|m\rangle = \delta_{nm}$$

Construct the state $|\psi\rangle = A|n\rangle$

$$H|\psi\rangle = HA|n\rangle = A(H-\hbar\omega)|n\rangle$$

$$= A(E_n-\hbar\omega)|n\rangle$$

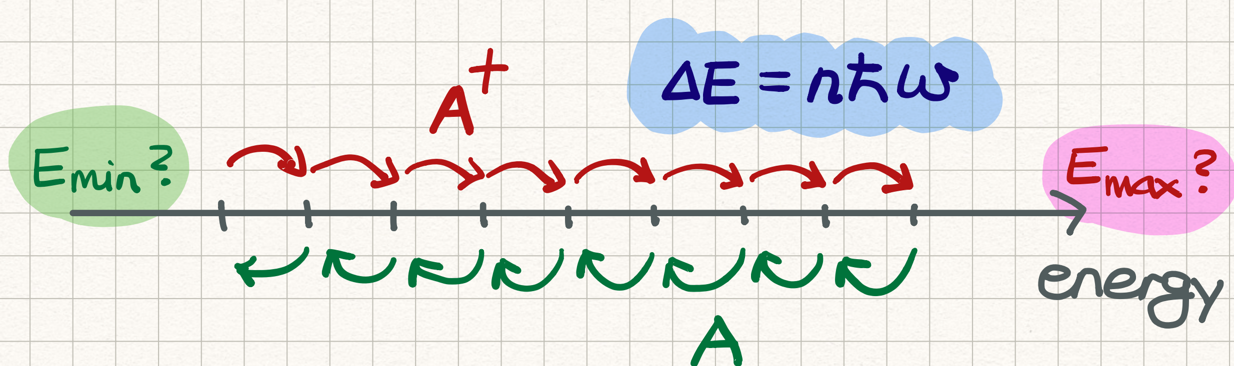
$$= (E_n-\hbar\omega)A|n\rangle = (E_n-\hbar\omega)|\psi\rangle$$

The constructed state $|\psi\rangle = A|n\rangle$ is still an eigenstate but the energy reduces $\hbar\omega$.

Similarly, one can construct $|\phi\rangle = A^{+}|n\rangle$

$$H|\phi\rangle = HA^{+}|n\rangle = A^{+}(H+\hbar\omega)|n\rangle$$

$$= A^{+}(E_n+\hbar\omega)|n\rangle = (E_n+\hbar\omega)|\phi\rangle$$



Because $\langle\psi|H|\psi\rangle \geq 0$, the energy must have a lowest value E_0 with corresponding eigenstate $|0\rangle$. But, the energy-lowering rule still holds ~

$$H A|0\rangle = (E_0 - \hbar\omega) A|0\rangle$$

To be consistent, we must have that $A|0\rangle = 0$.

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

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

Since $A|0\rangle = 0$, $A^\dagger A|0\rangle = 0$. Thus,

$$H|0\rangle = \omega\left(A^\dagger A + \frac{1}{2}\hbar\right)|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$$

The ground-state energy of a SHO is $E_0 = \frac{1}{2}\hbar\omega$. Since the energy changes are in units of $\hbar\omega$ ($\Delta E = n\hbar\omega$), the energy spectrum is

One can view n as the number of phonons with energy $\hbar\omega$.

$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega} \qquad n = 0, 1, 2, \cdots$$

Finding GS wave function

The ground state $|0\rangle$ is annihilated by the ladder operator A :

$$A|0\rangle = 0 \quad \longrightarrow \quad \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\, x + \frac{ip}{\sqrt{m\omega}}\right)|0\rangle = 0$$

Making use the x-space representation, $p = -i\hbar \frac{\partial}{\partial x}$, the GS wave function satisfies

$$\frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\, x + \frac{\hbar}{\sqrt{m\omega}}\frac{\partial}{\partial x}\right)\phi_0(x) = 0$$

$$\boxed{\frac{d\phi_0}{dx} + \frac{m\omega}{\hbar} x \phi_0 = 0}$$

One can thus solve the above ordinary differential equation (ODE) to find out the GS wave function

$$\phi_0(x) = N_0\, e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$$

The other eigenstates can be obtained as well,

$$\phi_n(x) = N_n \left(\sqrt{\frac{m\omega}{2}}\, x - \frac{\hbar}{\sqrt{2m\omega}}\frac{\partial}{\partial x}\right)^n \phi_0(x)$$

normalization const. $\quad\quad$ $\in (A^+)^n$ in x-space.