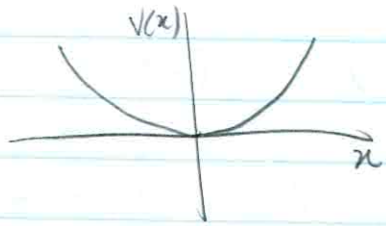
Lecture #15

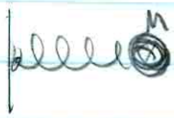
Quantum waves : Phonons

Quantum Harmonic oscillator

See e.g. Chapter 5 of "Quantum Mechanics" by Cohen-Tannoudji.

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 x^2$$





$$\omega_0 = \sqrt{\frac{k}{m}}$$

Classical to quantum : $\begin{cases} x \to \hat{x} \\ p \to \frac{\hbar}{i}\frac{\partial}{\partial x} \end{cases}$ $\qquad [x, p] = i\hbar$

Define dimensionless operators:

$$\begin{cases} \hat{x} = \frac{x}{\ell} \; ; \; \ell = \sqrt{\frac{\hbar}{m\omega_0}} \quad \text{"length scale" or harmonic potential.} \\ \hat{p} = \frac{p}{\left(\frac{\hbar}{\ell}\right)} \end{cases}$$

$$\Rightarrow H = \underbrace{\frac{1}{2m}\frac{\hbar^2}{\ell^2}}_{\frac{1}{2}\frac{1}{m}\frac{\hbar^2}{\frac{\hbar}{m\omega_0}}} \hat{p}^2 + \underbrace{\frac{1}{2} m \omega_0^2 \ell^2}_{\frac{1}{2} m \omega_0^2 \frac{\hbar}{m\omega_0}} \hat{x}^2 = \frac{1}{2}\hbar\omega_0 \left(\hat{x}^2 + \hat{p}^2\right) \qquad \text{and } [\hat{x}, \hat{p}] = i$$

Define creation and destruction operators : $\begin{cases} \hat{a} = \frac{1}{\sqrt{2}}\left(\hat{x} + i\hat{p}\right) \\ \hat{a}^{+} = \frac{1}{\sqrt{2}}\left(\hat{x} - i\hat{p}\right) \end{cases}$

From $[\hat{x}, \hat{p}] = i$ we get

$$[a, a^{+}] = 1$$

②

$$\hat{a}^\dagger \hat{a} = \frac{1}{2}(\hat{x} - i\hat{p})(\hat{x} + i\hat{p}) = \frac{1}{2}\Big\{ \hat{x}^2 + \underbrace{i\hat{x}\hat{p} - i\hat{p}\hat{x}}_{i[\hat{x},\hat{p}] = -1} + \hat{p}^2 \Big\} = \frac{1}{2}(\hat{x}^2 + \hat{p}^2) - \frac{1}{2}$$

$$\Rightarrow \mathcal{H} = \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right)\hbar\omega_0$$

From $[\hat{a}, a^\dagger] = 1$ prove (See Cohen-Tannoudji) that the eigenstates of $\hat{a}^\dagger\hat{a}$ are $|N\rangle$ where

$$\hat{a}^\dagger \hat{a}\,|N\rangle = N\,|N\rangle$$ "Fock states"

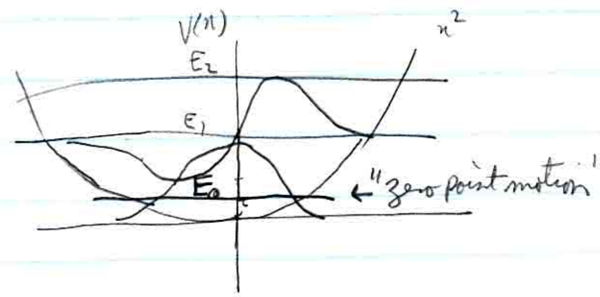
and
$$\begin{cases} \hat{a}\,|N\rangle = \sqrt{N}\,|N-1\rangle \\ \hat{a}^\dagger\,|N\rangle = \sqrt{N+1}\,|N+1\rangle \end{cases}$$

$\hat{a}$ is the "destruction operator"

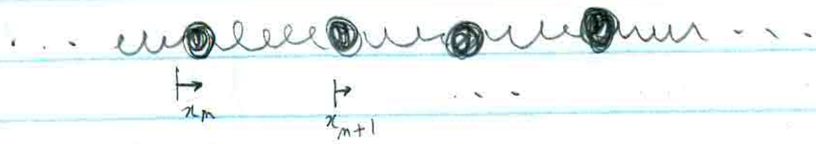
"$a^\dagger$ is the creation operator".

Hence $\mathcal{H}|N\rangle = \left(N + \frac{1}{2}\right)\hbar\omega_0$

▶ Equally spaced levels.



Phonons



$$H = \sum_n \left[\frac{1}{2m} p_n^2 + \frac{1}{2} K \left(x_n - x_{n-1} \right)^2 \right]$$

$$x_n(t) = \mathrm{Re}\left\{ x_0 e^{i(kan - \omega_k t)} \right\} \Rightarrow \omega_k = \omega_0 \left| \sin\left(\frac{ka}{2}\right) \right|$$

$$\omega_0 = 2\sqrt{\frac{K}{m}} \text{ here}$$

Let's decouple this Hamiltonian by rewriting it in terms of normal modes:

$$\begin{cases} x_k = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{n=1}^{N} x_n e^{-ikan} \\ p_k = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{n=1}^{N} p_n e^{-ikan} \end{cases} \qquad \begin{cases} x_{n+N} = x_N \Rightarrow e^{-ikaN} = 1 \\ k = \dfrac{2\pi}{Na} \nu, \quad \nu = -\dfrac{N}{2}, -\dfrac{N}{2}+1, \dots, \dfrac{N}{2} \\ k = -\dfrac{\pi}{a}, -\dfrac{\pi}{a} + \dfrac{2\pi}{Na}, \dots, \dfrac{\pi}{a} \quad (1^{st}\ BZ) \end{cases}$$

Inverse relation:

$$\begin{cases} x_n = \dfrac{1}{\sqrt{N}} \displaystyle\sum_k x_k e^{ikan} \\ p_n = \dfrac{1}{\sqrt{N}} \displaystyle\sum_k p_k e^{ikan} \end{cases}$$

Proof:

$$x_n = \frac{1}{\sqrt{N}} \sum_k x_k e^{ikan} = \frac{1}{\sqrt{N}} \sum_k e^{ikan} \frac{1}{\sqrt{N}} \sum_{n'} x_{n'} e^{-ikan'} = \sum_{n'} \underbrace{\left(\frac{1}{N} \sum_k e^{ika(n-n')} \right)}_{\delta_{n,n'}} x_{n'}$$

$$= x_n$$

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Plug into $\mathcal{H}$:

$$\mathcal{H} = \sum_n \left\{ \frac{1}{2m}\left[\frac{1}{N}\sum_{k,k'} p_k p_{k'} e^{i(k+k')an}\right] + \frac{1}{2}K\left(\frac{1}{\sqrt{N}}\sum_k x_k\left(1-e^{-ika}\right)\right)\left(\frac{1}{\sqrt{N}}\sum_{k'} x_{k'}\left(1-e^{-ik'a}\right)\right) \times e^{i(k+k')an} \right.$$

$$= \frac{1}{2m}\sum_{k,k'} p_k p_{k'} \underbrace{\left(\frac{1}{N}\sum_n e^{ima(k+k')}\right)}_{\delta_{k',-k}} + \frac{1}{2}K \sum_{k,k'} x_k x_{k'} \left(1-e^{-ika}\right)\left(1-e^{-ik'a}\right)\delta_{k',-k}$$

$$= \frac{1}{2m}\sum_k p_k^2 + \frac{1}{2}K\sum_k x_k x_{-k} \underbrace{\left(1-e^{-ika}\right)\left(1-e^{ika}\right)}_{4\sin^2\left(\frac{ka}{2}\right)}$$

$$x_{-k} = x_k^* = x_k \quad (x \text{ is real})$$

$$\boxed{\mathcal{H} = \frac{1}{2m}\sum_k p_k^2 + \frac{1}{2}m\sum_k \omega_k^2 x_k^2}$$

$$\omega_k^2 = \frac{4K}{m}\sin^2\left(\frac{ka}{2}\right) \Rightarrow \omega_k = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|.$$ (Identical to classical result!)

For each k,
Define $\hat{a}_k = \frac{1}{\sqrt{2}}\left(\frac{x_k}{\sqrt{\frac{\hbar}{m\omega_k}}} + \frac{p_k}{\sqrt{\hbar m\omega_k}}\right)$ <u>Note</u>: $[\hat{a}_k, a^\dagger_{k'}] = \delta_{k,k'}$

$$\Rightarrow \boxed{\mathcal{H} = \sum_k \hbar\omega_k\left(\hat{a}^\dagger_k \hat{a}_k + \frac{1}{2}\right)}$$

$$\mathcal{H}|\ldots, n_k, n_{k'}, \ldots\rangle = \underbrace{\sum_k \hbar\omega_k\left(n_k + \frac{1}{2}\right)}_{\text{Energy}} |\ldots, n_k, \ldots\rangle$$

$$|\ldots, n_k, n_{k'}, \ldots\rangle = |n_k\rangle|n_{k'}\rangle|n_{k''}\rangle|n_{k'''}\rangle \ldots$$