Approach 2: Operator Method

- Included here for its beauty and conceptual implications
- Many ideas are essential for studying advanced QM (e.g. QFT)
- In Exams, only fundamentals will be tested. Detailed manipulations are not necessary.

Harmonic Oscillator (Approach 2): Operator Method

Background/Motivation: Schrödinger solved HO by TISE

$[\hat{p} \to \frac{\hbar}{i}\frac{d}{dx}$, $\hat{x} \to x$ then TISE $\to$ Done$]$

Dirac: What is really important is $[\hat{x}, \hat{p}] = i\hbar$

[Other ways of solving HO?]

(Slightly deeper) Heisenberg and Born: QM can be done in Matrices

$$\left.\begin{array}{l}\text{Energy eigenvalues} \\ \text{are } (n+\tfrac{1}{2})\hbar\omega_0 \\ (n = 0, 1, 2, \cdots) \\ \text{[infinitely many]}\end{array}\right\} \begin{array}{l}\text{first learned} \\ \text{eigenvalues} \\ \text{from Matrices}\end{array} \left\{ \overleftrightarrow{H} = \begin{pmatrix} \frac{1}{2}\hbar\omega_0 & & & \\ & \frac{3}{2}\hbar\omega_0 & & \\ & & \frac{5}{2}\hbar\omega_0 & \\ & & & \ddots \end{pmatrix} \right.$$

"$\infty \times \infty$" Matrix

The Problem: Solve $\hat{H}\psi = E\psi$

$$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{x}^2} \qquad (1)$$

- <u>Introduce two new operators</u>

$$\hat{a} \equiv \sqrt{\frac{m\omega_0}{2\hbar}}\,\hat{x} + i\sqrt{\frac{1}{2\hbar m\omega_0}}\,\hat{p} = \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega_0}\hat{p}\right) \qquad (2)$$

$$\hat{a}^+ \equiv \sqrt{\frac{m\omega_0}{2\hbar}}\,\hat{x} - i\sqrt{\frac{1}{2\hbar m\omega_0}}\,\hat{p} = \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega_0}\hat{p}\right) \qquad (3)$$

You may wonder <u>why</u>? Stay tuned!

- This is similar to factorizing (1), $(c^2+d^2) = (c-id)(c+id)$
- The notation $\hat{a}^+$ [the "+"] has a deeper meaning in mathematics. For the present purpose, take (3) as definition of $\hat{a}^+$

$$\hat{a}^{+}\hat{a} = \frac{m\omega_0}{2\hbar}\left(\hat{x} - \frac{i}{m\omega_0}\hat{p}\right)\left(\hat{x} + \frac{i}{m\omega_0}\hat{p}\right)$$

$$= \frac{m\omega_0}{2\hbar}\left(\hat{x}^2 + \frac{1}{m^2\omega_0^2}\hat{p}^2 + \frac{i}{m\omega_0}\overbrace{(\hat{x}\hat{p} - \hat{p}\hat{x})}^{[\hat{x},\hat{p}] = i\hbar}\right)$$

[ordering of operators is important]

$$= \frac{\hat{p}^2}{2\hbar m\omega_0} + \frac{m\omega_0}{2\hbar}\hat{x}^2 - \frac{1}{2}$$

[first two terms resemble $\hat{H}$]

$$= \frac{1}{\hbar\omega_0}\left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2\right] - \frac{1}{2}$$

$$= \frac{1}{\hbar\omega_0}\hat{H} - \frac{1}{2}$$

$$\therefore \quad \boxed{\hat{H} = \hbar\omega_0\left(\hat{a}^{+}\hat{a} + \frac{1}{2}\right)} \qquad (4)$$

- $\frac{1}{2}\hbar\omega_0$ is ground state energy
- $\hat{H}$ is "factorized" into $(\hat{a}^{+}\hat{a})$

Commutators: $[\hat{a}, \hat{a}^+] = \frac{m\omega_0}{2\hbar}\left[\hat{x} + \frac{i}{m\omega_0}\hat{p}, \hat{x} - \frac{i}{m\omega_0}\hat{p}\right] = 1$ (5) (Ex.)

[using $[\hat{A}, \hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$, & $[\hat{x},\hat{p}] = i\hbar$]

$[\hat{a}, \hat{a}] = 0$, $[\hat{a}^+, \hat{a}^+] = 0$ (6)

[At this point, we have all we need about $\hat{a}$, $\hat{a}^+$, $\hat{H}$ to move on.]

- Look at $\hat{H}$, it has $(\hat{a}^+\hat{a})$ as a combination

(7) $[\hat{a}, \hat{a}^+\hat{a}] = \hat{a}^+\cancel{[\hat{a},\hat{a}]}^{\,0} + \overbrace{[\hat{a},\hat{a}^+]}^{1}\hat{a} = \hat{a}$ (LHS is $[\hat{a}, \frac{1}{\hbar\omega_0}\hat{H}]$)

(8) $[\hat{a}^+, \hat{a}^+\hat{a}] = \hat{a}^+[\hat{a}^+, \hat{a}] = -\hat{a}^+[\hat{a}, \hat{a}^+] = -\hat{a}^+$ (LHS is $[\hat{a}^+, \frac{1}{\hbar\omega_0}\hat{H}]$)

[(7) and (8) give the most important properties, as we see next]

Convenient to define $\boxed{\hat{N} \equiv \hat{a}^{+}\hat{a} \quad (9)}$ (will be called "number operator")

$$\therefore \quad \boxed{\hat{H} = \hbar\omega_0 \left(\hat{N} + \frac{1}{2}\right)} \quad (10) \qquad \text{OR} \quad \frac{\hat{H}}{\hbar\omega_0} = \underbrace{\hat{N} + \frac{1}{2}}_{\text{no units (just numbers)}}$$

- $\hat{N}$ has its eigenvalue problem
- Its eigenvalues are numbers

Write eigenvalue problem of $\hat{N}$ as

$$\hat{N}\,|n\rangle = n\,|n\rangle \quad (11)$$

eigenvalue

eigenstate associated with eigenvalue n

c.f. $$\underbrace{\hat{A}\,\phi_n = A_n\,\phi_n}_{\text{OR}} \ \text{(same)}$$

$$\hat{A}\,|\phi_n\rangle = A_n\,|\phi_n\rangle$$

- From Eq.(10) and Eq.(11), eigenstates of $\hat{N}$ are also energy eigenstates, i.e. also eigenstates of $\hat{H}$

(12)

$$\hat{H}|n\rangle = \hbar\omega_0\left(\hat{N}+\frac{1}{2}\right)|n\rangle = \underbrace{\hbar\omega_0\left(n+\frac{1}{2}\right)}_{\text{energy eigenvalues } E_n}\overbrace{|n\rangle}^{\text{also eigenstate of } \hat{H}} = E_n|n\rangle$$

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega_0$$

[started to "make sense"! <u>But what values of n?</u>]

remaining question

- Now, Eqs.(7), (8) enter!

<u>Key idea:</u> If $|n\rangle$ is an eigenstate, $(\hat{a}|n\rangle)$ and $(\hat{a}^{+}|n\rangle)$ <u>Generate</u> other energy eigenstates

This is really why $\hat{a}$, $\hat{a}^{+}$ were introduced!

Let's see why. $\hat{H}|n\rangle = E_n \underbrace{|n\rangle}_{\text{normalized}}$ $\quad E_n = (n+\frac{1}{2})\hbar\omega_0$

Want to find $\hat{H}(\hat{a}|n\rangle) = ?$ (Will it generate another eigenstate?)

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

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

$$= \hat{a}E_n|n\rangle - \hbar\omega_0\hat{a}|n\rangle \quad \left(\text{see (7)}, [\hat{a}, \tfrac{1}{\hbar\omega_0}\hat{H}] = [\hat{a}, \hat{a}^\dagger\hat{a}] = \hat{a}\right)$$

$$= \underbrace{(E_n - \hbar\omega_0)}_{\substack{\text{energy eigenvalue} \\ \text{lowered by } \hbar\omega_0}}\underbrace{(\hat{a}|n\rangle)}_{\text{another energy eigenstate}} \qquad (13)$$

$\therefore$ $\hat{a}$ takes an eigenstate of energy E_n and turns it into another eigenstate of energy $(E_n - \hbar\omega_0)$ ["one $\hbar\omega_0$ lower" in energy]

But $E_n - \hbar\omega_0 = n\hbar\omega_0 + \frac{1}{2}\hbar\omega_0 - \hbar\omega_0 = \underbrace{\left[(n-1) + \frac{1}{2}\right]\hbar\omega_0}_{\text{this is } E_{n-1} \text{ of } |n-1\rangle}$

- Formally, $\hat{H}|n-1\rangle = E_{n-1}|n-1\rangle$. We also saw $\hat{H}(\hat{a}|n\rangle) = E_{n-1}(\hat{a}|n\rangle)$.

  $\therefore$ $(\hat{a}|n\rangle)$ is proportional to $|n-1\rangle$

  Thus $\hat{a}|n\rangle = \underbrace{C_n}_{\text{to be determined}} |n-1\rangle = \underbrace{\sqrt{n}}_{\text{the result}^{+}} |n-1\rangle$ (14)

Names of $\hat{a}$: "lowering operator" [it lowers energy eigenvalue by $\hbar\omega_0$]

"destruction" or "annihilation" operator [it "destroys" a quanta $\hbar\omega_0$ of energy]

+ Not proven here. But the result is far more important than its derivation.

Similarly, Want to find $\hat{H}(\hat{a}^+|n\rangle) = ?$ (Will it generate another eigenstate?)

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

$$\therefore\ \hat{H}(\hat{a}^+|n\rangle) = E_n\,\hat{a}^+|n\rangle - [\hat{a}^+, \hat{H}]|n\rangle$$

$$= E_n\,\hat{a}^+|n\rangle - (-\hbar\omega_0\,\hat{a}^+)|n\rangle \quad \left(\text{See Eq. (8)}, \left[\hat{a}^+, \frac{\hat{H}}{\hbar\omega_0}\right] = [\hat{a}^+, \hat{a}^+\hat{a}] = -\hat{a}^+\right)$$

$$= \underbrace{(E_n + \hbar\omega_0)}_{\substack{\text{energy eigenvalue} \\ \text{raised by } \hbar\omega_0}}\ \underbrace{(\hat{a}^+|n\rangle)}_{\text{generates another energy eigenstate}} \qquad (15)$$

Names of $\hat{a}^+$: "raising operator" (it raises energy eigenvalue by $\hbar\omega_0$)

"creation operator" (it "creates" a quanta $\hbar\omega_0$ of energy)

$\boxed{\hat{a}^+ \text{ takes } |n\rangle \text{ (energy } E_n) \text{ and turns it into another energy eigenstate of energy } (E_n + \hbar\omega_0)}$

But $E_n + \hbar\omega_0 = \left[(n+1) + \frac{1}{2}\right]\hbar\omega_0$, which is E_{n+1} of $|n+1\rangle$

$\therefore$ $\hat{a}^\dagger|n\rangle$ is a state that is proportional to $|n+1\rangle$

Thus

$$\boxed{\hat{a}^\dagger|n\rangle = \underbrace{C'_n}_{\text{to be determined}}|n+1\rangle = \underbrace{\sqrt{n+1}}_{\text{the result (not proven here)}}\,|n+1\rangle \qquad (16)}$$

Take Eq.(14) and Eq.(16) as some "reserved results" for the time being. We don't need them to get the oscillator's E_n.

Eq.(14) $\Rightarrow$ $$\frac{\hat{a}}{\sqrt{n}}|n\rangle = \underbrace{|n-1\rangle}_{\text{normalized}} \qquad (14')$$

Eq.(16) $\Rightarrow$ $$\frac{\hat{a}^\dagger}{\sqrt{n+1}}|n\rangle = \underbrace{|n+1\rangle}_{\text{normalized}} \qquad (16')$$

- <u>What do we have?</u>

If E_n is an energy eigenvalue of $\hat{H}$, so are

"to very negative" $\leftarrow$ $\cdots, E_n - 2\hbar\omega_0, E_n - \hbar\omega_0, E_n, E_n + \hbar\omega_0, E_n + 2\hbar\omega_0, E_n + 3\hbar\omega_0, \cdots$ (17)

- But for Oscillator $U(x)$, <u>E_n cannot be negative</u> (18)

<u>Any contradiction?</u>

(17) and (18) are <u>consistent</u> if (17) breaks at some point

<u>How?</u> Physically, there must be a state (ground state) that it cannot be further lowered.

$\therefore$ Some $\underbrace{|n_{min}\rangle}_{\text{ground state}}$ such that $\hat{a}|n_{min}\rangle = 0$ [statement of "can't be further lowered"] (19)

Operating with $\hat{a}^+$, $\hat{a}^+\hat{a}|n_{min}\rangle = 0$ OR $\hat{N}|n_{min}\rangle = 0 = \underset{\text{eigenvalue } n_{min}=0}{0}|n_{min}\rangle$

$\therefore$ $\boxed{\hat{N} \text{ has } 0 \text{ as its } \underline{\text{minimum eigenvalue}}}$ (20)

Label this state by $|0\rangle$ (because its eigenvalue n is "0")

$$\hat{H}|0\rangle = \hbar\omega_0\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)|0\rangle = \frac{1}{2}\hbar\omega_0|0\rangle$$

$\therefore$ $|0\rangle$ is also an eigenstate of $\hat{H}$ associated with energy $\frac{1}{2}\hbar\omega_0$

This $|0\rangle$ is the <u>ground state</u> of energy $\frac{1}{2}\hbar\omega_0$.

- It follows from (17) that the allowed energies of an oscillator are

E_n:	$\frac{1}{2}\hbar\omega_0$,	$\frac{3}{2}\hbar\omega_0$,	$\frac{5}{2}\hbar\omega_0$,	$\frac{7}{2}\hbar\omega_0$,	$\cdots$,	$(n+\frac{1}{2})\hbar\omega_0$,	$\cdots$
n:	0,	1,	2,	3,	$\cdots$,	n,	$\cdots$
State $\|n\rangle$:	$\|0\rangle$,	$\|1\rangle$,	$\|2\rangle$,	$\|3\rangle$,	$\cdots$,	$\|n\rangle$,	$\cdots$

<u>Without</u> solving TISE (differential equation), we obtained the oscillators E_n.

energy

⋮	⋮	⋮
$E_n = (n+\frac{1}{2})\hbar\omega_0$	$\|n\rangle$	$\psi_n(x)$
⋮	⋮	⋮
$E_3 = \frac{7}{2}\hbar\omega_0$	$\|3\rangle$	$\psi_3(x)$
$E_2 = \frac{5}{2}\hbar\omega_0$	$\|2\rangle$	$\psi_2(x)$
$E_1 = \frac{3}{2}\hbar\omega_0$	$\|1\rangle$	$\psi_1(x)$
$E_0 = \frac{1}{2}\hbar\omega_0$	$\|0\rangle$	$\psi_0(x)$
	State	TISE solutions

Same results, of course.

- <u>Is there a way to find $\psi_0(x)$ from operator method?</u>

Short cut: $\hat{a}|0\rangle = 0$ (defines ground state as one that can't be further lowered)

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\,\hat{x} + i\sqrt{\frac{1}{\hbar m\omega_0}}\,\hat{p}\right)$$

$$\rightarrow \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\,x + \sqrt{\frac{\hbar}{m\omega_0}}\,\frac{d}{dx}\right) \quad \text{[Go Schrödinger]}$$

$\therefore$ $\psi_0(x)$ satisfies

$$\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\,x + \sqrt{\frac{\hbar}{m\omega_0}}\,\frac{d}{dx}\right)\psi_0(x) = 0$$

OR $y \equiv \sqrt{\frac{m\omega_0}{\hbar}}\,x$

$$\frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)\psi_0(y) = 0 \qquad (21)$$

$$\Rightarrow \frac{d\psi_0(y)}{\psi_0(y)} = -y\,dy$$

$$\Rightarrow \psi_0(y) = A_0\, e^{-y^2/2} \quad \text{(Solved!)}$$

$$\psi_0(x) = A_0\, e^{-\frac{m\omega_0}{2\hbar}x^2}$$

Done! ("Easier")

How about $\psi_1(x)$? $\quad \hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \quad$ (See (16))

With normalized $|0\rangle$, $\quad \hat{a}^+|0\rangle = \sqrt{0+1}\,|1\rangle = |1\rangle$ (raises energy from $\frac{1}{2}\hbar\omega_0$ to $\frac{3}{2}\hbar\omega_0$)

Meaning: $\hat{a}^+ \rightarrow \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)$, $\psi_1(y)$ is generated by

$$\psi_1(y) = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\psi_0(y)$$

Done! (Will generate $H_1(y)$)

$\therefore$ Starting from $|0\rangle$, <u>repeatedly operating</u> $\hat{a}^+$ leads to $|n\rangle$ ($\psi_n(y)$)

Use (16): $\quad \hat{a}^+|n-1\rangle = \sqrt{n}\,|n\rangle \quad$ OR $\quad |n\rangle = \frac{1}{\sqrt{n}}\hat{a}^+|n-1\rangle$

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

$$= \cdots$$

n^{th} excited state

$E_n = (n+\frac{1}{2})\hbar\omega_0$

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^+)^n|0\rangle} \qquad (22)$$

Ground state ($E_0 = \frac{1}{2}\hbar\omega_0$)

Summary

- Harmonic Oscillator can be solved by operator method
- $\hat{a}$, $\hat{a}^+$ $\qquad \hat{H} = \hbar\omega_0\left(\hat{a}^+\hat{a} + \frac{1}{2}\right) = \hbar\omega_0\left(\hat{N} + \frac{1}{2}\right)$
- $\hat{a}$ ($\hat{a}^+$) lowers (raises) energy of eigenstate by $\hbar\omega_0$
- Non-negative eigenvalues of $\hat{H}$ implies ladder of eigenvalues must break
- Ground state $|0\rangle$ is a state its energy cannot be further lowered

$$\hat{a}|0\rangle = 0$$ [futher applying $\hat{a}$ is still zero $\Rightarrow$ break ladder]

$E_n = \frac{1}{2}\hbar\omega_0$

- All eigenvalues are, therefore, $E_n = (n + \frac{1}{2})\hbar\omega_0$, $n = 0, 1, 2, \ldots$
- $|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$ is a short cut to get eigenstates $|n\rangle$ of energy E_n

By product: "Selection Rule"

- In Schrödinger's approach, we have $\psi_0(x), \psi_1(x), \psi_2(x), \ldots$
- In future applications, we will encounter integrals like

$$\int_{-\infty}^{\infty} \psi_1^*(x) \; x \; \psi_0(x)\, dx$$

different

[e.g. can light induce transition from $|0\rangle$ to $|1\rangle$]

- Short hand notations: $\langle 1 | \hat{x} | 0 \rangle$

Similarly, $\int \psi_1^*(x)\, \psi_1(x)\, dx = \langle 1 | 1 \rangle = 1$ (normalized)

We could have $\langle n' | \hat{a} | n \rangle = \sqrt{n}\langle n' | n-1\rangle$ ($\neq 0$ only when $\underbrace{n' = n-1}_{\text{eigenstates are orthogonal}}$)

$$= \sqrt{n}\, \delta_{n', n-1}$$

$$\langle n' | \hat{a}^{+} | n \rangle = \sqrt{n+1}\, \delta_{n', n+1}$$

$$\int_{-\infty}^{\infty} \psi_{n'}^{*}(x)\, \hat{x}\, \psi_n(x)\, dx = \langle n' | \hat{x} | n \rangle$$

[Will light induce transitions between $|n\rangle$ and $|n'\rangle$?]

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega_0}\hat{p} \right) \quad ; \quad \hat{a}^{+} = \sqrt{\frac{m\omega_0}{\hbar}} \left(\hat{x} - \frac{i}{m\omega_0}\hat{p} \right)$$

Express $\hat{x}$ and $\hat{p}$ in terms of $\hat{a}$ and $\hat{a}^{+}$:

$$\boxed{\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\hat{a} + \hat{a}^{+} \right) \quad ; \quad \hat{p} = -i\sqrt{\frac{\hbar m\omega_0}{2}} \left(\hat{a} - \hat{a}^{+} \right)} \qquad (23)$$

[Key ideas: $\hat{x}$ & $\hat{p}$ consist of $\hat{a}$ and $\hat{a}^{+}$ once

$\hat{a}$ connects states differ by "1" (by $\hbar\omega_0$ in energy)

$\hat{a}^{+}$ connects states differ by "1" (by $\hbar\omega_0$ in energy)

thus $\langle 2 | \hat{x} | 0 \rangle = 0$, $\langle 7 | \hat{x} | 2 \rangle = 0$ without calculations]
etc.

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left[\langle n'|\underbrace{\hat{a}|n\rangle}_{\sqrt{n}\,|n-1\rangle} + \langle n'|\underbrace{\hat{a}^{+}|n\rangle}_{\sqrt{n+1}\,|n+1\rangle}\right]$$

$$= \sqrt{\frac{\hbar}{2m\omega_0}}\left[\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right] \quad \text{Done!}$$

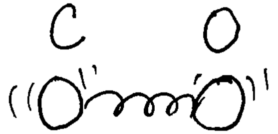
[<u>Much easier</u> than $\int_{-\infty}^{\infty}\psi^{*}_{n'}(x)\,x\,\psi_n(x)\,dx$ for general n', n]

Similarly,

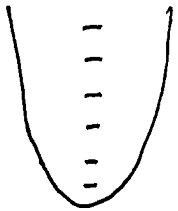
$$\langle n'|\hat{p}|n\rangle = -i\sqrt{\frac{\hbar m\omega_0}{2}}\left[\langle n'|\hat{a}|n\rangle - \langle n'|\hat{a}^{+}|n\rangle\right]$$

$$= -i\sqrt{\frac{\hbar m\omega_0}{2}}\left[\sqrt{n}\,\delta_{n',n-1} - \sqrt{n+1}\,\delta_{n',n+1}\right] \quad \text{Done!}$$

[<u>Much easier</u> than $\int_{-\infty}^{\infty}\psi^{*}_{n'}(x)\,\frac{\hbar}{i}\frac{d}{dx}\,\psi_n(x)\,dx$ for general n', n]

Remark: 

molecule $\Rightarrow$ oscillator



vibrational states are $\hbar\omega_0$ apart

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left[\sqrt{n}\,\underbrace{\delta_{n',n-1}} + \sqrt{n+1}\,\underbrace{\delta_{n',n+1}}\right]$$

$\boxed{\text{Selection Rule}}$ in Spectrum

- Transitions between vibrational states differ by $\Delta n = \pm 1$ are allowed in principle

Magical By-Product: $\infty \times \infty$ Matrices in Oscillator Problem

Take $\langle n' | \hat{x} | n \rangle \equiv x_{n'n} = (n'n)$ Matrix element of X

$\underbrace{n'n}_{\text{two indices}}$ $[n', n = 0, 1, 2, \cdots]$

$$X = \sqrt{\frac{\hbar}{2m\omega_0}} \begin{array}{c|cccccc} & |0\rangle & |1\rangle & |2\rangle & |3\rangle & \cdots & \\ \hline \langle 0| & & & & & & \\ \langle 1| & & & & & & \\ \langle 2| & & & & & & \\ \langle 3| & & & & & & \\ \vdots & & & & & & \end{array} \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots & & \\ \sqrt{1} & 0 & \sqrt{2} & \cdots & & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots & \\ 0 & 0 & \sqrt{3} & 0 & \cdots & \\ & & & & \ddots & \end{pmatrix}$$

An element is $\langle n | \hat{x} | n' \rangle$

$(\infty \times \infty)$ Matrix

$$P = -i\sqrt{\frac{\hbar m\omega_0}{2}} \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots & & \\ -\sqrt{1} & 0 & \sqrt{2} & \cdots & & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \cdots & \\ 0 & 0 & -\sqrt{3} & 0 & \cdots & \\ & & & & \ddots & \end{pmatrix}$$

An element is $\langle n | \hat{p} | n' \rangle$

$(\infty \times \infty)$ Matrix

In this way of expressing $\hat{x}$ and $\hat{p}$ ("in energy basis"),

$$\underset{\text{Matrix}}{H} = \frac{1}{2m}\underset{\text{Matrix}}{P^2} + \frac{1}{2}m\omega_0^2\underset{\text{Matrix}}{X^2} = \frac{\hbar\omega_0}{2}\underbrace{\begin{pmatrix} 1 & & & & \\ & 3 & & 0 & \\ & & 5 & & \\ & 0 & & 7 & \\ & & & & \ddots \end{pmatrix}}_{\underline{\text{eigenvalues}} \text{ of } H \text{ is } (n+\frac{1}{2})\hbar\omega_0} \quad \begin{matrix}(\infty\times\infty)\\ \text{Matrix}\end{matrix}$$

- This was Heisenberg and Born's way of approaching QM oscillator.
- This is the most explicit way of seeing the eigenvalues of $\hat{H}$ and that they correspond to the physically allowed energies

Even More Magical By-Product: A word on Quantum Field Theory

- $\hat{a}$ ($\hat{a}^+$) lowers (raises) energy of a state by $\hbar\omega_0$
- If we regard (which is unnecessary for our oscillator problem) an additional $\hbar\omega_0$ as creating a particle, then $\hat{a}^+$ acts on a state to create one more particle. Similarly, $\hat{a}$ acts to destroy a particle. In this way, we can do QM in a system in which the number of particles is not fixed. We know that situations like this do happen [particle + anti-particle $\rightarrow$ no particle (+ photons)]. We need Quantum Field Theories to handle such cases. Oscillator physics in operator method is the first step towards QFT. In this context, $|0\rangle$ is the "vacuum" state. $\hat{a}|0\rangle = 0$ means can't destroy a particle from vacuum. Make sense!