Appendix A: QM of a harmonic Oscillator

$$H = \frac{P^2}{2M} + \frac{1}{2} M\omega^2 X^2 \qquad (A1)$$

- From classical to quantum mechanics:

  Impose $[\hat{X}, \hat{P}] \equiv \hat{X}\hat{P} - \hat{P}\hat{X} = i\hbar \qquad (A2)$

  (Note: Using $\hat{X} \to X$; $\hat{P} = \frac{\hbar}{i}\frac{\partial}{\partial X}$ is a possible representation)

  Solving the Schrödinger Equation $\Rightarrow \varepsilon_n = (n+\frac{1}{2})\hbar\omega$; $n = 0, 1, 2, \ldots$

- One can also proceed by defining

$$\left.\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2\hbar M\omega}}(M\omega\hat{X} + i\hat{P}) \\ \hat{a}^+ &= \frac{1}{\sqrt{2\hbar M\omega}}(M\omega\hat{X} - i\hat{P}) \end{aligned}\right\} (A3)$$

Just replacing $\hat{X}, \hat{P}$ by $\hat{a}, \hat{a}^+$

$[\hat{a}, \hat{a}^+] = 1$ (A4) (followed from $[\hat{X}, \hat{P}] = i\hbar$)

- Expressing $\hat{X}$ and $\hat{P}$ in terms of $\hat{a}$ and $\hat{a}^+$:

$$\hat{X} = \sqrt{\frac{\hbar}{2M\omega}}(\hat{a}^+ + \hat{a}) \; ; \; \hat{P} = \frac{i}{2}\sqrt{2\hbar M\omega}(\hat{a}^+ - \hat{a}) \quad (A5)$$

- Then $\hat{H}$ can be expressed in terms of $\hat{a}$ and $\hat{a}^+$ as:

$$\hat{H} = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right) \qquad (A6)$$

- Defining $\hat{n} \equiv \hat{a}^+ \hat{a}$,

$$\hat{H} = \hbar\omega\left(\hat{n} + \frac{1}{2}\right) \qquad \text{(A7)}$$

- Energy eigenstates can be written as $|n\rangle$, which denotes the state with energy $(n+\frac{1}{2})\hbar\omega$
- $|n\rangle$ also denotes the state with <u>n excitations</u> ($n=0$, no excitation, i.e. ground state)
- $$\left.\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}\,|n-1\rangle \\ \hat{a}^+|n\rangle &= \sqrt{n+1}\,|n+1\rangle \end{aligned}\right\}\text{(A8)}$$
  ($\therefore$ $\hat{a}$ annihilates one excitation)
  ($\therefore$ $\hat{a}^+$ creates one excitation)
- It follows that $\hat{n}|n\rangle = n|n\rangle$
- $\underbrace{\text{Ground state}}_{|0\rangle}$: $\hat{a}|0\rangle = 0$ (A9) (nothing to annihilate)

  Use Eq. (A3) to write this as a differential equation, one can solve for the ground state wavefunction. Then Eq. (A8) gives the excited states.
- Applying Eq. (A8) repeatedly, the state $|n\rangle$ can be constructed from $|0\rangle$ as:

$$|n\rangle = \frac{1}{\sqrt{n!}} \underbrace{(\hat{a}^+)^n}\, |0\rangle \qquad \text{(A10)}$$

normalization factor

creating n excitations

- For a collection of <u>independent</u> Harmonic Oscillators:

$$\hat{H} = \sum_{\text{oscillators } i} \left(\frac{\hat{P}_i^2}{2M_i} + \frac{1}{2} M_i \omega_i^2 \hat{X}_i^2 \right) \quad \text{(A11)}$$

- For normal modes in a crystal, the modes are labelled by $(s, \vec{q})$

which branch $\to s$; $\vec{q} \in 1^{st}$ B.Z.

$$\hat{H} = \underbrace{\sum_{s} \sum_{\vec{q}}}_{\text{sum over all independent oscillators}} \underbrace{\hbar \omega_s(\vec{q}) \left(\hat{a}_s^{+}(\vec{q})\, \hat{a}_s(\vec{q}) + \frac{1}{2} \right)}_{\text{Carry out Eqs.(A1)-(A6) for each independent oscillator}} \quad \text{(A12)}$$