Appendix D

- **Does a normal mode carry Physical Momentum?**

Back to our 1D monatomic chain example

Physical momentum = Mass · Velocity

$$= \sum_{\text{all atoms } n} M \cdot \frac{du_n}{dt} \qquad (N \text{ atoms}) \quad (N \gg 1)$$

$$u_n = A e^{iqna} e^{-i\omega t} \equiv A(t)\, e^{iqna}$$

$$\therefore \text{Physical momentum} = M \frac{dA}{dt} \underbrace{\sum_{n=0}^{N-1} e^{iqna}}_{\frac{1-e^{iNqa}}{1-e^{iqa}}}$$

This is the same as:

$$\sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} \quad (\text{in } 1D)$$

- but now $\vec{q}$ is in 1^{st} B.Z.

Vanishes except $\vec{q} = \vec{G}$

(i) But for any $\vec{q} \neq 0$ in 1^{st} B.Z., $\vec{q} \neq \vec{G}$

$\therefore$ Physical momentum $= 0$ for any $\vec{q} \neq 0$

The physical reason is that only relative coordinates of the atoms are involved.

(ii) The Only $\vec{G}$ in the 1^{st} B.Z. is $\vec{G} = 0$.

$\therefore$ The $\vec{q} = 0$ mode is an exceptional case.

For $q = 0$ (1D chain),

$$\text{physical momentum} = M \frac{dA}{dt} \overbrace{\sum_{n=0}^{N-1} 1}^{N}$$

$$= MN \frac{dA}{dt}$$

representing a uniform translation of the crystal as a whole.

Remarks:

- Since the physical momentum is different from $\hbar\vec{q}$ and $\hbar\vec{q}$ appears in "selection rules" or "momentum conservation" rules, we call $\hbar\vec{q}$ the crystal momentum of a phonon in the mode $\vec{q}$ (or $(s\vec{q})$ where s labels the branches)
- Recall that when the media is dispersive (i.e. $\omega(\vec{q})$), the velocity of a wave packet is the group velocity:

$$\vec{V}_q = \vec{\nabla}_q\, \omega(\vec{q}) \leftarrow \text{dispersion relation}$$

$\vec{\nabla}_q$: gradient w.r.t. $\vec{q}$

OR $\frac{d\omega}{dq}$ in 1D