

Recap:  $H = \sum_n \frac{p_n^2}{2m_n} + \sum_{nm} \frac{\kappa_{nm}}{2} \underline{g_n g_m}$

- only  $\frac{\kappa_{nm} + \kappa_{mn}}{2}$  appears.  $\kappa_{nm} = (\kappa^T)_{nm}$   
 $\kappa_{nm} \in \mathbb{R}$

- let  $\left\{ \begin{array}{l} Q_n = \sqrt{m_n} g_n \\ P_n = p_n / \sqrt{m_n} \\ V_{nm} = \kappa_{nm} / \sqrt{m_n m_m} \end{array} \right.$   $\Rightarrow \underline{\kappa = \kappa^T}$   
 $[g_n, p_m] = i \delta_{nm}$   
 $\Leftrightarrow [Q_n, P_m] = i \delta_{nm}$

$H = \frac{1}{2} \left( \sum_n P_n^2 + \sum_{nm} V_{nm} Q_n Q_m \right)$

find  $U$  st.  $U V U^T = \text{diagonal}$ .

$\sum_{nm} U_{\alpha n} V_{nm} (U^T)_{m\beta} = \underline{\omega_\alpha^2} \delta_{\alpha\beta}$

$U U^T = \mathbb{1}$  i.e.  $\sum_n U_{\alpha n} (U^T)_{n\beta} = \delta_{\alpha\beta}$

$U^T U = \mathbb{1}$  i.e.  $\sum_\alpha (U^T)_{\alpha n} U_{\alpha m} = \delta_{nm}$   $\star$

normal modes  $\left\{ \begin{array}{l} \tilde{Q}_\alpha \equiv \sum_n U_{\alpha n} Q_n \\ \tilde{P}_\alpha \equiv \sum_n U_{\alpha n} P_n \end{array} \right. \xrightarrow{\star} \left\{ \begin{array}{l} Q_n = \sum_\alpha (U^T)_{n\alpha} \tilde{Q}_\alpha \\ P_n = \sum_\alpha (U^T)_{n\alpha} \tilde{P}_\alpha \end{array} \right.$

$$\begin{aligned}
 Q_n &= Q_n^+ = \sum_{\alpha} (U^+)_{n\alpha}^* \tilde{Q}_{\alpha}^+ \\
 P_n^+ &= \sum_{\alpha} (U^T)_{n\alpha} \tilde{Q}_{\alpha}^+ \\
 &= \sum_{\alpha} \tilde{Q}_{\alpha}^+ U_{\alpha n}
 \end{aligned}$$

Wichtig:

$$\sum_{n,m} V_{nm} Q_n Q_m = \sum_{n,m} V_{nm} Q_n^+ Q_m^+$$

$$= \sum_{\alpha,\beta} \underbrace{U_{\alpha n} V_{nm} (U^+)_{m\beta}}_{= \omega_{\alpha\beta}^2} \tilde{Q}_{\alpha}^+ \tilde{Q}_{\beta}$$

$$= \sum_{\alpha} \omega_{\alpha}^2 \tilde{Q}_{\alpha}^+ \tilde{Q}_{\alpha}$$

$$\sum_n P_n^2 = \sum_n P_n^+ P_n$$

$$= \sum_{\alpha} \sum_{\beta} \underbrace{U_{\alpha n} (U^+)_{n\beta}}_{= \delta_{\alpha\beta}} \tilde{P}_{\alpha}^+ \tilde{P}_{\beta}$$

$$= \sum_{\alpha} \tilde{P}_{\alpha}^+ \tilde{P}_{\alpha}$$

$$= \sum_n P_n \delta_{nm} P_n$$

special case

$$K_{nm} q_n q_m = \sum_n (q_{n+1} - q_n)^2 = \sum_n (\tau - a) q_n^2$$

- local
- transl. inv. :  $K_{nm} q_n q_m$  only depends on  $(q_n - q_m)$ .

$$U_{kn} = \frac{1}{\sqrt{N}} e^{ikna}$$

$$U_{kn}^* = \frac{1}{\sqrt{N}} e^{-ikna} = U_{-k, n}$$

$$Q_n = Q_n^\dagger \Rightarrow \underline{Q_k^\dagger = Q_{-k}}, \quad P_k^\dagger = P_{-k}$$

$$\rightarrow H = \sum_k \left( \tilde{P}_k \tilde{P}_{-k} + \frac{1}{2} m \omega_k^2 \tilde{Q}_k \tilde{Q}_{-k} \right)$$

and  $\omega_k \sim v_s |k|$  for  $k \ll \frac{1}{a}$ .

$$\tilde{Q}_n = \sum_k U_{nk} \tilde{Q}_k$$

$$[Q_n, P_m] = i \delta_{nm}$$

$$[\tilde{Q}_k, \tilde{P}_k] = i \delta_{kk}$$

$$H = \bigotimes_n H_{SHO}^{(n)} = \bigotimes_k H_{SHO}^{(k)}$$

for  $k \neq 0$ :

$$q_k \equiv \sqrt{\frac{\hbar}{2m\omega_k}} (a_k + a_{-k}^\dagger)$$

$$p_k \equiv \frac{1}{i} \sqrt{\frac{\hbar m \omega_k}{2}} (a_k - a_{-k}^\dagger)$$

$$\Leftrightarrow [a_k, a_{k'}^\dagger] = \delta_{kk'}$$

note: the form of  $p$  is fixed by

$$\dot{q}_k = i [H, q_k] = p_k / m$$

$$\Rightarrow H = \sum_k \underbrace{\hbar \omega_k (a_k^\dagger a_k + \frac{1}{2})}_{\text{oscillators}} + \underbrace{\frac{P_0^2}{2m}}_{\text{C.O.M.}}$$

Groundstate:  $a_k |0\rangle_{osc} = 0 \quad \forall k.$

is

$$\hat{P}_0 |p_0\rangle = p_0 |p_0\rangle$$

$$|0\rangle = |0\rangle_{osc} \otimes |p_0=0\rangle$$

Phonons:

$$\underline{a_k^\dagger} |0\rangle = | \text{one phonon of momentum } \hbar k \rangle$$

has energy  $E_0 + \hbar\omega_k$

$$| \hbar k \rangle.$$

$$| \text{one phonon at position } x \rangle = \sum_k e^{ikx} | \hbar k \rangle$$

" $|x\rangle$ ".

$$= \sum_k e^{ikx} a_k^\dagger |0\rangle$$

$$| \text{one phonon w/ wavefunction } \psi(x) \rangle = \int dx \psi(x) |x\rangle$$

$$= \int dx \sum_k e^{ikx} \psi(x) a_k^\dagger |0\rangle$$

$N_k = a_k^\dagger a_k$  counts phonons w/  $k$ .

$$|k, k'\rangle \equiv a_k^\dagger a_{k'}^\dagger |0\rangle$$

2 phonons

$$E = E_0 + \hbar\omega_k + \hbar\omega_{k'} \\ = =$$

A basis for  $\mathcal{H}$  is:

$$(a_{k_1}^+)^{n_{k_1}} (a_{k_2}^+)^{n_{k_2}} \dots |0\rangle \propto |n_{k_1}, n_{k_2}, \dots\rangle$$

$a_k^+$  creates phonons  
 $a_k$  annihilates phonons.

occupation #s.

$$\begin{aligned} |k, k'\rangle &= a_k^+ a_{k'}^+ |0\rangle \\ &\stackrel{n \neq k'}{\sim} = a_{k'}^+ a_k^+ |0\rangle = |k', k\rangle \end{aligned}$$

• phonons are indistinguishable.

• phonons are bosons.

$$\begin{cases} q_n = \sqrt{\frac{\hbar}{2m}} \sum_k \frac{1}{\sqrt{\omega_k}} (e^{ikx} a_k + e^{-ikx} a_k^+) + \frac{q_0}{\sqrt{N}} \\ p_n = \frac{1}{i} \sqrt{\frac{\hbar m}{2}} \sum_k \sqrt{\omega_k} (e^{ikx} a_k - e^{-ikx} a_k^+) + \frac{p_0}{\sqrt{N}} \end{cases}$$

$$\Delta H = \sum_{nml} \lambda_{nml} \underline{q_n q_m q_l}$$

$$= \sum (\underline{a^+ a a^+} + \underline{a a a^+} + \underline{a^+ a a} + \underline{a a a})$$

$$\Delta H = \sum_{n,m \neq 0} g_n g_m g_{-n} g_{-m}$$

$$= \sum (a^\dagger)^4 + \dots \quad \underbrace{a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}} + \dots$$

$$|k_3, k_4\rangle \longrightarrow |k_1, k_2\rangle$$

Gaplessness

$a_k^\dagger |0\rangle$  has energy  $\hbar \omega_k$

$$\Delta E \equiv E_1 - E_0$$

$$= \min_k \hbar \omega_k$$

$$= \frac{\hbar \cdot 2\pi}{L}$$

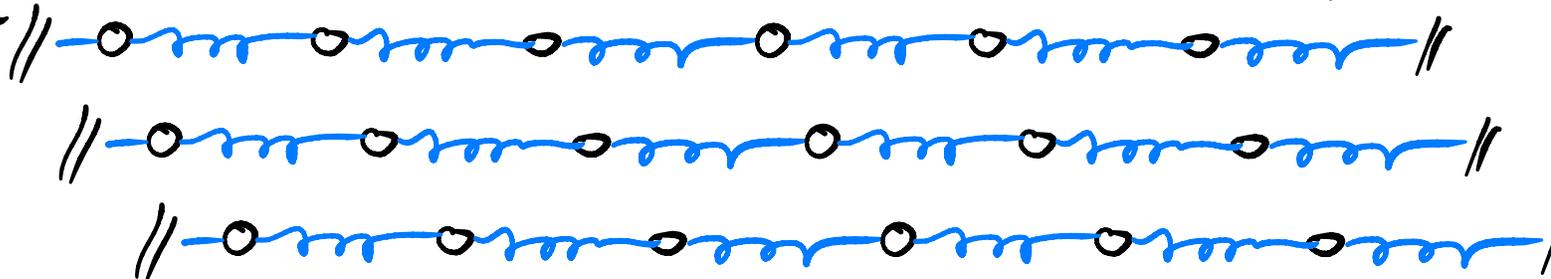
$$\xrightarrow{L \rightarrow \infty} 0$$

$$L = Na$$



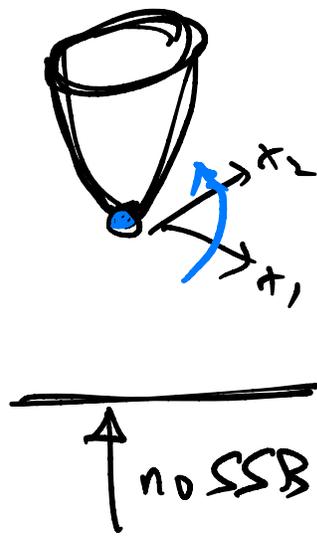
$$k = \frac{2\pi j}{Na} \quad j = 1 \dots N$$

"Energy gap"  $\equiv \Delta E$  is finite as  $L \rightarrow \infty$ .



Goldstone's theorem:

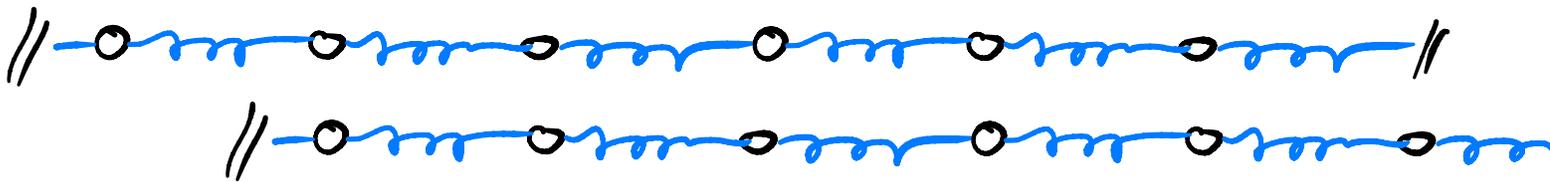
spontaneously breaking  
a continuous symmetry  
→ gapless



Tower of states:

$q_0, p_0$

$$\frac{\partial \mathcal{L}}{\partial q_0} = 0$$



$$|\{q_n\}\rangle \equiv |\{q_n + a\}\rangle$$

$$q_0 = \frac{1}{\sqrt{N}} \sum_{n=1}^N q_n e^{-i0x_n} \equiv \frac{1}{\sqrt{N}} \left( \sum_{n=1}^N q_n + Na \right)$$

$$= q_0 + \sqrt{Na}$$

$$\Rightarrow e^{ip_0 q_0} = e^{ip_0 (q_0 + \sqrt{Na})}$$

$$\Rightarrow p_0 \in \frac{2\pi}{\sqrt{Na}} \mathbb{Z}$$

1st exc. state:

$$\frac{p_0^2}{2m} \Big|_{p_0 = \frac{2\pi\hbar}{\sqrt{Na}}} = \frac{1}{2} \left( \frac{2\pi\hbar}{a} \right)^2 \frac{1}{Nm}$$

$Nm =$  total mass

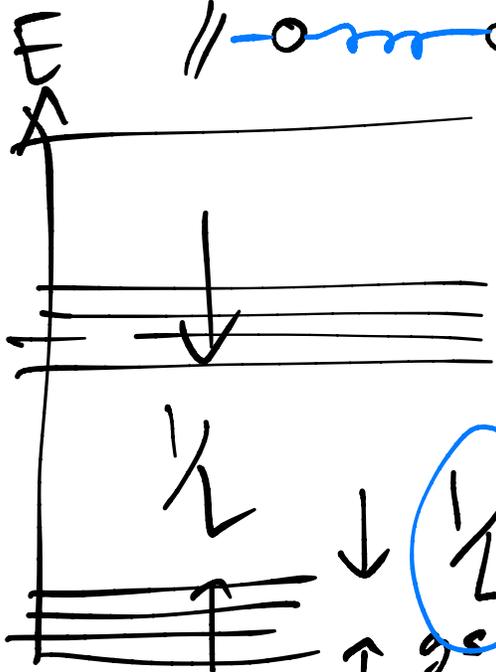
Rigid translation of the whole solid.

$$L = Na$$

more generally:

total mass =  $Nm$

$$N = L^d$$



$$\omega \sim k = \frac{2\pi}{L}$$

Rigid translation.

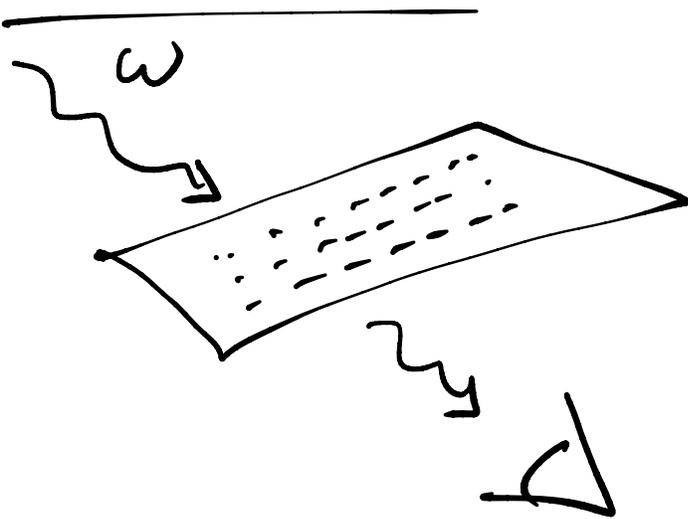
• Heat capacity of solids

$$\langle \hat{H} \rangle_T = \sum_k \langle \hbar \omega a_k^\dagger a_k \rangle + \text{const}$$

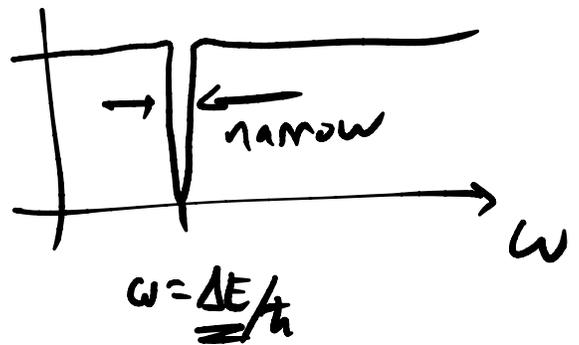
$$C_v = \partial_T E \xrightarrow{T \rightarrow 0} 0$$

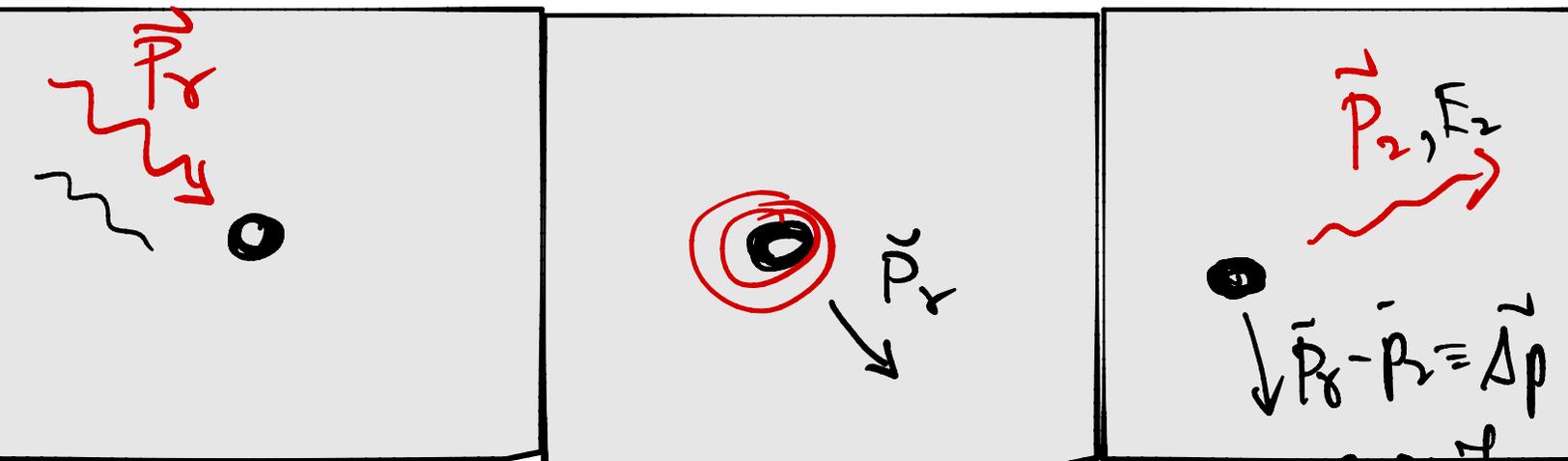


• Mössbauer effect (Bragg scattering...)



Fact:





$$|\vec{p}_r| = E_\gamma / c$$

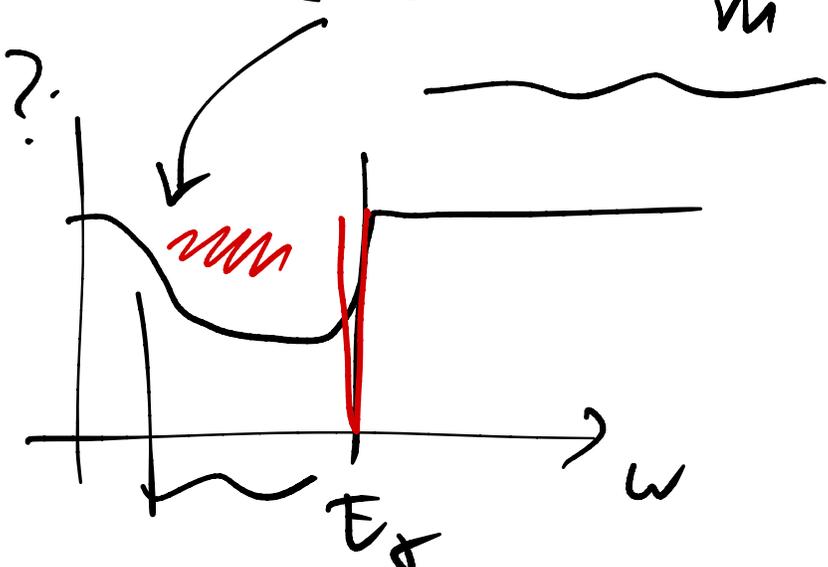
Recoil!

$$E_2 = E_\gamma - \frac{(\Delta p)^2}{2m}$$

KE of atom

$$|\Delta p|_{\max} = 2|p_\gamma|$$

$$E_2 \in \left( E_\gamma - 2 \frac{(E_\gamma / c)^2}{m}, E_\gamma \right)$$



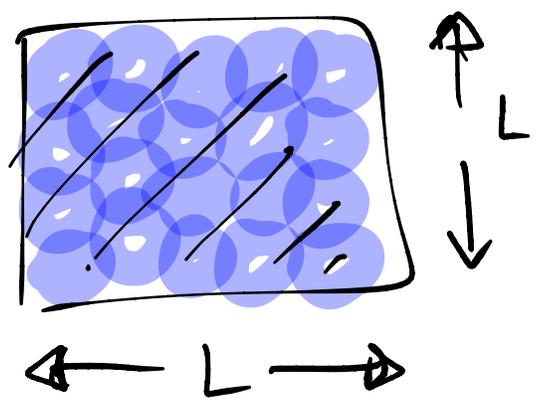
Resolution: Prob (zero phonon process) ≠ 0.

$$E_2 = E_\gamma - \frac{(\Delta p)^2}{2M}$$

$M = Nm$   
 $N \sim 10^{26}$

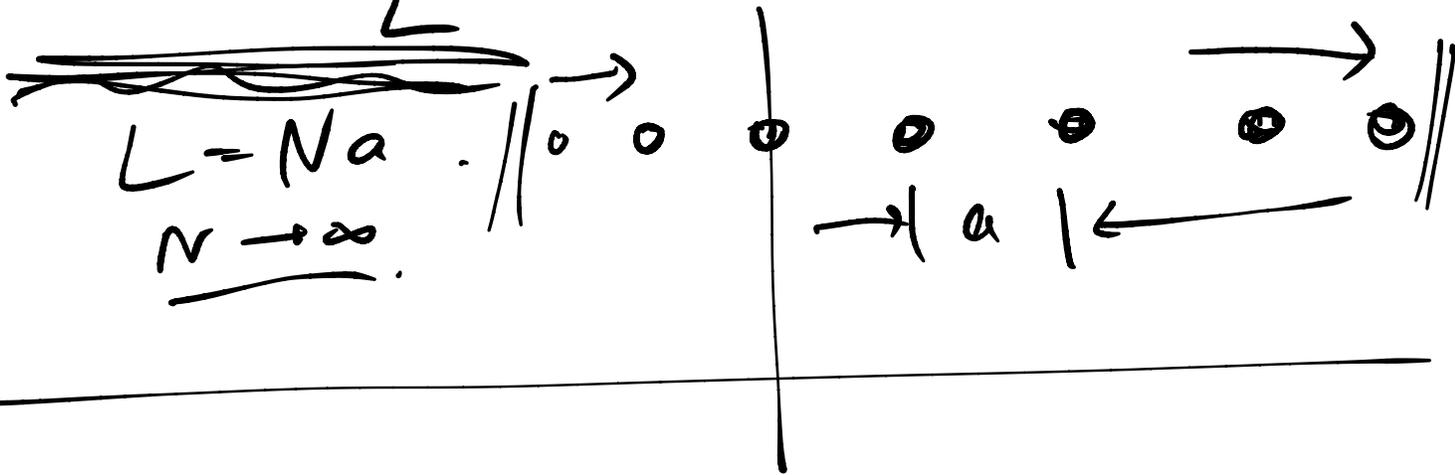
$$\mathcal{H} = \bigotimes_{x \in \text{space}}^L \mathcal{H}_x$$

$$H = \sum_x^L h_x$$

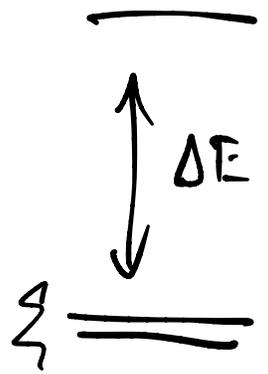


$$\Delta E \equiv E_1 - E_0 \xrightarrow{L \rightarrow \infty} \begin{cases} \text{finite, gap} \\ 0, \text{gaps} \end{cases}$$

$$\Delta E \sim \frac{1}{L} \xrightarrow{L \rightarrow \infty} 0$$



$x=0$



$$\begin{aligned}
 & \sum_n \left( (T - 1) q_n \right)^2 \\
 &= \sum_{kk'} \left[ \sum_n \frac{1}{\sqrt{N}} e^{-ikna - ik'a} \right] \\
 & \quad \left( (T - 1) q_k \right) \left( (T - 1) q_{k'} \right) \\
 & \quad \left( e^{-ika} - 1 \right) q_k \left( e^{-ik'a} - 1 \right) q_{k'} \\
 &= \sum_k q_k q_{-k} \left[ \left( e^{-ika} - 1 \right) \left( e^{+ika} - 1 \right) \right] \\
 \omega_k^2 &= \left( e^{-\frac{ika}{2}} - e^{\frac{ika}{2}} \right) \left( e^{\frac{ika}{2}} - e^{-\frac{ika}{2}} \right) \\
 &= -4(i)^2 \sin^2 \frac{ka}{2} \\
 &= 4 \sin^2 \frac{ka}{2} \quad [p^2, q] = 2p(-i)
 \end{aligned}$$

$$(1) \dot{q}_n = i [H, q_n] = i \left[ \sum_{m'} \frac{p_{m'}^2}{2m}, q_n \right] = p_n/m$$

$$(2) \dot{p}_n = i [H, p_n] = i \left[ \left( (q_n - q_{n-1})^2 + (q_{n+1} - q_n)^2 \right), p_n \right]$$

$$(1) \downarrow = - \left[ 2(q_n - q_{n-1}) - 2(q_{n+1} - q_n) \right]$$

$$= m \ddot{q}_n$$