## Quantized Hamiltonian

$$\mathcal{H} = \sum_{\vec{k}} \hbar\omega_{\vec{k}} \left( \hat{b}^\dagger_{\vec{k}} \hat{b}_{\vec{k}} + \frac{1}{2} \right) = \sum_{\vec{k}} \hbar\omega_{\vec{k}} \left( \hat{n}_{\vec{k}} + \frac{1}{2} \right)$$

Debye wavevector

$$\omega_{\vec{k}} = c_l |\vec{k}| \qquad |\vec{k}| \leq k_D$$

### creation/annihilation operators

$$[\hat{b}_{\vec{k}}, \hat{b}^\dagger_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$$

$$[\hat{b}_{\vec{k}}, \hat{b}_{\vec{k}'}] = [\hat{b}^\dagger_{\vec{k}}, \hat{b}^\dagger_{\vec{k}'}] = 0$$

like bosonic particles

**Phonons**

### displacement field operator

$$\widehat{\vec{u}}(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\vec{k}} \vec{e}_{\vec{k}} \sqrt{\frac{\hbar}{2\rho_m \omega_{\vec{k}}}} \left[ \hat{b}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \hat{b}^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \right]$$

## Correlation function

$$g(\vec{r}-\vec{r}') = \langle \hat{\vec{u}}(\vec{r}) \cdot \hat{\vec{u}}(\vec{r}') \rangle - \langle \hat{\vec{u}}(\vec{r}) \rangle \cdot \langle \hat{\vec{u}}(\vec{r}') \rangle = \langle \vec{u}(\vec{r}) \cdot \vec{u}(\vec{r}') \rangle$$

$$= \frac{1}{\Omega} \sum_{\vec{k},\vec{k}'} \frac{\hbar \vec{e}_{\vec{k}} \cdot \vec{e}_{\vec{k}'}}{2\rho_m \sqrt{\omega_{\vec{k}} \omega_{\vec{k}'}}} \langle \left[ \hat{b}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \hat{b}^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \right] \left[ \hat{b}_{\vec{k}'} e^{i\vec{k}'\cdot\vec{r}'} + \hat{b}^\dagger_{\vec{k}'} e^{-i\vec{k}'\cdot\vec{r}'} \right] \rangle$$

$$= \frac{\hbar}{(2\pi)^2 \rho_m c_l} \int dk \frac{\sin(k|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|} \left(1 + 2\langle \hat{n}_{\vec{k}} \rangle\right)$$

$$g(R) \approx \frac{k_B \Theta_D}{(2\pi)^2 \lambda k_D} \times \begin{cases} \dfrac{1}{R^2} & T \ll T^*(R) \quad \text{quantum} \\ \dfrac{\pi T k_D}{\Theta_D R} & T \gg T^*(R) \quad \text{thermal} \end{cases}$$

$$T^*(R) = \frac{\Theta_D}{2 k_D R}$$

## melting transition in 3D:

mean square displacement

$$\langle \vec{u}(\vec{r})^2 \rangle = \frac{\hbar}{(2\pi)^2 \rho_m c_l} \int_0^{k_D} dk\ k\ \coth\left(\frac{\beta\hbar c_l k}{2}\right) = \begin{cases} \dfrac{k_D k_B T}{2\pi^2 \lambda} & T \gg \Theta_D\ , \\ \dfrac{k_D k_B \Theta_D}{8\pi^2 \lambda} & T \ll \Theta_D\ , \end{cases}$$

**Lindemann criterion**

lattice stable for

$$\langle \vec{u}(\vec{r})^2 \rangle < L_m^2 a^2$$

$$L_m \sim 0.1$$

→

melting temperature $\quad k_B T_m = 2\pi\lambda a^3 L_m^2$

quantum melting $\quad k_B \Theta_D < 8\pi\lambda a^3 L_m^2$

see He $\begin{cases} \text{solid} & \text{at high pressure} \\ \text{liquid} & \text{at low pressure} \end{cases}$

## Anharmonic elastic energy - phonon-phonon interaction

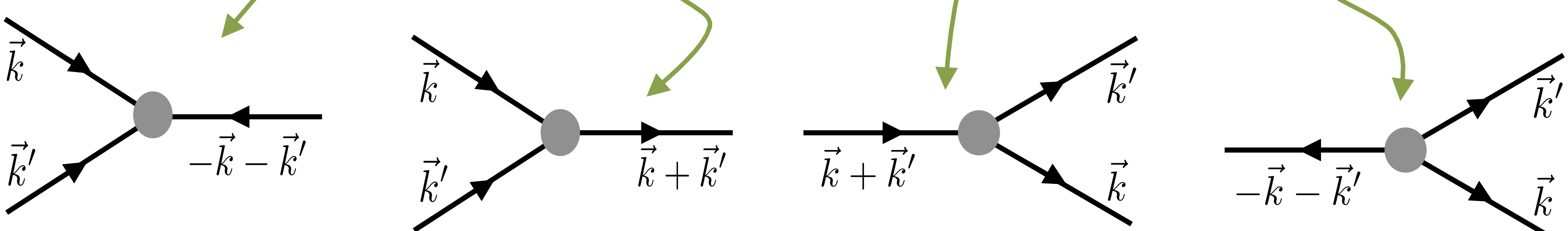
$$E'_{\mathrm{el}} = \frac{C'}{3} \int d^3 r (\vec{\nabla} \cdot \vec{u})^3$$

third-order anharmonic coupling

quantization →

$$\mathcal{H}'_{\mathrm{el}} = \frac{C}{3} \left( \frac{\hbar}{2 \rho_m c_l \Omega} \right)^{3/2} \sum_{\vec{k}, \vec{k}'} \left( |\vec{k}| \, |\vec{k}'| \, |\vec{k} + \vec{k}'| \right)^{1/2}$$

$$\times \left\{ \hat{b}_{\vec{k}} \hat{b}_{\vec{k}'} \hat{b}_{-\vec{k}-\vec{k}'} + 3 \, \hat{b}_{\vec{k}} \hat{b}_{\vec{k}'} \hat{b}^\dagger_{\vec{k}+\vec{k}'} + 3 \, \hat{b}_{\vec{k}+\vec{k}'} \hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{\vec{k}'} + \hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{\vec{k}'} \hat{b}^\dagger{}_{-\vec{k}-\vec{k}'} \right\} .$$




$\hat{b}_{\vec{k}} \hat{b}_{\vec{k}'} \hat{b}_{-\vec{k}-\vec{k}'}$ | $\hat{b}_{\vec{k}} \hat{b}_{\vec{k}'} \hat{b}^\dagger_{\vec{k}+\vec{k}'}$ | $\hat{b}_{\vec{k}+\vec{k}'} \hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{\vec{k}'}$ | $\hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{\vec{k}'} \hat{b}^\dagger{}_{-\vec{k}-\vec{k}'}$