Phonons

- Phonon bandstructure
- Second quantization of phonons
- Thermodynamics
- Electron-phonon interaction
- Scattering rate
- Electron spectrum
- 1D metal
- Umklapp processes

Phonons

Phonons: Lattice displacement or vibrations

What do they induce?

✓ Deformation
✓ Sound
✓ Heat

What are they involved into?

✓ Electron transport
✓ Heat transfer
✓ Structural phase transitions
✓ Melting

Phonon band structure

Total energy of a solid: function of coordinates of all the atoms *i*: x_i^α

$E = E\{x_i^\alpha\}$ *i* numbers all the atoms; $\alpha = x, y, z$

Small deviations from equilibrium positions: $x_i^\alpha = x_i^{\alpha(0)} + u_i^\alpha$

Expand energy in *u* up to 2nd order and get equations of motion:

$M_i \ddot{u}_i^\alpha = -\partial E / \partial x_i^\alpha = F_{ij}^{\alpha\beta} u_j^\beta$

For a periodic solid, $u_i^\alpha(t) \simeq \exp(-i\omega t + i q^\alpha x_i^\alpha) u_k^\alpha(\vec{q})$

$\boxed{\omega^2 M_k u_l^\alpha = F_{kl}^{\alpha\beta}(\vec{q}) u_l^\beta}$ *k,l* label the atoms in the elementary cell!!!

Eigenvalues: $\boxed{\omega(\vec{q})}$ Phonon band structure

Phonon band structure

Features of the phonon band structure:

- Energy scale involved: $M\Omega^2 x \sim Fx$ *F* – force at atomic scale

$F \sim E_{at}/a, E_{at} \sim \hbar^2/ma^2$ *a* – interatomic distance

$\boxed{\hbar\Omega \sim E_{at}\sqrt{m/M} \ll E_{at}}$ - Debye frequency

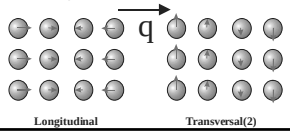
- # of modes=3 polarizations times # of atoms in the elementary cell
- Always 3 sound (acoustic) modes – since the lattice can move as a whole for free

$\boxed{\omega_{sound}(\vec{q}=0)=0}$

- Other modes (if any): optical

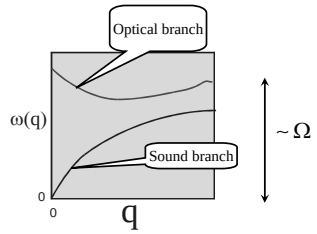
$\boxed{\omega_{opt}(\vec{q}=0)\neq 0}$

Polarizations: 1 longitudinal, 2 transverse



Longitudinal Transversal(2)

Phonon band structure



$\boxed{\omega = qs}$ *s* – speed of sound

Second quantization of phonons

Second quantization: is performed as for any oscillator set
Phonons are bosons.

A system of phonons is characterized by the number of quanta $N_{\vec{q}m}$
(*m* – phonon branch)

Hamiltonian: $\boxed{\hat{H} = \sum_{qm} \hbar\omega_{qm} \hat{b}_{qm}^\dagger \hat{b}_{qm} = \sum_{qm} \hbar\omega_{qm} \hat{N}_{qm}}$

$\hat{b}$ - creation/annihilation operators for bosons $\boxed{\left[\hat{b}_{qm}, \hat{b}_{q'm'}^\dagger\right] = \delta_{qq'}\delta_{mm'}}$

An important relation from comparison of classical and quantum energy:

$\boxed{u^\alpha(q) = \frac{1}{\sqrt{V}}\sqrt{\frac{\hbar}{2\rho\omega_{qm}}}(e_{qm}^\alpha \hat{b}_{qm} + h.c.)}$

ρ - density

$\vec{e}_{qm}$ - polarization vector

Thermodynamics of phonons

Bose statistics: Planck distribution function $\boxed{\langle N_q \rangle \equiv f_q = \frac{1}{\exp\left(\frac{\hbar\omega_q}{k_B T}\right)-1}}$

Energy density: $\boxed{\frac{E}{V} = \sum_m \int \frac{d^3\vec{q}}{(2\pi)^3} f_q \hbar\omega_q = \int d\varepsilon \frac{\varepsilon g(\varepsilon)}{\exp\left(\frac{\varepsilon}{k_B T}\right)-1}}$

Density of states: $\boxed{\begin{aligned} &g(\varepsilon) = \int \frac{d^3\vec{q}}{(2\pi)^3} \sum_m \delta(\varepsilon - \hbar\omega_{qm}); \\ &g \propto q^3/\varepsilon \propto \varepsilon^2 \text{ if } \varepsilon \to 0; \\ &\int d\varepsilon \nu(\varepsilon) = 3 \cdot N_{AT}/V \end{aligned}}$

Specific heat

$\boxed{c(T) = \partial E / V \partial T}$ Two limits: $k_B T \ll \Omega$ vs $k_B T \gg \Omega$

Ω - typical phonon energy (Debye frequency/temperature)

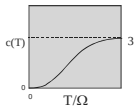
Low temperatures: only small wave vectors are important

$g \propto q^3/\varepsilon \propto \varepsilon^2 \Rightarrow \boxed{E \propto T^4, c \propto T^3}$ Electrons produce $\boxed{c \propto T}$!

$\boxed{c(T) \sim \frac{12\pi^4}{5} k_B \left(\frac{T}{\Theta}\right)^3}$ Θ - Debye temperature

High temperatures: classical limit

$\boxed{\frac{E}{V} = k_B T \int d\varepsilon g(\varepsilon) \to c(T) = 3 \cdot N_{AT}/V}$



(Einstein model of phonons)

Electron spectrum of a deformed solid

Small deformation in terms of the displacement: $\boxed{\delta V/V \sim \partial u^\alpha / \partial x^\alpha}$

Spectrum change: $\boxed{\delta\varepsilon(\vec{q},x) = -E_D(\vec{q}) \partial u^\alpha / \partial x^\alpha}$

Proportional to the deformation!

Second quantization for electrons:

$$\hat{H} = \sum_q \varepsilon(\vec{q}) \hat{a}_q^\dagger \hat{a}_q$$

$$\delta\hat{H} = \sum_{q,k} \delta\varepsilon(\vec{q},\vec{k}) \hat{a}_q^\dagger \hat{a}_{q-k}$$

Fourier component

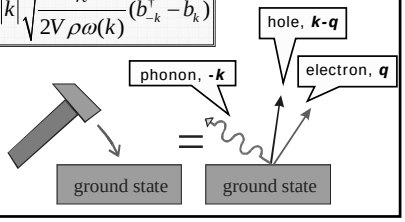
Electron-phonon interaction

Now substitute quantized displacement:

$$\hat{H}_{e-ph} = \sum_{q,k} E_D(\vec{q},\vec{k}) \hat{a}_q^\dagger \hat{a}_{q-k} i k^\alpha u^\alpha(k)$$

$$= \sum_{q,k} E_D(\vec{q},\vec{k}) \hat{a}_q^\dagger \hat{a}_{q-k} i|k| \sqrt{\frac{\hbar}{2V\rho\omega(k)}} (\hat{b}_{-k}^\dagger - \hat{b}_k)$$

What does this mean?



Electron-phonon interaction

Write it differently:

$$\hat{H}_{e-ph} = V^{-1/2} \sum_{q,k} g(\vec{q},\vec{k}) \sqrt{\hbar\omega(k)} \hat{a}_q^\dagger \hat{a}_{q-k} i(\hat{b}_{-k}^\dagger - \hat{b}_k)$$

$$g(\vec{q},\vec{k}) \equiv \frac{E_D|k|}{\omega(k)} \sqrt{\frac{1}{2\rho}} \equiv \sqrt{\frac{\lambda}{g}}$$

Dimensionless parameter of electron-phonon interaction

Electron density of states

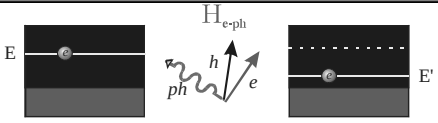
k cancels; atomic mass cancels

Estimates for metals: $\boxed{\lambda \sim 0.2}$: Weak coupling

This is why we can usually treat electron-phonon interaction as perturbation!

But not always!!

Electron-phonon scattering rate



An electron with energy E above the Fermi level loses its energy by emitting a phonon with the wave vector ***k***.

The rate is determined by the Golden rule,

$$\Gamma = \frac{2\pi}{\hbar} \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{\lambda}{g} \hbar\omega(\vec{k}) \, \delta(E(\vec{q}) - E(\vec{q}-\vec{k}) - \hbar\omega(\vec{k}))$$

Summation over final states

Matrix element of the interaction

Energy conservation

Electron-phonon scattering rate

Low energies: $E \ll \Omega$

Typical energy loss is of order of E $\Rightarrow$ $k \sim E/s$

$$\Gamma = \frac{2\pi}{\hbar}\frac{\lambda}{g} E g_{ph}(E) \sim \lambda \frac{E}{\hbar}\left(\frac{E}{\Omega}\right)^2$$

Since $\Gamma \ll \frac{E}{\hbar}$, the quasiparticles are well defined.

Typically $E \sim k_B T$: at which temperature it catches up the elastic rate $\tau^{-1} \sim v/l$?

$$T \sim k_B^{-1}\left(\frac{\hbar\Omega^2 g}{l\lambda}\right)^{1/3}$$

$l = 10\mu m$

$\Omega / k_B = 1000K$

$\lambda = 0.2$

$T \sim 150K$!

Electron-phonon scattering rate

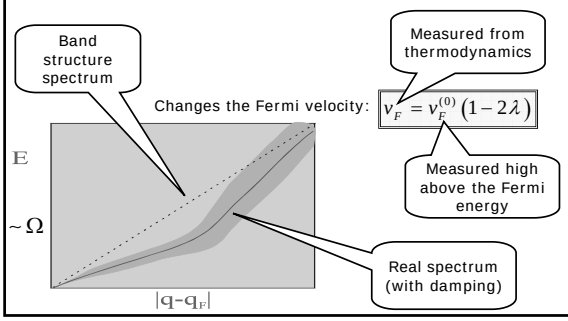
High energies: $E \gg \Omega$

Typical energy loss is of order of Ω

$$\Gamma \sim \frac{\lambda\Omega}{\hbar}$$

Again $\Gamma \ll \frac{E}{\hbar}$, the quasiparticles are well defined.

Electron spectrum



Umklapp processes

$$\sigma_{ph} = e^2\left(g v^2 \tau\right)_{\varepsilon=\mu}/3 \rightarrow (e^2/3)(g v^2 \hbar/\Gamma)\,?$$

The same problem as with electron-electron interactions:

Phonons have to be at equilibrium: How the equilibrium is established?

- Phonon-impurity collisions; Too weak
- Phonon-phonon interaction; For low temperatures no Umklapp
- Electron-phonon interactions.

If the total momentum of electron and phonon systems is conserved, we do not get any dissipation and do not equilibrate phonons.

⇓

Need Umklapp processes

$$\vec{q}_1 - \vec{q}_2 - \hbar\vec{k} = \hbar\vec{K}$$

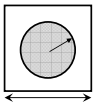
Umklapp processes

$$\vec{q}_1 - \vec{q}_2 - \hbar\vec{k} = \hbar\vec{K}$$

Low temperatures:

$|\hbar\vec{k}| \ll p_F$ $\Rightarrow$ $\vec{q}_1 - \vec{q}_2 \approx \hbar\vec{K}$ $2q_{\max} > \hbar K_{\min}$

Not fulfilled in e.g. alkali metals!
We can only fulfill the condition if short-wave length phonons are involved. Probability to find a phonon with $\hbar K$:



$p_F = \hbar K_{min}(3/8\pi)^{1/3}$

$K_{\min} = 2\pi/a$

$(\exp(\hbar\omega/k_B T) - 1)^{-1} \approx \exp(-\hbar\omega/k_B T)$ $\quad \hbar\omega \sim k_B T_D$ $\Rightarrow$ $\sigma_{ph} \propto \exp(-T_D/T)$

More than one electron per atom: condition fulfilled