Lattice thermal conductivity

treated in the Debye approximation:

just 3 acoustic modes $\quad \omega_s(\vec{k}) = c\,k \quad s = 1,2,3$

$$\vec{j}(\vec{r}) = -\kappa \vec{\nabla} T(\vec{r})$$

thermal "current": the flow of thermal energy density

gradient of T

kinetic coefficient: thermal conductivity

$$[\vec{j}] \sim \text{velocity} \times \text{energy density} = \frac{\text{cm}}{\text{sec}} \cdot \frac{\text{erg}}{\text{cm}^3}$$

$$[\vec{\nabla} T] \sim \frac{\text{Temperature}}{\text{Distance}} = \frac{\text{K}}{\text{cm}}$$

$$[\kappa] \cdot \frac{\text{K}}{\text{cm}} = \frac{\text{cm}}{\text{sec}} \cdot \frac{\text{erg}}{\text{cm}^3} \Rightarrow [\kappa] = \frac{\text{erg}}{\text{sec}} \cdot \frac{1}{\text{cm} \cdot \text{K}}$$

$$[\kappa] = \frac{\text{Power}}{\text{cm} \cdot \text{K}} \dashrightarrow \frac{\text{W}}{\text{cm} \cdot \text{K}}$$

Local temperature $T(\vec{r})$: collisions maintain local quasi-equilibrium

Energy density $u(\vec{r}) = u^{eq}[T(\vec{r})]$

Local distribution of phonons

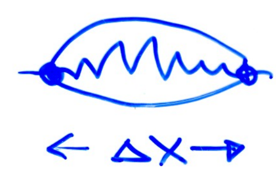
time t!

$n_s(\vec{k};\vec{r})$ ← kinetic equation

plane wave $e^{i\vec{k}\cdot\vec{r}}$ $\overset{?}{\Longleftrightarrow}$ particle with a specified position.

can be reconciled?

Yes, by constructing wave-packets



$\Delta k \approx \dfrac{1}{\Delta x}$

Meaning of $\sum_s n_s(\vec{k};\vec{r};t)$:

$$dN = \sum_s n_s(\vec{k};\vec{r};t)\,\frac{d\vec{k}\cdot d\vec{r}}{(2\pi)^3}$$

# of phonons

Semiclassical approach

19.2.1

Kinetic equation: Boltzmann 1872

$$\frac{dn_s(\vec{k};\vec{r};t)}{dt} = \frac{\partial n_s}{\partial t} + \underbrace{\frac{\partial n_s}{\partial \vec{k}}\cdot\dot{\vec{k}}}_{\text{vanishes for phonons}} + \frac{\partial n_s}{\partial \vec{r}}\dot{\vec{r}} = St\{n\}$$

collision integral

$\dot{\vec{r}} = \vec{u} = \frac{\partial\omega}{\partial\vec{k}}$ group velocity

thermal energy density

$$U = \sum_s \int \frac{d^3k \cdot V}{(2\pi)^3} \hbar\omega_s(\vec{k})\, n_s = U(\vec{r},t)$$

thermal energy density flow (current)

$$\vec{J} = \sum_s \int \frac{d^3k}{(2\pi)^3} \hbar\omega_s(\vec{k}) \cdot \frac{\partial\omega_s(\vec{k})}{\partial\vec{k}}\, n_s = J(\vec{r},t)$$

....

Conservation laws? in collisions:

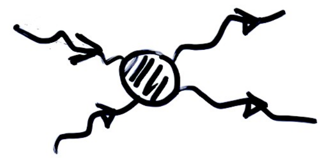
Total
- Number of phonons $N = \sum_s \int \frac{d\vec{r}\,d\vec{k}}{(2\pi)^3} n_s$ No
- quasi-momentum $\vec{k}_{tot} = \sum_s \int \frac{d\vec{r}\,d\vec{k}}{(2\pi)^3} \vec{k}\, n_s$ No
- Energy $E = \sum_s \int \frac{d\vec{r}\,d\vec{k}}{(2\pi)^3} \hbar\omega_s(\vec{k})\, n_s$ Yes

Relaxation time approximation

$$St\{n\} = -\frac{n-n^0}{\tau}$$

Scattering of phonons

- By phonons (anharmonic effect

( three-phonon processes, u^3 e.g.  four-phonon processes, u^4)

- Imperfections in the crystal
  - atoms of different elements
  - isotopes of the same element
  - dislocations

  ...

- Surface of the crystal

Eeach process is characterized by the rate of scattering (frequency) $\frac{1}{\tau_i}$

τ_i: mean time between collisions of sort "i"

- Total rate $\frac{1}{\tau} = \sum_i \frac{1}{\tau_i}$
- In each collision the phonon momentum $\vec{k}$ is not conserved

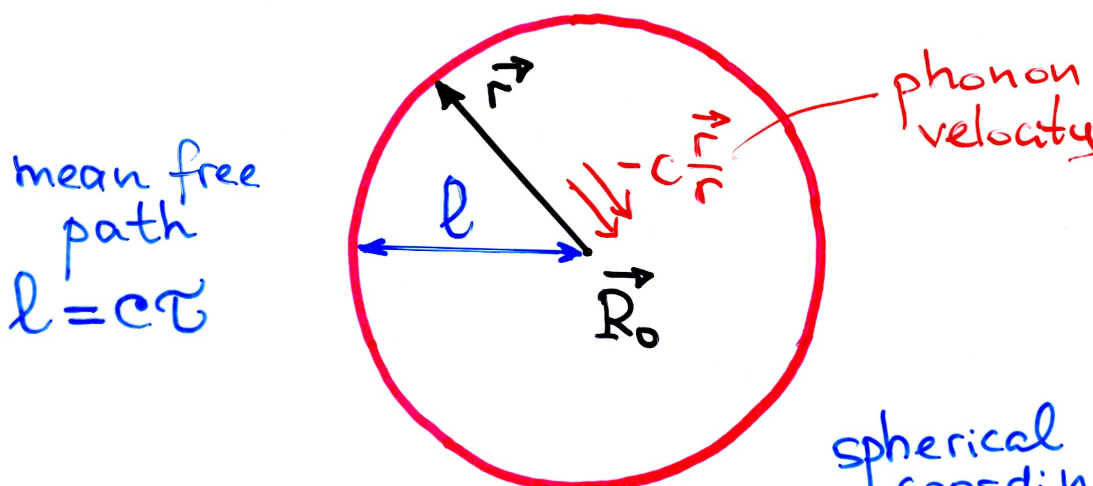
Simple calculation of thermal energy current in the presence of $\vec{\nabla}T$

Debye approx.

(Fast) collisions maintain local quasi-equilibrium:

local temperature $T(\vec{r})$ can be introduced

energy density $u(\vec{r}) = u^{eq}[T(\vec{r})]$



spherical coordinates

$$\vec{J}(\vec{R}_0) = \int_{|\vec{r}|=\ell=c\tau} \frac{d\Omega}{4\pi}\, u(\vec{R}_0+\vec{r})\left[-\frac{\vec{r}}{r}c\right]$$

thermal energy density current

$$u^{eq}[T(\vec{R}_0+\vec{r})] \simeq u^{eq}[T(\vec{R}_0)] + \frac{\partial u^{eq}}{\partial T}\cdot(\vec{r}\cdot\vec{\nabla}_{R_0})T$$

$$\frac{\partial u^{eq}}{\partial T} = c_v \quad \text{specific heat}$$

$$\vec{J}(\vec{R_0}) = \int\limits_{|\vec{r}|=\ell} \frac{d\Omega}{4\pi}\, c_v (\vec{r}\cdot\vec{\nabla}_{R_0})\left[-\frac{\vec{r}}{r} c\right] T(\vec{R_0})$$

$$\vec{J}(\vec{R_0}) = \left(-\int\limits_{|\vec{r}|=\ell} \frac{d\Omega}{4\pi} \cdot \frac{r_i r_j}{r^2}\right) \hat{e}_i\, c_v c \ell \frac{\partial T}{\partial R_{0j}}$$

$$\boxed{\begin{gathered} \vec{r} = \hat{e}_i r_i \qquad i = x, y, z \\ (\vec{r}\cdot\vec{\nabla}_{R_0}) T = r_j \frac{\partial T}{\partial R_{0j}} \end{gathered}}$$

averaging over directions:

$$\int \frac{d\Omega}{4\pi} \frac{r_i r_j}{r^2} \equiv \overline{\frac{r_i r_j}{r^2}} = \frac{1}{3}\delta_{ij}$$

$$\overline{\frac{xy}{r^2}} = \Big|_{x\to -x} -\overline{\frac{xy}{r^2}} = 0$$

$$\overline{\frac{x^2}{r^2}} = \frac{1}{3}\cdot\overline{\frac{x^2+y^2+z^2}{r^2}} = \frac{1}{3}$$

$$\vec{J}(\vec{R}) = -\underbrace{\frac{1}{3} C_v c \ell}_{\text{thermal conductivity } \kappa} \vec{\nabla} T(\vec{R})$$

$$\vec{J} = -\kappa \vec{\nabla} T \qquad \boxed{\kappa = \frac{1}{3} C_v c^2 \tau}$$

$$\ell = c\tau$$

T- dependence of κ: ①. $C_v(T)$

②. $\tau(T)$

I. High T: $T \gg \Theta_D$

$$C_v(T) = 3k_B$$

$$n_s(\vec{k}) = \frac{1}{\exp\left(-\frac{\hbar\omega_s(\vec{k})}{k_B T}\right) - 1} \approx \frac{k_B T}{\hbar\omega_s(\vec{k})}$$

# of scatterers increases $\sim T$

$\Rightarrow$ τ decreases with T

$$\boxed{\kappa \sim \frac{1}{T^x} \qquad \begin{array}{c} 1 < x < 2 \\ T \gg \Theta_D \end{array}}$$

II. Low T : $T \ll \Theta_D$

τ: U processes are frozen out $\sim e^{-\frac{\Theta_D}{T}} \ll 1$

② N processes conserve total crystal momentum

$\Downarrow$

do not give finite κ !

In the absence of U processes an ideal infinite crystal would have $\kappa = \infty$!

U processes: $\tau \sim e^{\frac{T_0}{T}}$, $T_0 \sim \Theta_D$

$l = c\tau \sim e^{\frac{T_0}{T}}$

phonon-phonon scattering

Once l is sufficiently large, other scattering processes [defects, surface, isotopes] become important : $\tau \to \tau_0 = \mathrm{const}$

C_v

① $C_v \sim T^3$

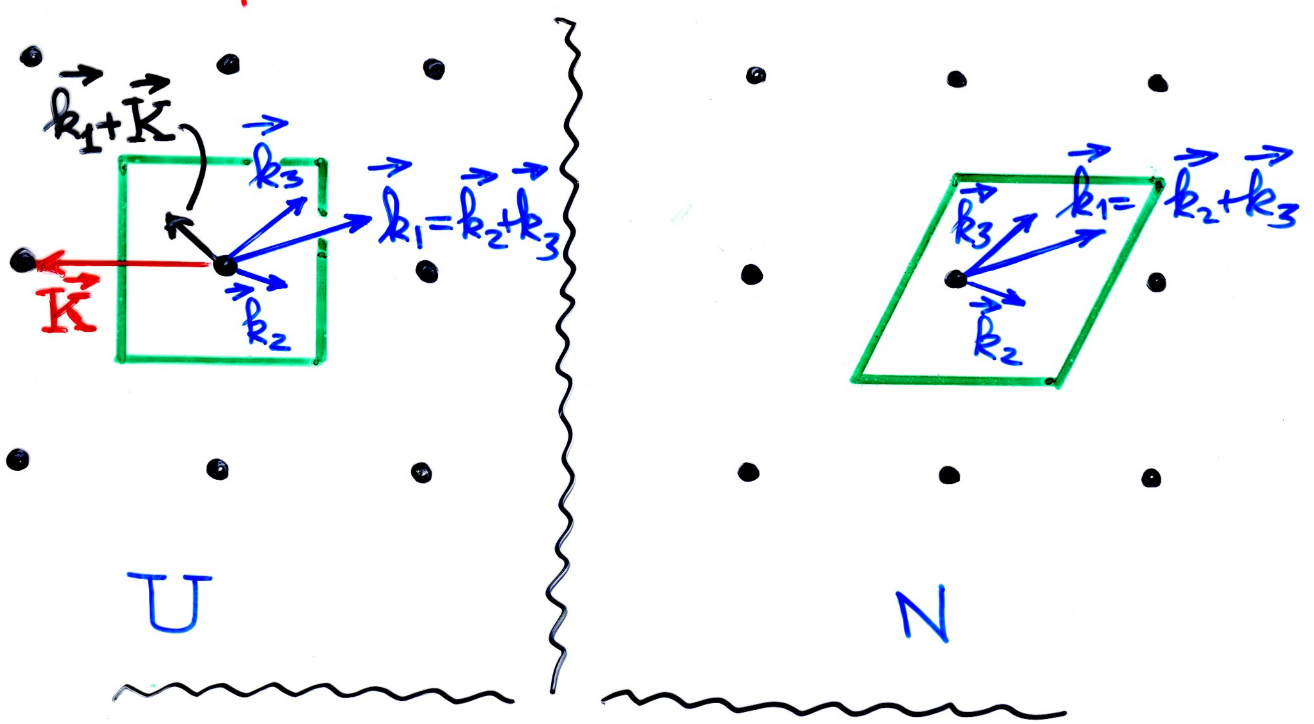
<u>N</u>ormal processes: $\vec{K} = 0$

$$\vec{k}_1 = \vec{k}_2 + \vec{k}_3 \qquad \sum_i \vec{k}_i = \sum_f \vec{k}_f$$

<u>U</u>mklapp processes: $\vec{K} \neq 0 \in RL$

$$\vec{k}_1 = \vec{k}_2 + \vec{k}_3 + \vec{K} \qquad \sum_i \vec{k}_i = \sum_f \vec{k}_f + \vec{K}$$

Distinction between N and U processes depends on a choice of a unit cell



However: $\exists$ choice to make <u>all</u> processes normal

A reasonable choice of a $\underline{\underline{RL}}$ primitive cell:

$\vec{k}=0$ in the center:

- all low-energy (ω) acoustic phonons have also small $|\vec{k}| \ll 1/a$
- short-wavelengths $|\vec{k}| \sim \pi/a$ have large $\omega(\vec{k}) \sim \Theta_D$

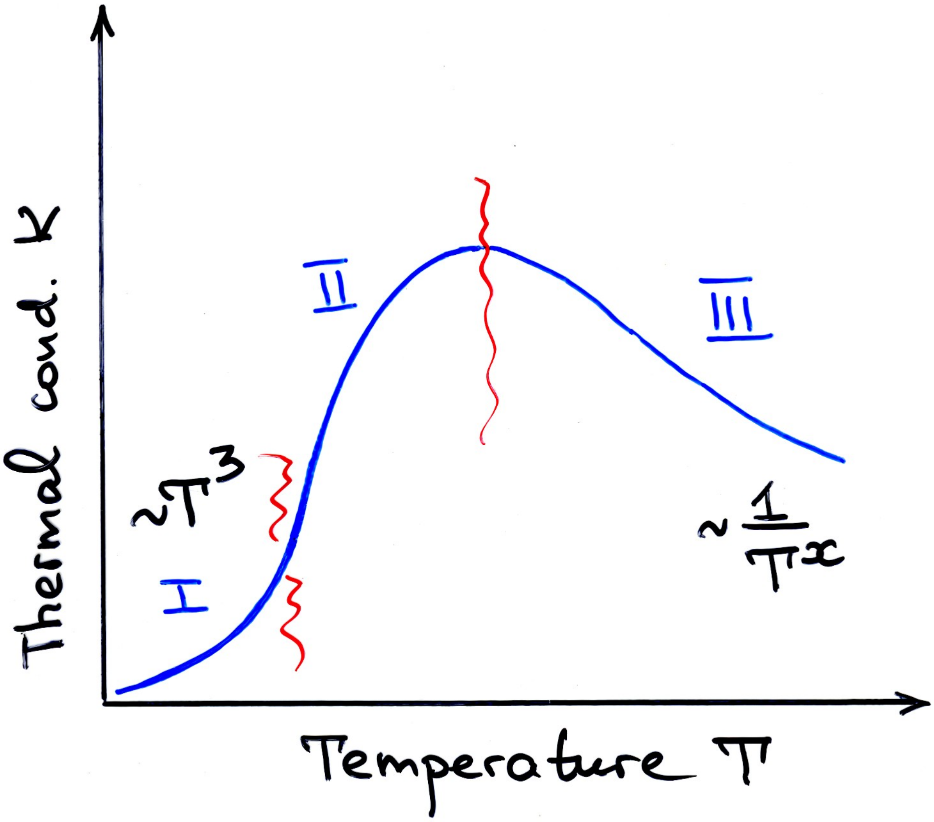
all processes with low-energy phonons are N.

② U: $\sum_i \vec{k}_i = \sum_f \vec{k}_f + \vec{K}$, $\vec{K} \neq 0$

$\Rightarrow$ at least one of phonons should have $|\vec{k}| \sim \pi/a \Rightarrow \omega \sim \Theta_D$

at $T \ll \Theta_D$ $\quad n_s \approx \exp\left(-\frac{\hbar\omega}{k_B T}\right) \approx e^{-\frac{\Theta_D}{T}}$

U processes are exponentially frozen out



I: Surface scattering with $\tau(T) = \tau_0 = \text{const}$

$$\kappa \sim C_v \sim T^3$$

II: U processes step in

κ reaches max when $\tau_U \sim \tau_0$

III: Ph-Ph scattering dominates

$$\kappa \sim \frac{1}{T^x} \quad 1 < x < 2$$

Isotopically pure LiF:

I: $T \lesssim 10\,K$

II: $10\,K \lesssim T \lesssim 20\,K$ $\quad \kappa_{max} \simeq 1.5 \times 10^2 \frac{W}{cm \cdot K}$