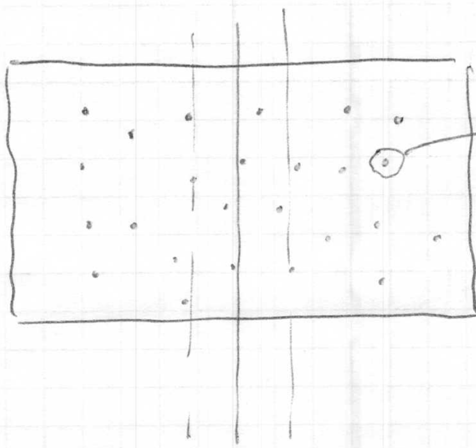
heat flow is due to random motion of molecules

→ recall wave - particle duality + simple harmonic oscillator.

→ as long as crystal dimension >> phonon wavelength, we can consider a phonon "gas", analogous to an electron gas or a molecular gas (fluid)

let's consider a small box of "gas"



carrier has energy E

molecules moving at average velocity v_x

half going right, half going left.

$x-\Delta x \quad x \quad x+\Delta x, \quad \Delta x = v_x \tau$

q_x = heat flux = (# carriers)(energy per carrier)(velocity)

$$= -\frac{1}{2}\left(nEv_x\right)\Big|_{x+\Delta x} + \frac{1}{2}\left(nEv_x\right)\Big|_{x-\Delta x}$$

$$= -\frac{1}{2}\cdot 2\cdot \Delta x\left(\frac{dEn\,v_x}{dx}\right)$$

$\Delta x = v_x \tau$, v_x is independent of x

$$\Rightarrow \quad q_x = -v_x^2 \tau \cdot \frac{d(En)}{dx}, \qquad v_x^2 = \frac{1}{3}v^2$$

average random molecular velocity

$En = U$: internal energy

$$q_x = -\frac{1}{3}v^2\tau\frac{dU}{dx}$$

definition of specific heat

$$= -\frac{1}{3}v^2\tau\frac{dU}{dT}\frac{dT}{dx}$$

so $q_x = \underbrace{-\frac{v^2}{3} c\tau}_{\text{definition of thermal conductivity}} \frac{dT}{dx} = -k\frac{dT}{dx}$ (1D problem)

so $k = \frac{v^2}{3} c\tau = \frac{vc}{3}\underbrace{(v\tau)}_{\text{mean free path}}$

$v \approx 10^4$ m/s (speed of sound in solid)

$\lambda \approx 10^{-6}$ m (1 μm)

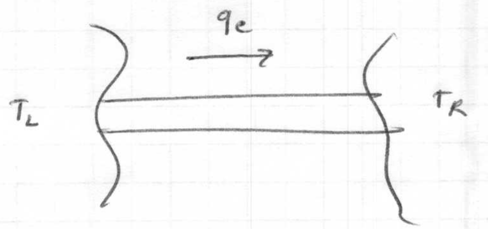
relaxation time $= \frac{\lambda}{v} = \tau \approx 10^{-10}$ s

much slower than a fast laser pulse (~ femtosecond pulse)

but this all assumes a conductor $\gg$ mean free path.

what happens at the opposite size limit?

let's approximate a very small size conductor, at very low temperature



Fourier's law

$$k_e = \frac{q_e}{\Delta T}$$ (only electron modes for now)

$\Delta T = T_L - T_R$

get same result for phonons, but difficult to solve by definition, heat flux is change in energy per unit time,

$$q_e = \frac{dE}{dt} = \frac{\Delta E}{\Delta t} \quad (\text{as } \Delta t \to 0)$$

also by definition, $\Delta E = k_b \Delta T$ ← $= 1.38 \times 10^{-23}$ J/K

for a single carrier

$$\text{so,} \quad q_e = \frac{k_b \Delta T}{\Delta t}$$

$$\text{say} \quad E_{wire} = k_b T_{wire} = k_b \left(\frac{T_L + T_R}{2} \right) = k_b T$$

$$\text{so,} \quad q_e = \frac{k_b \Delta T}{\Delta t} \left(\frac{E_{wire}}{E_{wire}} \right) = \frac{k_b^2 T \Delta T}{E \Delta t}$$

$$\text{from above,} \quad q_e = k_e \Delta T \implies k_e = \frac{q_e}{\Delta T}$$

$$\implies k_e = \frac{k_b^2 T}{E \Delta t}$$

by heisenberg's uncertainty principle, $\Delta E \Delta t = \frac{\hbar}{2}$ ✗ uncertainty in position and momentum of a carrier

$$\text{therefore,} \quad k_e = \frac{2 k_b^2 T}{\hbar}$$

More formally derived, we get $k_e = \frac{\pi^2}{3} \left(\frac{k_b^2 T}{\hbar} \right)$

recall the quantum of electrical conductance, per channel

$G = \frac{2e^2}{h}$, so $W = \frac{\text{electron thermal conductivity}}{\text{electrical conductivity}}$

$W = \frac{\kappa_e}{\sigma} = \frac{k_b^2 T}{e^2}$

roughly true for metals

e.g. Cu higher κ, σ than steel

<u>not true</u> for insulators, which do not conduct heat by electrons (only phonons)

for CNTs, it was determined that

$q = 2 M k_q T$ quantum of thermal conductivity

$M =$ # of occupied phonon "branches"

$M = \frac{1.5 \pi k_b T R^3}{h a c}$

$c = 1.5\text{e}4$ m/s = speed of sound in graphite

0.34 nm

in the diffusive limit, the thermal conductance is (1/resistance)

$\frac{\kappa A}{L} = \frac{\lambda M k_q}{L} \Rightarrow \kappa = \frac{\lambda M k_q}{A}$

experimental fit to both regimes

$$q = 2 M k_q L^{-1} \Big/ \left(L^{-1} + \frac{3}{8}\lambda \right) = \frac{\frac{2 M k_q}{L}}{\underbrace{\frac{1}{L}}_{\text{ballistic + non-length dependent}} + \frac{3}{8}\lambda}$$