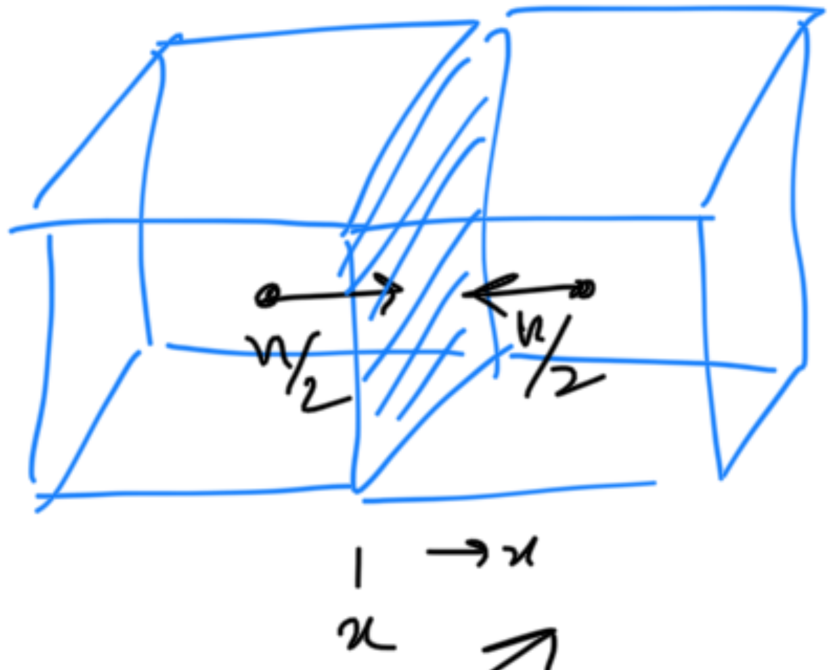
# Thermal conductivity




Heat flux:

Thermal current density $\overleftarrow{j}^{th}$ at $x$ from right

$$\overleftarrow{j}^{th} = \left(\frac{n}{2}\right) v\, \bar{U}\left(T(x+v\tau)\right)$$ assuming collision suffered $\tau$ times back

$$\overrightarrow{j}^{th} = \left(\frac{n}{2}\right) v\, \bar{U}\left(T(x-v\tau)\right)$$

Temp: $T(x)$

$$\vec{J}^{th} = \vec{J} - \overleftarrow{J} = \frac{1}{2} n v\left[\bar{U}\left(T(x-v\tau)\right) - \bar{U}\left(T(x+v\tau)\right)\right]\hat{x}$$

$$= \frac{1}{2} n v\left[\bar{U}(T(x)) - \frac{d\bar{U}}{dT}\frac{dT}{dx}v\tau - \bar{U}(T(x)) - \frac{d\bar{U}}{dT}\frac{dT}{dx}v\tau\right]\hat{x}$$

$$= -n v^2 \tau \frac{d\bar{U}}{dT}\frac{dT}{dx}\hat{x}$$ Note: $n\frac{d\bar{U}}{dT} = \frac{1}{V}\frac{dU}{dT} = c_v$

$$= v^2 c_v \left(-\frac{dT}{dx}\right)\hat{x}$$

3D: $v \equiv v_x$ to be averaged over all directions: $\langle v_x^2\rangle = \langle v_y^2\rangle = \langle v_z^2\rangle = \langle v^2\rangle \frac{1}{3}$

assuming isotropic medium

$$\Rightarrow \vec{J}^{th} = \frac{1}{2} v^2 c_v(-\nabla_x T)$$

Thermal conductivity $(k)$: $J^{th} = -k\nabla T$

$$\therefore\ k = \frac{1}{3} v^2 c_v \tau$$ Recall $\sigma_{DC} = ne^2\tau/m$

$$\therefore\ \frac{k}{\sigma_{DC}} = \frac{\frac{1}{2}v^2 c_v \tau}{ne^2\tau/m} = \frac{1}{3}\frac{c_v m v^2}{ne^2}$$ independent of $\tau$!

Putting $c_v = \frac{3}{2} n k_B$ and $\frac{1}{2} m v^2 = \frac{3}{2} k_B T$ (Too approximate for electron) not applicable.

$$\frac{\kappa}{\sigma_{DC}} = \frac{1}{3}\left(\frac{3}{2} n k_B\right) \cancel{\tau} \left(\frac{3 k_B T}{\cancel{m}}\right) \Big/ n e^2 = \frac{3}{2}\left(\frac{k_B}{e}\right)^2 T$$

$\Rightarrow$ Wiedemann Franz Law : $\frac{\kappa}{\sigma_{DC}} \propto T$ prop constant off by factor of 2 but it is accidental.

$\left\{ \begin{array}{l} c_v \text{ is roughly } 100 \text{ times smaller} \\ v^2 \text{ is } \quad " \quad 100 \quad " \quad \text{bigger.} \end{array} \right\}$

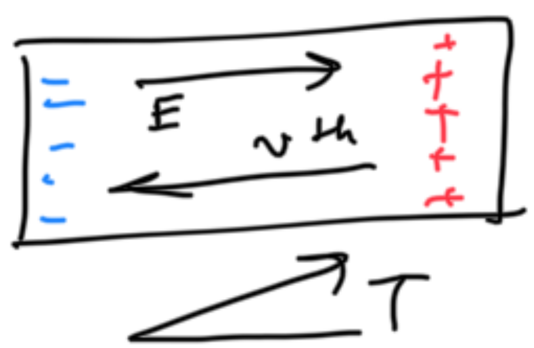
## Thermoelectric current:

velocity flux:

$$\vec{v}^{\,th}_x = \frac{1}{n}\left(\frac{n}{2}\right)\left[\vec{v}_x(x - v\tau) - \overleftarrow{v_x}(x + v\tau)\right]\hat{x} = -\hat{x}\,\tau v_x \frac{dv_x}{dx} = -\hat{x}\frac{\tau}{2}\frac{d}{dx}\left(v_x^2\right) = -\hat{x}\frac{\tau}{2}\frac{dv_x^2}{dT}\frac{dT}{dx}$$

3D: $\vec{v}^{\,th} = -\frac{\tau}{2}\frac{d}{dT}\left(\frac{v^2}{3}\right)\nabla(T) \longrightarrow$ Drude model explain thermoelectricity

At steady state this will be balanced by electric field caused by the thermal migration of charge. Let the field be $E$




$$\therefore -\vec{v}^{\,th} = \vec{v}_E \Rightarrow \frac{\tau}{6}\frac{dv^2}{dT}\nabla T = -\frac{eE}{m}\tau$$

$\therefore$ Thermopower : $\frac{E}{\nabla T} = \left(-\frac{1}{3e}\right)\frac{d}{dT}\left(\frac{1}{2}mv^2\right) = \left(-\frac{1}{3en}\right)\frac{d}{dT}\left(n\frac{1}{2}mv^2\right) = -\frac{c_v}{3ne}$

off by 100
corrected by Q Statmech.

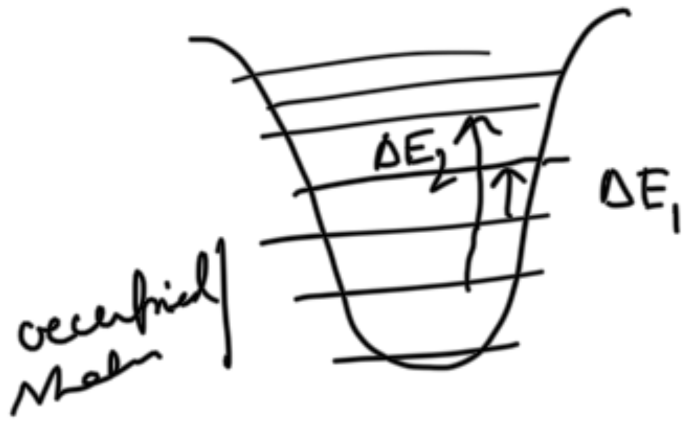
## Nature of corrections

In real system electrons are in discrete levels:

Discrete levels: Limited scope for absorption of energy

It can absorb energy only exactly equal to energy difference $\Delta E$ between available states.

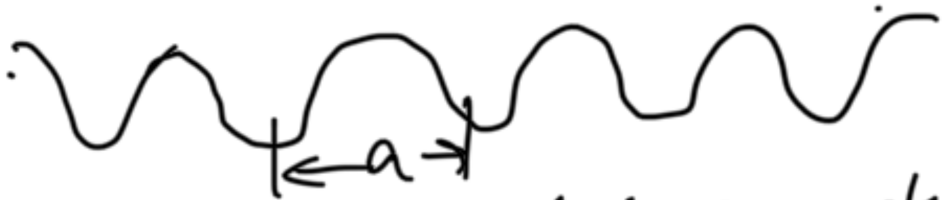
$\Rightarrow$ Deviation from Dulong Petit law as we saw in Einstein and Debye models of sp. heat.





$\therefore$ If $\Delta E \uparrow$ then $\Delta Q$ amount of heat will need to occupation of higher energy state $\Rightarrow \Delta T \uparrow \Rightarrow C \downarrow \because C = \frac{\Delta Q}{\Delta T}$ $\quad \Delta T \propto \frac{1}{\Delta E}$ approx

We will see soon that the quantum treatment of electrons in the periodic potential limits the momentum $p = \frac{2\pi}{a}$ where $a$ is the lattice constant:



.... Other available values are $p = \frac{2\pi}{na}$ $n = 1, \ldots \infty$

$a$ is order of Å $= 10^{-10}$ m $\approx 2$ Bohr (atomic units)

Using atomic units: $\hbar = 1, m = 1$, 1 a.u. of E is 1 Hartree (Ha) $\approx 27$ eV

$k_B$ in a.u. $\approx 10^{-6}$ Ha/K

$k_BT \approx 10^{-4}$ Ha

Approximate Quantum estimate:

$$\left.\frac{\hbar^2 k^2}{2m}\right|_{max} \approx 10 \text{ Ha}$$

$\therefore$ Classical estimate: $\sqrt{\frac{3k_BT}{m}} \approx 10^{-2}$ Ha

$$\therefore \frac{\text{Q estimate of } E}{\text{Cl estimate of } E\ (\sim \frac{1}{2}mv^2)} \approx 100 \text{ to } 1000$$

$$\therefore \frac{\Delta E_{Quantum}}{\Delta E_{Cl}} \approx 100 \Rightarrow \frac{\Delta T_{Qu}}{\Delta E_{Cl}} \approx 10^{-2} \Rightarrow \frac{C_{Cl}}{C_{Qu}} \approx 10^{2}$$