Thermal transport

- Interested in flow of heat (thermal energy) across sample
- Response of heat flow, electrical current flow to applied thermal gradients.

First: Define heat current. (Following A&M Ch. 13)

- Consider small, fixed volume of our system.
- Infinitesimal change in energy (in a time dt) is:

$$dE = T\,dS + \mu\,dN \qquad \left(\begin{array}{c} dV = 0 \text{ since} \\ \text{volume fixed}\end{array}\right)$$

- Heat in $= dQ = T\,dS = dE - \mu\,dN$

- Energy current density: $\vec{J}_{\text{Energy}} = \int \frac{d^3\vec{k}}{4\pi^3}\, \varepsilon_{\vec{k}}\, \vec{v}_{\vec{k}}\, g(\vec{r}, \vec{k}, t)$

- Number current density: $\vec{J}_{\text{Num}} = \int \frac{d^3\vec{k}}{4\pi^3}\, \vec{v}_{\vec{k}}\, g(\vec{r}, \vec{k}, t)$

$$\Rightarrow \boxed{\text{Heat current density } \vec{J}_Q = \int \frac{d^3\vec{k}}{4\pi^3} (\varepsilon_{\vec{k}} - \mu)\, \vec{v}_{\vec{k}}\, g(\vec{r}, \vec{k}, t)}$$

- Now suppose we apply $\vec{E}$ and $\vec{\nabla}T$. This will **also** induce a gradient in μ, $\vec{\nabla}\mu$. (For now consider $\vec{B} = 0$.)

- Semiclassical force on electron due to $\vec{\nabla}\mu$ is

$$\vec{F}_\mu = -\vec{\nabla}\mu$$

- Define $\vec{\mathcal{E}} = \vec{E} + \frac{\vec{\nabla}\mu}{e}$, then total force on electron due to $\vec{E}$ & $\vec{\nabla}\mu$ is just $\vec{F} = -e\vec{\mathcal{E}}$.

Expect linear relations between currents & applied fields:

$$\boxed{\begin{aligned} \vec{J} &= \overleftrightarrow{L}_{EE}\cdot\vec{\mathcal{E}} + \overleftrightarrow{L}_{ET}\cdot(-\vec{\nabla}T) \\ \vec{J}_Q &= \overleftrightarrow{L}_{TE}\cdot\vec{\mathcal{E}} + \overleftrightarrow{L}_{TT}\cdot(-\vec{\nabla}T) \end{aligned}}$$

I use this notation because E stands for electrical, T for thermal.

So $\overleftrightarrow{L}_{ET}$ gives the electrical current due to the thermal gradient $\vec{\nabla}T$.

Next: Linearize Boltzmann equation in $\vec{\nabla} T$ and $\vec{\nabla}\mu$.

- These enter through $\frac{\partial g}{\partial \vec{r}}$ term:

$$\frac{\partial g}{\partial \vec{r}} \approx \frac{\partial g^{(0)}}{\partial T} \vec{\nabla} T + \frac{\partial g^{(0)}}{\partial \mu} \vec{\nabla}\mu$$

- Note: $g^{(0)}$ is independent of position. Weak $\vec{\nabla} T$ means

$T(\vec{r}) = T_0 + \vec{\alpha} \cdot \vec{\nabla} T$, $g^{(0)}$ depends only on T_0,

i.e. $g^{(0)}(\vec{r},\vec{k},t) = f(\varepsilon_{\vec{k}})$

Using relations:

$$\frac{\partial f(\varepsilon)}{\partial T} = -\left(\frac{\varepsilon-\mu}{T}\right) f'(\varepsilon)$$

$$\frac{\partial f(\varepsilon)}{\partial \mu} = -f'(\varepsilon)$$

Have:

$$\frac{\partial g}{\partial \vec{r}} \approx \left[-f'(\varepsilon_k)\right]\left[\left(\frac{\varepsilon_k-\mu}{T}\right)\vec{\nabla} T + \vec{\nabla}\mu\right]$$

Assuming steady state, Boltzmann equation is:

$$\cancelto{0}{\frac{\partial g}{\partial t}} + \vec{v}_{\vec{k}} \cdot \frac{\partial g}{\partial \vec{r}} + \overbrace{\dot{\vec{k}} \cdot \frac{\partial g}{\partial \vec{k}}}^{-e f'(\varepsilon_{\vec{k}})\, \vec{v}_{\vec{k}} \cdot \vec{E}} = -\frac{1}{\tau}\left(g - g^{(0)}\right)$$

$$\Rightarrow \boxed{g - g^{(0)} = \tau\left[-f'(\varepsilon_{\vec{k}})\right] \vec{v}_{\vec{k}} \cdot \left[\left(\frac{\varepsilon_{\vec{k}} - \mu}{T}\right)(-\vec{\nabla} T) - e\vec{\mathcal{E}}\right]}$$

- We can now calculate coefficients $\overleftrightarrow{L}_{EE}$, $\overleftrightarrow{L}_{TT}$, etc.
  - Plug expression for $g - g^{(0)}$ into expressions for electrical and thermal currents.
  - To get, say, $\overleftrightarrow{L}_{TE}$, find the term in the <u>thermal</u> current proportional to $\vec{\mathcal{E}}$.

- In the free electron gas, we have spherical symmetry, so

$$(\overleftrightarrow{L}_{EE})_{ij} = \delta_{ij} L_{EE}, \quad (\overleftrightarrow{L}_{ET})_{ij} = \delta_{ij} L_{ET}, \text{ etc.}$$

- Results (you will calculate these on the homework!)

- $L_{EE} = \sigma = \frac{ne^2\tau}{m}$ (already did it!)

- $L_{TT} = \frac{\pi^2}{3} \frac{n\tau}{m} k_B^2 T$

- $L_{ET} = \frac{ne^2\tau}{m}\left[-\frac{\pi^2}{2e}\frac{k_B^2 T}{\varepsilon_F}\right] = \sigma\left[-\frac{\pi^2}{2e}\frac{k_B^2 T}{\varepsilon_F}\right]$

- $L_{TE} = T \cdot L_{ET}$

Discuss measurable quantities/effects ....

Thermal conductivity

Under open circuit conditions, apply $\vec{\nabla}T$, measure $\vec{J}_Q$:

Open circuit: $\vec{J} = 0 = L_{EE}\vec{\mathcal{E}} + L_{ET}(-\vec{\nabla}T)$

$$\Rightarrow \quad \vec{\mathcal{E}} = \frac{L_{ET}}{L_{EE}}\vec{\nabla}T$$

$$\vec{J}_Q = L_{TT}(-\vec{\nabla}T) + L_{TE}\vec{\mathcal{E}}$$

$$= \left[L_{TT} - \frac{L_{ET}L_{TE}}{L_{EE}}\right](-\vec{\nabla}T) \equiv -\underbrace{K}_{\text{thermal conductivity}}\vec{\nabla}T$$

2nd term in K not very important for metals:

$$K = L_{TT}\left[1 - \frac{L_{ET}L_{TE}}{L_{EE}L_{TT}}\right]; \quad \frac{L_{ET}L_{TE}}{L_{EE}L_{TT}} = \frac{\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2$$

$$\sim \begin{cases} 10^{-3} & ; T \approx 300\,K \\ 10^{-5} & ; T \approx 100\,K \end{cases}$$

$$\Rightarrow \quad \boxed{K \approx L_{TT}}$$

Wiedemann–Franz "Law"

$$\frac{\kappa}{\sigma T} = \underbrace{\frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2}_{\text{"Lorenz number"}} = 2.44 \times 10^{-8} \ \frac{\text{Watt} \cdot \text{Ohm}}{K^2}$$

- Often violated, but obeyed well in many metals at low-T.
- Physics: elastic scattering degrades $\vec{J}$ and $\vec{J}_Q$ the same way ...

$$\vec{J} = \int \frac{d^3k}{4\pi^3} \underbrace{(-e v_k)} g \quad ; \quad \vec{J}_Q = \int \frac{d^3k}{4\pi^3} \underbrace{(\varepsilon_k - \mu)} v_k \cdot g$$

$-e$ is charge of electron — no scattering ever changes it!

If scattering conserves energy, then $(\varepsilon_k - \mu)$ is like charge, it never changes.

- Elastic scattering only changes v_k, affects $\vec{J}$ & $\vec{J}_Q$ the same way.

Thermopower:

Again open circuit → apply $\vec{\nabla} T$, measure voltage

$$0 = \vec{J} = L_{EE}\vec{\mathcal{E}} + L_{ET}(-\vec{\nabla} T)$$

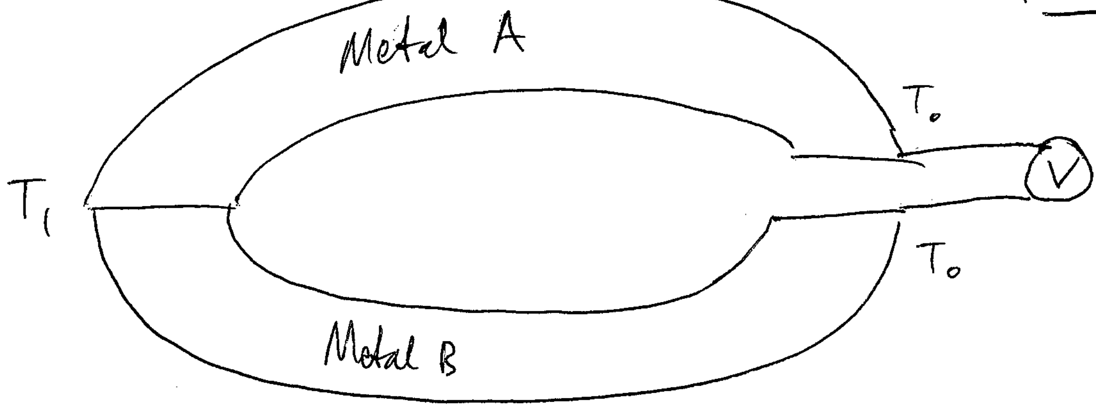
$$\vec{\mathcal{E}} = \underbrace{Q}_{\text{thermopower}} \vec{\nabla} T \quad ; \quad Q = \frac{L_{ET}}{L_{EE}} = -\frac{\pi^2}{2e}\frac{k_B^2 T}{\varepsilon_F}$$

- Order of magnitude: $Q \sim \frac{\mu V}{K}$

If relaxation time depends on energy, form of Q is modified.

- Practically, can measure Q in this setup:

  ↳ This is a thermocouple!



(Actually measures $Q_A - Q_B$.)

- Q depends on sign of electron charge. But, empirically, it's not always negative...