

Physics 460/560

Lecture 4

Thermal conductivity

Thermal gradient:

$$\vec{F} = 0 \quad \frac{\partial f}{\partial \vec{r}} = \frac{\partial f}{\partial T} \nabla T$$

Boltzmann equation:

$$\underbrace{\frac{\partial f}{\partial t}}_0 + \nabla \cdot \frac{\partial f}{\partial \vec{r}} + \underbrace{\vec{F} \cdot \frac{\partial f}{\partial \vec{p}}}_0 = \frac{\partial f}{\partial t} \Big|_{\text{collisions}}$$

steady state

$$\nabla \cdot \nabla T \frac{\partial f}{\partial T} = - \frac{f - f_0}{\tau}$$

$$f_1 = -\tau \frac{\partial f_0}{\partial T} \nabla \cdot \nabla T + \mathcal{O}[(\nabla T)^2]$$

1st order correction to the distribution function.

Heat current

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$$dQ = T ds = dE - \mu dN \quad (\text{constant volume})$$

$$\vec{J}_Q = \vec{J}_E - \mu \vec{J}_N$$

$$\vec{J}_N = \int \frac{d^3 p}{h^3} f(\vec{r}, \vec{p}) \vec{v}$$

$$\vec{J}_E = \int \frac{d^3 p}{h^3} \epsilon(\vec{p}) f(\vec{r}, \vec{p}) \vec{v}$$

$$\vec{J}_Q = \int \frac{d^3 p}{h^3} (\epsilon(\vec{p}) - \mu) f_1(\vec{r}, \vec{p}) \vec{v}$$

$$= - \int \frac{d^3 p}{h^3} \tau (\epsilon(\vec{p}) - \mu) \frac{\partial f_0}{\partial T} (\vec{v} \cdot \nabla T) \vec{v}$$

$$f_0 = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}$$

Fermi-Dirac
distribution

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$$\begin{aligned} \frac{\partial f_0}{\partial T} &= -\frac{1}{k_B T^2} \frac{\partial f_0}{\partial \beta} + \frac{\partial f_0}{\partial \mu} \frac{\partial \mu}{\partial T} \\ &= -\frac{\epsilon - \mu}{T} \frac{\partial f_0}{\partial \epsilon} - \frac{\partial \mu}{\partial T} \frac{\partial f_0}{\partial \epsilon} \\ &= -\frac{\partial f_0}{\partial \epsilon} \left(\frac{\epsilon - \mu}{T} + \frac{\partial \mu}{\partial T} \right) \end{aligned}$$

$$\begin{aligned} \vec{J}_Q &= - \int \frac{d^3 p}{h^3} \tau(\vec{p}) (\epsilon(\vec{p}) - \mu) \left(\frac{\epsilon(\vec{p}) - \mu}{T} + \frac{\partial \mu}{\partial T} \right) \\ &\quad \times \left(- \frac{\partial f_0}{\partial \epsilon} \right) (\vec{v} \cdot \nabla T) \vec{v} \end{aligned}$$

The thermal conductivity tensor is defined by

$$(\vec{J}_Q)_i = - \sum_j K_{ij} \frac{\partial T}{\partial x_j},$$

where

$$K_{ij} = \int \frac{d^3p}{h^3} \tau(\vec{p}) (\epsilon(\vec{p}) - \mu) \left(\frac{\epsilon(\vec{p}) - \mu}{T} + \frac{\partial \mu}{\partial T} \right) \times \left(-\frac{\partial f_0}{\partial \epsilon} \right) v_i v_j$$

$$= \frac{\delta_{ij}}{3} \int \frac{d^3p}{h^3} \tau(\vec{p}) (\epsilon(\vec{p}) - \mu) \left(\frac{\epsilon(\vec{p}) - \mu}{T} + \frac{\partial \mu}{\partial T} \right) \times \left(-\frac{\partial f_0}{\partial \epsilon} \right) \vec{v}^2$$

(provided $\tau = \tau(|\vec{p}|)$, $\epsilon = \epsilon(|\vec{p}|)$)

Further, assuming free particles

with $\epsilon = \frac{m\vec{v}^2}{2}$ and $\tau(\vec{p}) = \tau$ (constant)

we have

$$K = \frac{2\tau}{3m} \int \frac{d^3p}{h^3} (\epsilon(\vec{p}) - \mu) \left(\frac{\epsilon(\vec{p}) - \mu}{T} + \frac{\partial \mu}{\partial T} \right) \times \left(-\frac{\partial f_0}{\partial \epsilon} \right) \epsilon(\vec{p})$$

(dropping matrix notation)

The integrand now depends only on energy, so we can simplify to

$$K = \frac{2\pi}{3m} \int_0^{\infty} d\varepsilon D(\varepsilon) (\varepsilon - \mu) \left(\frac{\varepsilon - \mu}{T} + \frac{\partial \mu}{\partial T} \right) \times \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \varepsilon$$

$$-\frac{\partial f_0}{\partial \varepsilon} = \frac{\beta e^{\beta(\varepsilon - \mu)}}{(e^{\beta(\varepsilon - \mu)} + 1)^2}$$

$$\text{Let } x = \beta(\varepsilon - \mu)$$

$$K = \frac{2\pi}{3m} k_B \beta^{-1} \int_{-\beta\mu}^{\infty} dx D\left(\mu + \frac{x}{\beta}\right) \times \left(x + \frac{\partial \mu}{\partial k_B T}\right) \times \left(\mu + \frac{x}{\beta}\right) \frac{e^x}{(e^x + 1)^2}$$

For low temperatures, $k_B T \ll \varepsilon_F$, we have $\beta\mu \gg 1$ and we can

take $D\left(\mu + \frac{x}{\beta}\right) \approx D(\varepsilon_F)$. Then

$$K = \frac{2\pi D(\epsilon_F) k_B^2 T}{3m} \int_{-\infty}^{\infty} dx \frac{e^x}{(e^x + 1)^2}$$

$$\times \left(\frac{x^3}{\beta} + \frac{\mu \frac{\partial \mu}{\partial k_B T}}{\partial k_B T} x + \left(\mu + T \frac{\partial \mu}{\partial T} \right) x^2 \right)$$

odd terms
integrate to zero

$$K = \frac{2\pi D(\epsilon_F) \left(\mu + T \frac{\partial \mu}{\partial T} \right) k_B^2 T}{3m} \int_{-\infty}^{\infty} dx \frac{x^2 e^x}{(e^x + 1)^2}$$

$\frac{\pi^2}{3}$

$$D(\epsilon_F) = \frac{3n}{2\epsilon_F} \quad (\text{density of states per unit volume})$$

$$\mu \approx \epsilon_F, \quad T \frac{\partial \mu}{\partial T} \rightarrow \text{higher order in } T \text{ (neglect)}$$

$$K = \frac{\pi^2}{3} \frac{n\tau}{m} k_B^2 T$$

$$\frac{\kappa}{\sigma T} = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right)^2$$

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Wiedemann-Franz law rederived.

General formulation of transport

Steady state: $\frac{\partial f}{\partial t} = 0$

relaxation-time approx: $\frac{df}{dt} = - \frac{f - f_0}{\tau}$

$$\vec{\nabla} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = - \frac{f - f_0}{\tau}$$

$$f = f_0 + f_1, \quad f_0(\vec{r}, \vec{p}) = f_0(\vec{r}, \epsilon(\vec{p}))$$

$$\frac{\partial f_0}{\partial \vec{r}} = \frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu \quad \text{e.g.} \quad \frac{1}{e^{\beta(\vec{r})(\epsilon(\vec{p}) - \mu(\vec{r}))} + 1}$$

$$\frac{\partial f_0}{\partial T} = - \frac{\epsilon - \mu}{T} \frac{\partial f_0}{\partial \epsilon}$$

$$\frac{\partial f_0}{\partial \mu} = - \frac{\partial f_0}{\partial \epsilon}$$

$$\frac{\partial f}{\partial \vec{r}} = \frac{\partial f_1}{\partial \vec{r}} - \frac{\partial f_0}{\partial \epsilon} \left[\frac{\epsilon - \mu}{T} \nabla T + \nabla \mu \right]$$

$$\frac{\partial f_0}{\partial \vec{p}} = \frac{\partial f_0}{\partial \epsilon} \frac{\partial \epsilon}{\partial \vec{p}} = \frac{\partial f_0}{\partial \epsilon} \vec{v}$$

$$\vec{F} = q (\vec{E} + \frac{\vec{v}}{c} \times \vec{B})$$

$$\vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = q \vec{E} \cdot \vec{v} \frac{\partial f_0}{\partial \epsilon} + q \left(\frac{\vec{v}}{c} \times \vec{B} \right) \cdot \frac{\partial f_1}{\partial \vec{p}} + \mathcal{O}(\vec{E}^2)$$

Linearized Boltzmann equation

$$\vec{v} \cdot \left[q \vec{E} - \nabla \mu - \frac{\epsilon - \mu}{T} \nabla T \right] \left(- \frac{\partial f_0}{\partial \epsilon} \right)$$

$$= \frac{f_1}{\tau} + \vec{v} \cdot \frac{\partial f_1}{\partial \vec{r}} + \frac{q}{c} (\vec{v} \times \vec{B}) \cdot \frac{\partial f_1}{\partial \vec{p}}$$

(neglects terms $\mathcal{O}(\vec{E}^2)$, $\mathcal{O}(vT^2)$, etc.)

The term $\vec{\nabla} \cdot \frac{\partial f_1}{\partial \vec{r}}$ describes boundary effects. If the specimen is large enough, we can neglect this term.

Special case: $\vec{B} = 0$

$$f_1 = \tau \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \vec{\nabla} \cdot \left[g \vec{E} - \nabla \mu - \frac{\varepsilon - \mu}{T} \nabla T \right]$$

$$g \vec{E} - \nabla \mu = -\nabla V, \text{ where}$$

V is the electrochemical potential.

As far as a particle is concerned, only the combination $g \vec{E} - \nabla \mu$ counts: it cannot distinguish between an electric field and a gradient of chemical potential.

The electric current and heat current are

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$$\vec{J}_e = g \int \frac{d^3p}{h^3} \vec{v} f_1,$$

$$\vec{J}_Q = \int \frac{d^3p}{h^3} (\epsilon(\vec{p}) - \mu) \vec{v} f_1.$$

Inserting f_1 from above, we find

$$\vec{J}_e = g^2 (K_0) (-\nabla V) + \frac{g}{T} (K_1) (-\nabla T)$$

$$\vec{J}_Q = g (K_1) (-\nabla V) + \frac{1}{T} (K_2) (-\nabla T)$$

where

$$(K_n)_{ij} = \int \frac{d^3p}{h^3} \tau(\vec{p}) v_i v_j \left(-\frac{\partial f_0}{\partial \epsilon} \right) (\epsilon - \mu)^n$$

with $\epsilon = \epsilon(\vec{p})$, $v_i = v_i(\vec{p})$.

Thus, there is an intimate relation between electrical and thermal transport: the electric current induced by a unit temperature gradient is $\frac{1}{T}$ times the heat current induced by a unit electric field.

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Limitations of Boltzmann equation

The Boltzmann eq. gives a semiclassical description of transport.

The distribution function $f(\vec{r}, \vec{p})$ has been coarse grained over cells with $d^3r d^3p > h^3$, so it can not describe quantum wave

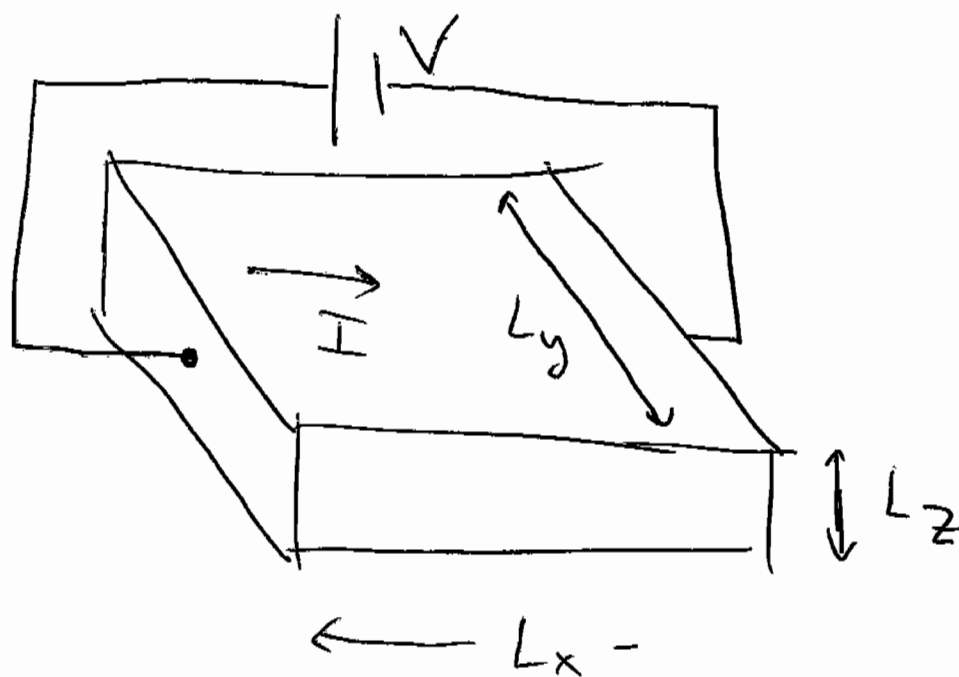
effects. Furthermore, it is only suitable to describe specimens with dimensions

$$L_x, L_y, L_z \gg l = \text{mean-free path}$$

For Fermions, $l = v_F \tau$.

For example, Ohm's law states

$$V = IR, \quad R = \frac{\rho L_x}{L_y L_z}$$



Substantial deviations from 13
Ohm's law are to be
expected if the conditions

$$L_x, L_y, L_z \gg l, \lambda$$

are not satisfied, where

λ is the de Broglie wavelength
of a typical charge carrier.