Physics 460/560 Lecture 3

Boltzmann equation of transport

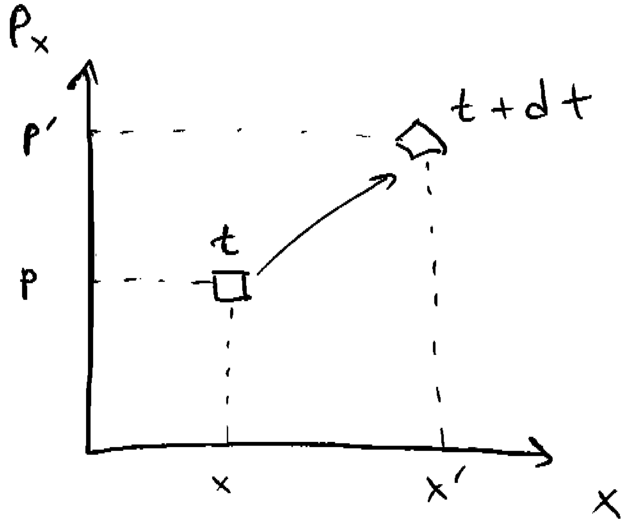
The derivations we have given for Ohm's law, the Hall effect, and the Wiedemann-Franz law have been quite rough. It is worthwhile to be more rigorous

A more precise treatment of transport can be obtained by considering the (semiclassical) distribution of particles in phase space:

Let the number of particles in an element of "volume" $d^3\mathbf{r}\, d^3p$ about the point $\vec{\mathbf{r}}, \vec{p}$ be

$$f(\vec{r},\vec{p},t)\, d^3r\, d^3p / h^3$$

How does the distribution function $f(\vec{r},\vec{p},t)$ evolve with time (in the absence of collisions — we'll include them later)?



$$\vec{r}\,' = \vec{r} + \vec{v}\,dt + \cdots$$

$$\vec{p}\,' = \vec{p} + \frac{d\vec{p}}{dt}\,dt + \cdots$$

$$= \vec{p} + \vec{F}\,dt + \cdots$$

Conservation of particles implies

$$f(\vec{r}\,',\vec{p}\,',t')\,d^3r'\,d^3p' = f(\vec{r},\vec{p},t)\,d^3r\,d^3p.$$

The element of volume in phase space $d^3r'd^3p'$ may become distorted as a result of the motion. The new volume is

$$d^3r'\,d^3p' = |J|\,d^3r\,d^3p$$

- $$J = \begin{vmatrix} \dfrac{\partial \vec{r}'}{\partial \vec{r}} & \dfrac{\partial \vec{r}'}{\partial \vec{p}} \\[2ex] \dfrac{\partial \vec{p}'}{\partial \vec{r}} & \dfrac{\partial \vec{p}'}{\partial \vec{p}} \end{vmatrix}$$

From the equations of motion on page 2, we have

- $$\frac{\partial \vec{r}'}{\partial \vec{r}} = \underline{\mathbb{1}} \qquad \frac{\partial \vec{r}'}{\partial \vec{p}} = \frac{\partial \vec{v}}{\partial \vec{p}}\, dt$$

$$\frac{\partial \vec{p}'}{\partial \vec{r}} = \frac{\partial \vec{F}}{\partial \vec{r}}\, dt \qquad \frac{\partial \vec{p}'}{\partial \vec{p}} = \underline{\mathbb{1}}$$

$$\Rightarrow \quad J = 1 + \mathcal{O}(dt^2)$$

$$\Rightarrow \quad d^3r'\, d^3p' = d^3r\, d^3p$$

- $$\boxed{f(\vec{r}', \vec{p}', t') = f(\vec{r}, \vec{p}, t)}$$

Liouville's theorem

In words, Liouville's theorem states that, in the absence of collisions, the local density of particles in phase space is invariant, as seen by a test particle, which moves with the flow. In differential form, we have:

$$f(\vec{r}+\vec{v}\,dt,\ \vec{p}+\vec{F}dt,\ t+dt) - f(\vec{r},\vec{p},t) = 0$$

$$\left[\vec{v}\cdot\frac{\partial f}{\partial \vec{r}} + \vec{F}\cdot\frac{\partial f}{\partial \vec{p}} + \frac{\partial f}{\partial t}\right]dt = 0$$

$$\Rightarrow \quad \frac{\partial f}{\partial t} + \vec{v}\cdot\frac{\partial f}{\partial \vec{r}} + \vec{F}\cdot\frac{df}{d\vec{p}} = 0$$

$$\left[\text{or} \quad \frac{df}{dt} = 0\right]$$

More generally, $\frac{df}{dt} = \frac{\partial f}{\partial t}\Big|_{collisions}$

$$\boxed{\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = \frac{\partial f}{\partial t}\Big|_{collisions}}$$

Boltzmann equation

Note that for free particles, $\vec{v} = \frac{\vec{p}}{m}$. In general, for a particle with energy $\varepsilon(\vec{p})$, $\vec{v} = \frac{\partial \varepsilon}{\partial \vec{p}}$.

<u>relaxation-time approximation</u>

$$\frac{\partial f}{\partial t}\Big|_{collisions} = -\frac{f - f_0}{\tau(\vec{p})}$$

f_0 = distribution function locally in equilibrium

For Fermions,

$$f_0(\vec{r},\vec{p}) = \frac{1}{e^{\beta(\vec{r})(\varepsilon(\vec{p})-\mu(\vec{r}))}+1}$$

$\tau = \tau(\vec{p}) =$ relaxation time

This form of $\frac{\partial f}{\partial t}\Big|_{collisions}$ is motivated by the fact that collisions cause the distribution function to relax toward a local equilibrium with a time constant of order the collision time.

i) If $f = f_0$, then $\frac{df}{dt} = 0$ (equilibrium)

ii) If $\underset{f(\vec{p},t_0)}{\underset{\shortparallel}{f(\vec{r},\vec{p},t_0)}} \neq f_0$ and $\vec{F} = 0$

(No external force), then

$$\frac{\partial f}{\partial t} = - \frac{f - f_0}{\tau(\vec{p})}$$

$$\Rightarrow f(\vec{p}, t) = f_0(\vec{p}) + [f(\vec{p}, t_0) - f_0(\vec{p})] e^{-\frac{(t-t_0)}{\tau(\vec{p})}}$$

Hence τ = relaxation time.

For a system near equilibrium, we write $f = f_0 + f_1$, where $f_1 \ll f_0$.

Remark: The relaxation-time approx. is a very useful approx. to calculate transport coefficients. In principle, we should derive it from a microscopic treatment of scattering. This is, however, nontrivial.

Hopefully, one of our esteemed graduate students will have more to say on this subject later in the semester

Electrical conductivity

$\vec{F} = q\vec{E}$ $\quad$ $\vec{E}$ independent of $\vec{r}$ & t

$\Rightarrow \quad f = f(\vec{p}) \qquad \tau = \tau(\vec{p})$

$$q\vec{E}\cdot\frac{\partial f}{\partial \vec{p}} = -\frac{f-f_0}{\tau(\vec{p})}$$

$$q\vec{E}\cdot\left(\frac{\partial f_0}{\partial \vec{p}} + \frac{\partial f_1}{\partial \vec{p}}\right) = -\frac{f_1}{\tau(\vec{p})}$$

Clearly $f_1 \propto |\vec{E}|$, so

$\vec{E}\cdot\frac{\partial f_1}{\partial \vec{p}} \propto \vec{E}^2 \rightarrow$ neglect

Neglecting higher order terms in $\vec{E}$ is known as the limit of linear response.

$$\Rightarrow \quad f_1 = -q\,\tau(\vec{p})\,\vec{E}\cdot\frac{\partial f_0}{\partial \vec{p}}$$

Normalization of f

If $f\, d^3r\, d^3p/h^3$ is the number of particles in a volume $d^3x\, d^3p$ of phase space, then the density of particles in real space is $n(\vec{r}) = \int \frac{d^3p}{h^3} f(\vec{r},\vec{p})$.

The total number of particles is

$$N = \int d^3r\, n(\vec{r}) = \int \frac{d^3r\, d^3p}{h^3} f(\vec{r},\vec{p})$$

Note that $\frac{d^3p}{h^3} = \frac{d^3k}{(2\pi)^3}$.

Electrical current

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

$$= q \int \frac{d^3p}{h^3}\, \frac{\partial \varepsilon}{\partial \vec{p}}\, f(\vec{r},\vec{p})$$

$$= \frac{q}{m} \int \frac{d^3p}{h^3}\, \vec{p}\, f(\vec{r},\vec{p}) \quad \text{(for free particles)}$$

Now $\int d^3p\, \vec{p}\, f_0(\vec{r},\vec{p}) = 0$ by symmetry since $f_0(\vec{r},-\vec{p}) = f_0(\vec{r},\vec{p})$.

Thus $$\vec{J}_e = q \int \frac{d^3p}{h^3}\, \frac{\partial \varepsilon}{\partial \vec{p}}\, f_1$$

$$\vec{J}_e = q\int \frac{d^3p}{h^3}\frac{\partial \varepsilon}{\partial \vec{p}}\left(-q\tau(\vec{p})\,\vec{E}\cdot\frac{\partial f_o}{\partial \vec{p}}\right)$$

In general, we have the matrix relation

$$(\vec{J}_e)_i = \sum_j \sigma_{ij} E_j$$

$$\boxed{\sigma_{ij} = -q^2\int \frac{d^3p}{h^3}\,\tau(\vec{p})\,\frac{\partial \varepsilon}{\partial p_i}\,\frac{\partial f_o}{\partial p_j}}$$

Conductivity tensor

If $\tau(\vec{p}) = \tau$ (constant) and

$\frac{\partial \varepsilon}{\partial \vec{p}} = \frac{\vec{p}}{m}$ (free particles), then

$$\sigma_{ij} = -\frac{q^2\tau}{m}\int \frac{d^3p}{h^3}\, p_i\,\frac{\partial f_o}{\partial p_j}$$

Now, $\int_{-\infty}^{\infty} dp_j \; p_i \frac{\partial f_0}{\partial p_j} = \cancel{p_i f_0(\vec{p}) \Big|_{-\infty}^{\infty}}^{\,0}$

$$- \delta_{ij} \int_{-\infty}^{\infty} dp_i \, f_0$$

$$\Rightarrow \sigma_{ij} = \frac{q^2 \tau}{m} \delta_{ij} \underbrace{\int \frac{d^3p}{h^3} f_0(\vec{p})}_{n}$$

$$\boxed{\sigma_{ij} = \frac{n q^2 \tau}{m} \delta_{ij} \quad \text{for } \tau(\vec{p}) = \tau \text{ (constant)}}$$

<u>Remark on spin</u>: If we consider particles with nonzero spin, then

$$\vec{J}_e = \sum_{\sigma=-s}^{s} q \int \frac{d^3p}{h^3} \frac{\partial \varepsilon}{\partial \vec{p}} f_\sigma(\vec{r},\vec{p})$$

and $n(\vec{r}) = \sum_{\sigma=-s}^{s} \int \frac{d^3p}{h^3} f_\sigma(\vec{r},\vec{p})$.

Again, $\sigma_{ij} = \frac{nq^2\tau}{m} \delta_{ij}$

independent of spin.

Hall effect

Let $\vec{B} = B\hat{z}$ and $E_z = 0$, as in the discussion in lecture 11.

No explicit dependence on $\vec{r}$ or t

$\Rightarrow \quad f = f(\vec{p}), \quad \tau = \tau(\vec{p})$

$$\vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = -\frac{f - f_0}{\tau(\vec{p})}$$

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

$$q\left(\vec{E} + \frac{\vec{V}}{c}\times\vec{B}\right)\cdot\left(\frac{\partial f_0}{\partial\vec{p}} + \frac{\partial f_1}{\partial\vec{p}}\right) = -\frac{f_1}{\tau(\vec{p})}$$

For free particles,

$\frac{\partial f_0}{\partial\vec{p}} \propto \vec{V}$, since $f_0 = f(\vec{p}^2)$,

so $(\vec{V}\times\vec{B})\cdot\frac{\partial f_0}{\partial\vec{p}} = 0$. Also,

$\vec{E}\cdot\frac{\partial f_1}{\partial\vec{p}} \propto \vec{E}^2$, so we can

neglect it. We obtain:

$$f_1 = -\tau(\vec{p})\left[q\vec{E}\cdot\frac{\partial f_0}{\partial\vec{p}} + q\frac{\vec{V}}{c}\times\vec{B}\cdot\frac{\partial f_1}{\partial\vec{p}}\right]$$

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

- $$\vec{J}_e = -q^2 \int \frac{d^3p}{h^3} \tau(\vec{p})\, \vec{v} \left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right) \cdot \frac{\partial f}{\partial \vec{p}}$$

If we demand $J_y = 0$, then

$$0 = J_y = -q^2 \int \frac{d^3p}{h^3} \tau(\vec{p})\, v_y \left(E_x \frac{\partial f_0}{\partial p_x} + E_y \frac{\partial f_0}{\partial p_y} + \frac{B}{c} v_y \frac{\partial f_1}{\partial v_x} - \frac{B}{c} v_x \frac{\partial f_1}{\partial v_y} \right)$$

- Suppose $\tau(\vec{p}) = \tau$ (constant):

$$0 = \int \frac{d^3p}{h^3} v_y \left(E_x \frac{\partial f_0}{\partial p_x} + E_y \frac{\partial f_0}{\partial p_y} + \frac{B}{c} v_y \frac{\partial f_1}{\partial p_x} - \frac{B}{c} v_x \frac{\partial f_1}{\partial p_y} \right)$$

(integrating by parts)

- $$0 = -\frac{n E_y}{m} + \frac{B}{cm} \int \frac{d^3p}{h^3} f_1 v_x$$

$$0 = -nE_y + \frac{B}{c}\frac{j_x}{q}$$

$$E_y = \frac{B}{nqc} j_x$$

$$\rho_H = \frac{E_y}{j_x} = \frac{B}{nqc}$$

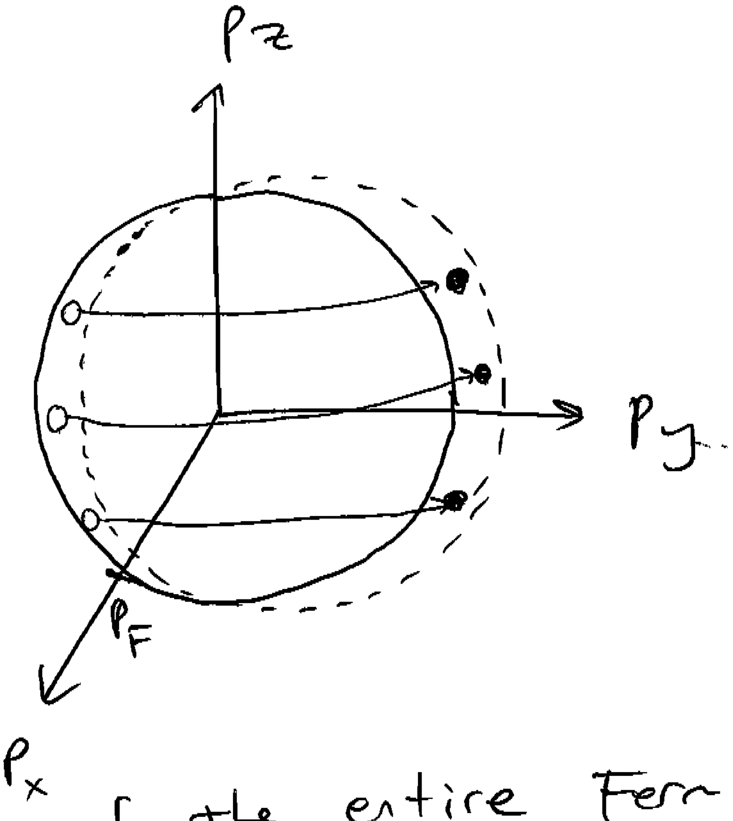
$$\boxed{R_H = \frac{\rho_H}{B} = \frac{1}{nqc}}$$

Remark: The results $\sigma = \frac{nq^2\tau}{m}$ and $R_H = \frac{1}{nqc}$ are identical to those obtained from Newton's equations,

$$m\frac{d\vec{V}}{dt} = q\left(\vec{E} + \frac{\vec{V}}{c}\times\vec{B}\right) - \frac{m\vec{V}}{\tau}.$$

Q: How can this result be reconciled with Fermi-Dirac statistics, which say that electrons cannot accelerate freely in every case, since they are prohibited from entering filled states?

Answer:



Acceleration of the entire Fermi sphere can be considered as taking some electrons from filled states on one side and putting them in empty states on the other side.