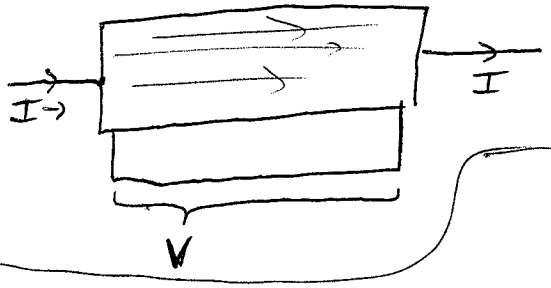
Transport in Free Fermi Gas

- "Transport" refers to the ability (or lack thereof) of a material to support motion of electric charge, energy, or other quantities from one point in the material to another.

- Familiar examples:

  - Ohm's Law

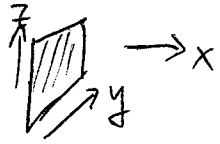


$V = IR$ (resistivity)

$\vec{E} = \rho \vec{J}$ or $\vec{J} = \sigma \vec{E}$ ($\sigma = \frac{1}{\rho}$) (conductivity)

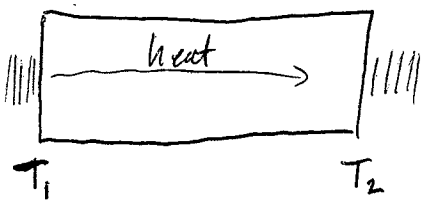
$\vec{J}$: current density, has units of current/area

- J_x measures current passing thru small square



$(I_x = J_x \, dy \, dz)$

  - Fourier's Law



$\vec{J}_Q = -K \vec{\nabla} T$

$\vec{J}_Q$: heat current density

K: thermal conductivity

(units: $\frac{\text{Energy}}{\text{Time}} \cdot \frac{1}{\text{Length}^2}$)

- Empirically, metals obey both Ohm's & Fourier's Laws.

- Calculate response of free gas to applied E-field ...

$$\frac{d\vec{P}_{tot}}{dt} = -Ne\vec{E} \Rightarrow \vec{P}_{tot} = -Ne\vec{E}t \Rightarrow \vec{P}_{avg} = -e\vec{E}t$$

$$\vec{J} = -\frac{ne\vec{p}_{avg}}{m} = \frac{ne^2t}{m}\vec{E} \Rightarrow \text{"}\sigma = \frac{ne^2t}{m}\text{"}!$$

N.t^m Ohm's Law → electrons are accelerated by E-field.

- Need mechanism to reduce total momentum → collisions with impurities, ions, motion of ions, ...
  ↳ focus on this for now

NB: Electron-electron collisions won't help us here → they conserve momentum.

Simple model of impurities:

$$\hat{H} = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

↑ 1-electron Hamiltonian

↑ impurity potential

- Solving for general $V(\vec{r})$ is hard.
- Possible to work out properties for a random $V(\vec{r})$. Outside scope of this course...

Instead .....

Take semiclassical approach

Why?
- Easier (conceptually & technically) to extract transport properties
- It can be justified for many cases of interest

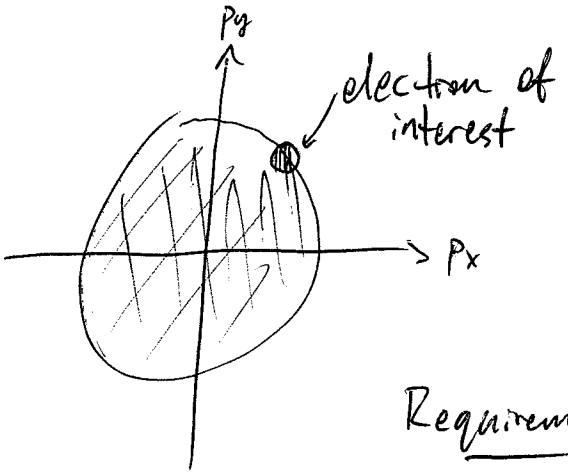
Basic idea:
(1) Understand semiclassical motion of single electron
(2) " " " " many electrons
(construct distribution function)
(3) Incorporate scattering of electrons by impurities (& other kinds of scattering)

#(1) — Construct single electron wavepackets

- Need to localize position and momentum with restriction $\Delta p \Delta r \geq \hbar$
- There are other conditions on Δp and Δr. Need to see if they allow us to proceed ...

- Condition on Δp

  - We want to be able to talk about electrons on a particular piece of Fermi surface. If we can't do this, then we can't even specify correct ground state (i.e., states full below p_F) in our semiclassical description.



Requirement: $\Delta p \ll p_F$

- Condition on Δr

  - Suppose applied $\vec{E}$, $\vec{B}$, $\vec{\nabla}T$ vary on a length scale longer than L_f. (So, spatially constant fields means $L_f = \infty$.) → (So, we are introducing the length scale L_f to characterize the spatial variation of the fields.)
  - We must require: $\Delta r \ll L_f$
  - If we don't require this, the fields will affect internal structure of wavepacket quantum ~~mechanically~~ mechanically.

#

Combine conditions on Δp & Δr

- Suppose $L_f = 100$ nm (UV light), and $p_F \sim \hbar[10^8 \text{ cm}^{-1}]$

Then: $L_f p_f \sim 10^3 \hbar >> \Delta r \Delta p \geq \hbar$

- gives "room" to construct wavepackets satisfying both conditions
- As L_f gets bigger (and it's often much bigger), situation gets better.

Semiclassical equations of motion

- Want $\frac{d\vec{r}}{dt}$ and $\frac{d\vec{k}}{dt}$ as functions of $\vec{k}, \vec{r}$ and applied fields.

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m} = \frac{\hbar\vec{k}}{m} = \frac{1}{\hbar}\frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} \equiv \vec{v}(\vec{k})$$

$$\vec{F} = \frac{d\vec{p}}{dt} = \hbar\frac{d\vec{k}}{dt} = -e\vec{E}(\vec{r}) - \frac{e\vec{v}(\vec{k})}{c} \times \vec{B}(\vec{r})$$

Move on to task #2 — Semiclassical motion of many electrons

- Nonequilibrium distribution function $g(\vec{r},\vec{k},t)$

~ $dN(\vec{r},\vec{k},t) = g(\vec{r},\vec{k},t)\,(d^3\vec{r})\cdot 2\,\frac{d^3k}{(2\pi)^3}$

↓ # electrons at $\vec{r}$ occupying state $|\vec{p}=\hbar\vec{k}\rangle$ at time t.

↑ for spin

$\Rightarrow N = \int d^3\vec{r}\,\frac{d^3k}{4\pi^3}\,g(\vec{r},\vec{k},t)$

~ Equilibrium: $g(\vec{r},\vec{k},t) = f(\varepsilon_{\vec{k}})$ (independent of $\vec{r},t$)

Express physical quantities in terms of g:

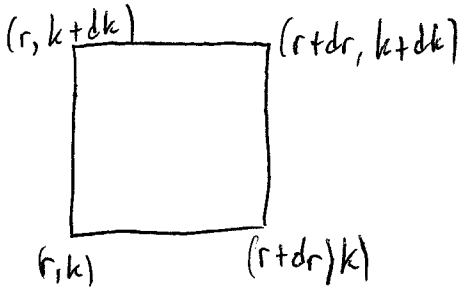
- Density: $n(\vec{r},t) = \int \frac{d^3\vec{k}}{4\pi^3}\,g(\vec{r},\vec{k},t)$

- Current density: $\vec{J}(\vec{r},t) = \int \frac{d^3\vec{k}}{4\pi^3}\,(-e\vec{v}(\vec{k}))\,g(\vec{r},\vec{k},t)$

⋮

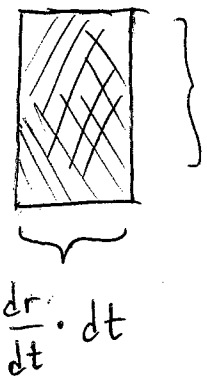
Need to understand time-evolution of $g(\vec{r},\vec{k},t)$

- Specialize to one dimension (generalization to higher-dimensions will follow immediately). Coordinates r, k.
- Consider region of (r,k) space:



$$\frac{dN(r,k,t)}{dt} = \frac{\partial g}{\partial t}(r_x,k_x,t)\, dr\, \frac{dk}{(2\pi)} \cdot 2$$

- dN changes only by particles entering/leaving at the edges.
- Consider flow of particles in through left edge



☆ # particles per unit time that come in thru left edge is:

$$\left[g(r,k,t)\frac{dr}{dt}\right] \cdot dt\, \frac{dk}{(2\pi)} \cdot 2$$

~~the one using the fact~~

☆ Similarly, # leaving thru right edge: $\left[-g(r+dr,k,t)\frac{dr}{dt}\right] dt\, \frac{dk}{(2\pi)} \cdot 2$

$\Rightarrow$ total # per time going in (left & right edges only) $= \left[-\frac{\partial g}{\partial r}(r,k,t)\frac{dr}{dt}\right] dr\, \frac{dk}{(2\pi)} \cdot 2 \cdot dt$

Note: We neglected all dependence of $g(r,k,t)$ on coordinates in the "strip".

Why dk?

- We should assume dt is "extremely small," even smaller than infinitesimals dr, dk. (More precisely, $\left|\left(\frac{dr}{dt}\right)dt\right| \ll dr$.)

This is fine since we just want to compute a rate, and in this case we can neglect dependence on r inside the strip.

Note 2: Why did we neglect dependence of $g(r,k,t)$ on k?

→ If we include this, it contributes a term $\propto dk^2$, which should be dropped compared to leading term $\propto dk$.

Same analysis for top and bottom edges yields:

$$\left(\begin{array}{c}\text{total \# per unit}\\ \text{time going in}\end{array}\right) = \frac{dN}{dt}(r,k,t) = \left[-\frac{\partial g}{\partial r}\frac{dr}{dt} - \frac{\partial g}{\partial k}\frac{dk}{dt}\right] dr\left(\frac{dk}{2\pi}\right)\cdot 2$$

$$\Rightarrow \quad \frac{\partial g}{\partial t} = -\frac{\partial g}{\partial r}\frac{dr}{dt} - \frac{\partial g}{\partial k}\frac{dk}{dt}$$

"Collisionless Boltzmann equation"

- Comments:

(1) In this equation, we should substitute for $\frac{dr}{dt}$ and $\frac{dk}{dt}$ using semiclassical equations of motion (e.g. $\frac{dr}{dt} = v(k)$). This gives a differential equation for $g(r,k,t)$ involving known functions of (r,k,t) – e.g. $\vec{v}(k)$, $\vec{E}(\vec{r})$, $\vec{B}(\vec{r})$.

(2) We actually showed in our derivation that the flow in (r,k) space is incompressible:

density at time t_i = density at time t_f.

- This is true more generally, for any equations of motion derived from a Hamiltonian → "Liouville's Theorem"

see below ↓

↳ A&M Appendix H; "Statistical Mechanics" by Huang.

- The equation we derived is a restatement of incompressibility. Write:

$$0 = \frac{\partial g}{\partial t} + \frac{\partial g}{\partial r}\frac{dr}{dt} + \frac{\partial g}{\partial k}\frac{dk}{dt} \equiv \frac{dg}{dt}$$

$\frac{dg}{dt}$ is time derivative of g following the path of the semiclassical trajectory $(r(t), k(t))$.

NB: Don't confuse $\frac{dg}{dt}$ and $\frac{\partial g}{\partial t}$! Usually we'll work with $\frac{\partial g}{\partial t}$, which is just the rate of change of $g(r,k,t)$ at the fixed point (r,k).

Generalization to 3 dimensions

$$\boxed{\frac{\partial g}{\partial t} + \frac{\partial g}{\partial \vec{r}} \cdot \frac{d\vec{r}}{dt} + \frac{\partial g}{\partial \vec{k}} \cdot \frac{d\vec{k}}{dt} = 0}$$

Now for task #3 – Scattering

Abstractly, one generally writes:

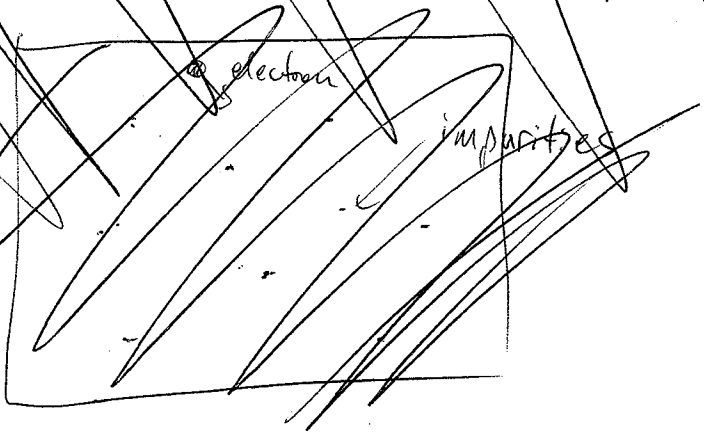
$$\frac{\partial g}{\partial t} + \frac{\partial g}{\partial \vec{r}} \cdot \frac{d\vec{r}}{dt} + \frac{\partial g}{\partial \vec{k}} \cdot \frac{d\vec{k}}{dt} = \left(\frac{\partial g}{\partial t}\right)_{coll}$$

"collision integral"

- This is the Boltzmann equation
- Collision integral gives rate of change of g due to all collisions. In general it's a nonlinear function of g.

Collision integral for impurity scattering

- Consider single electron with momentum $\vec{k}$. It scatters off a random set of impurities.



Collision integral for impurity scattering

- Define probability for electron at $\vec{k}$ to scatter to (volume element around) $\vec{k}'$ in time dt:

$$\text{Prob} = W_{\vec{k}\vec{k}'} \frac{d^3\vec{k}'}{(2\pi)^3} dt$$

- Consider electrons in infinitesimal box near $(\vec{r}, \vec{k})$.

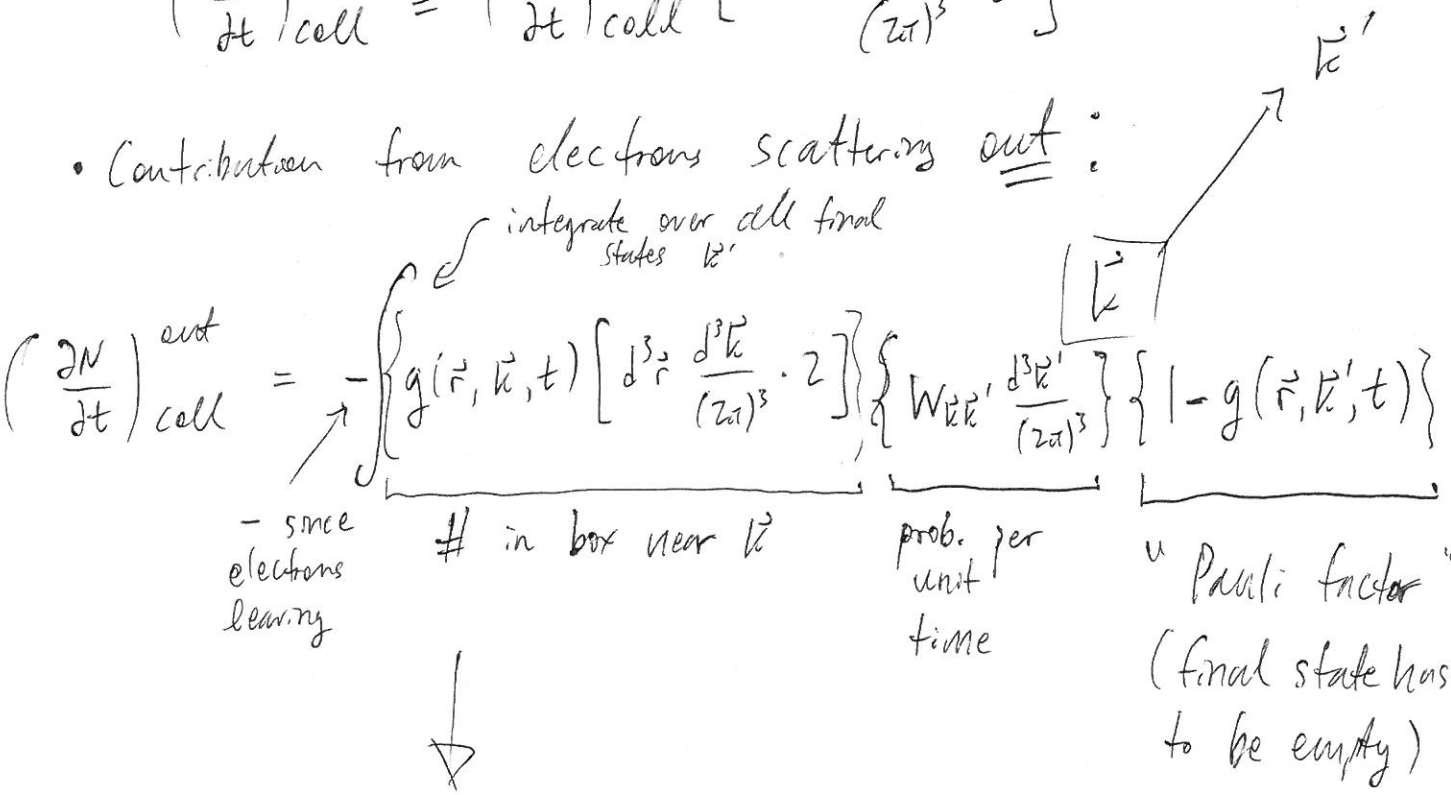
$$N = g(\vec{r}, \vec{k}, t) \left[d^3\vec{r} \frac{d^3\vec{k}}{(2\pi)^3} \cdot 2 \right]$$

(2 ↑ sp.n.)

- Rate of change of N due to collisions:

$$\left(\frac{\partial N}{\partial t}\right)_{coll} \equiv \left(\frac{\partial g}{\partial t}\right)_{coll} \left[d^3\vec{r} \frac{d^3\vec{k}}{(2\pi)^3} \cdot 2 \right]$$

- Contribution from electrons scattering <u>out</u>:



$$\left(\frac{\partial N}{\partial t}\right)^{out}_{coll} = \left[d^3\vec{r}\,\frac{d^3\vec{k}}{(2\pi)^3}\cdot 2\right]\left[-\int \frac{d^3\vec{k}'}{(2\pi)^3} W_{\vec{k}\vec{k}'}\, g(\vec{r},\vec{k},t)\left[1-g(\vec{r},\vec{k}',t)\right]\right]$$

$$\equiv -R_{out}$$

- Contribution from electrons scattering into $\vec{k}$:

$$\left(\frac{\partial N}{\partial t}\right)^{in}_{coll} = \int \left\{ g(\vec{r},\vec{k}',t)\left[d^3\vec{r}\,\frac{d^3\vec{k}'}{(2\pi)^3}\cdot 2\right]\right\} \left\{ W_{\vec{k}'\vec{k}}\,\frac{d^3\vec{k}}{(2\pi)^3}\right\} \cdot \left\{1-g(\vec{r},\vec{k},t)\right\}$$

integrate over initial states $\vec{k}'$

prob. per time

in box near $\vec{k}'$ (initial state)

"Pauli factor" for final state

$$= \left[d^3\vec{r}\,\frac{d^3\vec{k}}{(2\pi)^3}\cdot 2\right]\left[\int \frac{d^3\vec{k}'}{(2\pi)^3} W_{\vec{k}'\vec{k}}\, g(\vec{r},\vec{k}',t)\left[1-g(\vec{r},\vec{k},t)\right]\right]$$

$$\equiv R_{in}$$

Combining these: $\left(\frac{\partial N}{\partial t}\right)_{coll} = \left(\frac{\partial N}{\partial t}\right)^{out}_{coll} + \left(\frac{\partial N}{\partial t}\right)^{in}_{coll}$

$$\Rightarrow \left(\frac{\partial g}{\partial t}\right)_{coll} = R_{in} - R_{out}$$

- Note: $W_{\vec{k}\vec{k}'} = W_{\vec{k}'\vec{k}}$

- Assume: (1) Time reversal symmetry
  (2) Inversion symmetry ($\vec{r} \to -\vec{r}$) about scattering center

(1) $\Rightarrow$ $W_{\vec{k},\vec{k}'} = W_{-\vec{k}',-\vec{k}}$

(2) $\Rightarrow$ $W_{-\vec{k}',-\vec{k}} = W_{\vec{k}'\vec{k}}$ ✓

- Impurity scattering is elastic — conserves energy.

$$\Rightarrow \quad W_{\vec{k}\vec{k}'} = \delta(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'})\, \tilde{W}_{\vec{k}\vec{k}'}$$

Collision integral is:

$$\left(\frac{\partial g}{\partial t}\right)_{coll} = R_{in} - R_{out}$$

$$= \int \frac{d^3\vec{k}'}{(2\pi)^3} \left[g(\vec{r},\vec{k},t) - g(\vec{r},\vec{k}',t) \right] W_{\vec{k}\vec{k}'}$$

$$= \int \frac{d^3\vec{k}'}{(2\pi)^3} \left[g(\vec{r},\vec{k},t) - g(\vec{r},\vec{k}',t) \right] \delta(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'})\, \tilde{W}_{\vec{k}\vec{k}'}$$

- Nonlinear terms cancel out → Boltzmann equation is a linear integral equation. Special for impurity scattering.
- $\left(\frac{\partial g}{\partial t}\right)_{coll}$ vanishes in equilibrium, as it should.

(Left-hand side of Boltzmann equation vanishes in equilibrium, so collision integral must also vanish. → Role of collisions is to establish equilibrium.)

Relaxation time approximation

- While our ~~eqn~~ linear Boltzmann equation is in principle solvable, it's still complicated.
- We'll make a simplifying assumption — for now it's phenomenological, after we get some experience solving the Boltzmann equation, we'll justify it.

Assume: $$\left(\frac{\partial g}{\partial t}\right)_{coll} = -\frac{1}{\tau}\left[g(\vec{r},\vec{k},t) - g^{(0)}(\vec{r},\vec{k},t)\right]$$

- $g^{(0)}$ is local equilibrium distribution function, i.e.

$$g^{(0)}(\vec{k}) = f(\varepsilon_{\vec{k}}), \text{ where } T = T(\vec{r}),\ \mu = \mu(\vec{r})$$

"Role of collisions is to restore local equilibrium!"

- τ is phenomenological relaxation time. Can have $\tau = \tau(\varepsilon_{\vec{k}})$, or $\tau = \tau(\vec{k})$, but for simplicity we consider (for now) τ constant.