Lecture 15
Transport Phenomena

Relaxation Time Approx – Assumption

Left alone, non-equilibrium will tend to go to equilibrium

- Collisions will happen at time scale τ.
- Collisions wipe out all information about previous distribution.
- If equilibrium (Fermi-Dirac), then stay equilibrium.

$$dg_n(\vec{r},\vec{k},t)|_{coll} = \frac{dt}{\tau_n(\vec{r},\vec{k})} g_n^0(\vec{r},\vec{k}) - \frac{dt}{\tau_n(\vec{r},\vec{k})} g_n(\vec{r},\vec{k})$$

g is the distribution function; 0 means (local) equilibrium

Working Formula

$$g(t) = \int_{-\infty}^{t} \frac{dt'}{\tau(t')} g^0(t') P(t,t')$$

$$P(t,t') = P(t,t'+dt')[1 - \frac{dt'}{\tau(t')}]$$

$$\frac{\partial P(t,t')}{\partial t'} = \frac{P(t,t')}{\tau(t')}$$

$$P(t,t') = \exp(-\int_{t'}^{t} \frac{dx}{\tau(x)})$$

Examine the property of P and apply the semi-classical EOM

$$g(t) = \int_{-\infty}^{t} dt' g^0(t') \frac{\partial P(t,t')}{\partial t'}$$

$$g(t) = g^0(t) - \int_{-\infty}^{t} dt' P(t,t') \frac{dg^0(t')}{dt'}$$

$$g(t) = g^0 + \int_{\infty}^{t} dt' P(t,t')[-\frac{\partial f}{\partial \varepsilon} \vec{v} \cdot (-e\vec{E} - \nabla\mu - (\frac{\varepsilon - \mu}{T})\nabla T)]$$

Simplify, assuming

- Weak E and temperature gradient (also $\nabla\mu \sim O(\nabla T)$)
- No spatial dependence in field and τ
- $\tau = \tau(\varepsilon(k))$

$$\mu(\vec{x},t) = \mu_{equilibrium}(n, T(\vec{x},t))$$

$$g(\vec{k},t) = g^0(\vec{k}) + \int_{\infty}^{t} dt' e^{-(t-t')/\tau(\varepsilon(\vec{k}))} \left(-\frac{\partial f}{\partial \varepsilon}\right) \vec{v}(\vec{k}(t')) \cdot \left[(-e\vec{E}(t') - \nabla\mu(t') - (\frac{\varepsilon - \mu}{T})\nabla T(t')\right]$$

DC Electrical Conductivity

$$g(\vec{k}) = g^0(\vec{k}) - e\vec{E}\cdot\vec{v}(\vec{k})\tau\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$\vec{j} = -e\int \frac{d\vec{k}}{4\pi^3}\vec{v}(\vec{k})g$$

$$\begin{aligned}
\overleftrightarrow{\sigma} &= e^2\int \frac{d\vec{k}}{4\pi^3}\tau\vec{v}(\vec{k})\vec{v}(\vec{k})\left(-\frac{\partial f}{\partial \varepsilon}\right) \\
&\approx e^2\tau(\varepsilon_F)\int \frac{d\vec{k}}{4\pi^3\hbar}\frac{\partial\vec{v}(\vec{k})}{\partial\vec{k}}f(\varepsilon(\vec{k})) \\
&\approx e^2\tau(\varepsilon_F)\int_{occupied} \frac{d\vec{k}}{4\pi^3}\overleftrightarrow{M}^{-1} \\
&= e^2\tau(\varepsilon_F)\int_{unoccupied} \frac{d\vec{k}}{4\pi^3}(-\overleftrightarrow{M}^{-1})
\end{aligned}$$

Conductivity tensor

- Generally anisotropic
- Electron and Hole view
- Reduces to Drude in simple case

$$\int_{unit\,cell} d\vec{k}\nabla P(\vec{k}) = 0,\ for\,a\,periodic\,function\,P$$

Currents, Electric and Thermal

- For a volume element

  dQ=TdS=dE- μdN

$$\vec{j} = \overleftrightarrow{L}_{11}\vec{\varepsilon} + \overleftrightarrow{L}_{12}(-\nabla T)$$

$$\vec{j}_q = \overleftrightarrow{L}_{21}\vec{\varepsilon} + \overleftrightarrow{L}_{22}(-\nabla T)$$

$$\vec{j}_q = T\vec{j}_s = \vec{j}_\varepsilon - \mu\vec{j}_n$$

$$\vec{j}_q = \sum_n \int \frac{d\vec{k}}{4\pi^3}[\varepsilon_n(\vec{k}) - \mu]\vec{v}_n(\vec{k})g_n(\vec{k})$$

$$g(\vec{k}) = g_0(\vec{k}) + \tau(\varepsilon(\vec{k}))(-\frac{\partial f}{\partial \varepsilon})\vec{v}(\vec{k}) \cdot [-e\vec{\varepsilon} + \frac{\varepsilon(\vec{k}) - \mu}{T}(-\nabla T)]$$

$$\vec{\varepsilon} = \vec{E} + \frac{\nabla \mu}{e}$$

Currents, Electric and Thermal

$$\vec{j} = \overleftrightarrow{L}_{11}\vec{\mathcal{E}} + \overleftrightarrow{L}_{12}(-\nabla T)$$

$$\vec{j}_q = \overleftrightarrow{L}_{21}\vec{\mathcal{E}} + \overleftrightarrow{L}_{22}(-\nabla T)$$

$$\overleftrightarrow{\sigma}(\varepsilon) \equiv e^2\tau(\varepsilon)\int \frac{d\vec{k}}{4\pi^3}\delta(\varepsilon - \varepsilon(\vec{k}))\vec{v}(\vec{k})\vec{v}(\vec{k})$$

$$\overleftrightarrow{L}_{\alpha} = \int d\varepsilon\left(-\frac{\partial f}{\partial \varepsilon}\right)(\varepsilon - \mu)^{\alpha}\overleftrightarrow{\sigma}(\varepsilon)$$

$$\overleftrightarrow{L}_{11} = \overleftrightarrow{L}_{0}$$

$$\overleftrightarrow{L}_{21} = T\overleftrightarrow{L}_{12} = -\frac{1}{e}\overleftrightarrow{L}_{1}$$

$$\overleftrightarrow{L}_{22} = \frac{1}{e^2 T}\overleftrightarrow{L}_{2}$$

$$\overleftrightarrow{L}_{11} \approx \overleftrightarrow{\sigma}(\varepsilon_F) = \overleftrightarrow{\sigma}$$

$$\overleftrightarrow{L}_{21} = T\overleftrightarrow{L}_{12} = -\frac{\pi^2}{3e}(k_B T)^2\overleftrightarrow{\sigma}'(\varepsilon_F)$$

$$\overleftrightarrow{L}_{22} = \frac{\pi^2}{3}\frac{k_B^2 T}{e^2}\overleftrightarrow{\sigma}$$

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon) \approx \int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 H'(\mu)$$

Thermal Conductivity

- Temperature gradient and no electric current

$$\vec{\varepsilon} = -\left(\overleftrightarrow{L}_{11}\right)^{-1}\overleftrightarrow{L}_{12}(-\nabla T)$$

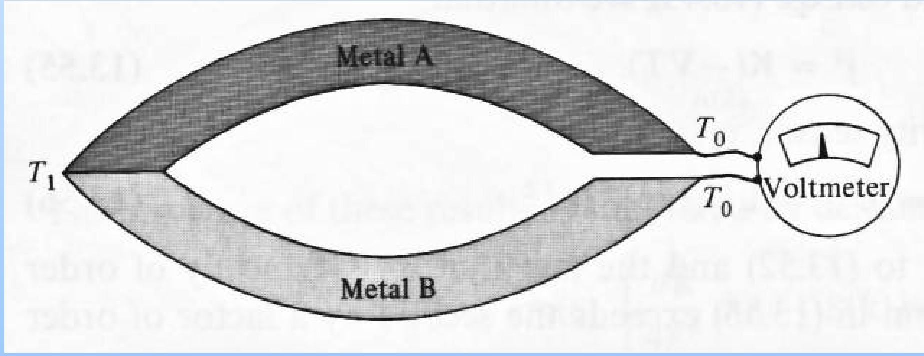
$$\vec{j}_q = -\overleftrightarrow{L}_{21}\left(\overleftrightarrow{L}_{11}\right)^{-1}\overleftrightarrow{L}_{12}(-\nabla T) + \overleftrightarrow{L}_{22}(-\nabla T) \equiv -\overleftrightarrow{K}\nabla T$$

$$\overleftrightarrow{K} = \overleftrightarrow{L}_{22} - \overleftrightarrow{L}_{21}\left(\overleftrightarrow{L}_{11}\right)^{-1}\overleftrightarrow{L}_{12}$$

$$\overleftrightarrow{K} \approx \overleftrightarrow{L}_{22} = \frac{\pi^2}{3}\frac{k_B^2 T}{e^2}\overleftrightarrow{\sigma}$$

Wiedenmann-Franz law again – under very general condition

Thermoelectric Power

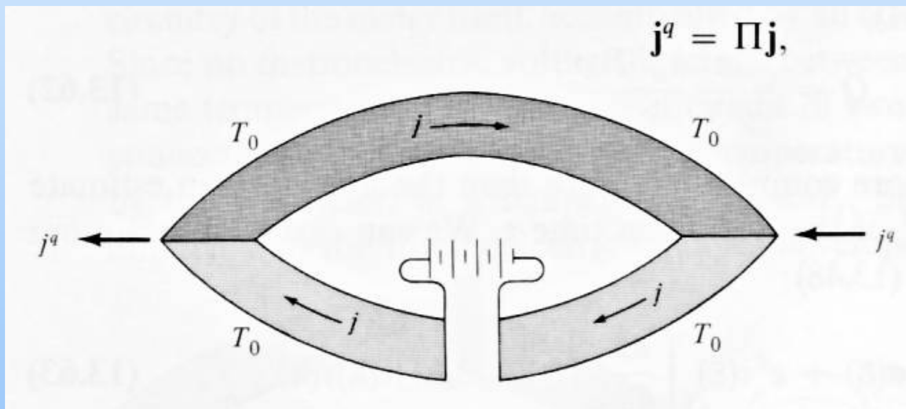


$$\vec{\varepsilon} = Q\nabla T$$

$$Q = \frac{L_{12}}{L_{11}}$$

$$Q = -\frac{\pi^2}{3}\frac{k_B^2 T}{e}\frac{\sigma'}{\sigma}$$

Peltier Effect



$$\vec{j}_q = \Pi \vec{j}$$

$$\Pi = L_{21}/L_{11}$$

$$\Pi = TQ$$

Boltzmann Equation

$$\frac{dg}{dt} = \left(\frac{\partial g}{\partial t}\right)_{coll}$$

$$g(\vec{r}, \vec{k}, t) = g(\vec{r} - \vec{v}(\vec{k})dt, \vec{k} - \vec{F}dt/\hbar, t - dt) + \left(\frac{\partial g}{\partial t}\right)_{out} dt + \left(\frac{\partial g}{\partial t}\right)_{in} dt$$

$$\frac{\partial g}{\partial t} + \vec{v} \cdot \frac{\partial g}{\partial \vec{r}} + \vec{F} \cdot \frac{1}{\hbar}\frac{\partial g}{\partial \vec{k}} = \left(\frac{\partial g}{\partial t}\right)_{coll}$$

W: prob per unit time

$$W_{\vec{k},\vec{k}'}$$

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

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

$$\left(\frac{\partial g}{\partial t}\right)_{in} = \int \frac{d\vec{k}'}{(2\pi)^3} W_{\vec{k}',\vec{k}}\, g'[1 - g] \qquad \left[\equiv \frac{g_0}{\tau(\vec{k})}\right]$$

Impurity Scattering

- Elastic, and weak scattering

$$W_{\vec{k},\vec{k}'} = \frac{2\pi}{\hbar} n_i \delta(\varepsilon(\vec{k}) - \varepsilon(\vec{k}')) |\langle \vec{k}|U|\vec{k}'\rangle|^2$$

Due to symmetry, the collision term

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

becomes

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

Impurity Scattering in Isotropic Material

Assume W depends on |k| and angle only, then

Relaxation time approximation is <u>exact</u>!!

$$g(\vec{k}) = g_0(\vec{k}) + \vec{a}(\varepsilon)\cdot\vec{k}$$

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

$$-\vec{a}(\varepsilon)\cdot\int \frac{d\vec{k}'}{(2\pi)^3}W_{\vec{k},\vec{k}'}[\vec{k}-\vec{k}']$$

Need to show $-\frac{1}{\tau}(g-g_0) = -\frac{1}{\tau}\vec{a}\cdot\vec{k}$

$$\int d\vec{k}' W_{\vec{k},\vec{k}'}\vec{k}' = \vec{k}\int d\vec{k}' W_{\vec{k},\vec{k}'}\hat{k}\cdot\hat{k}'$$

$$\frac{1}{\tau(\vec{k})} = \int \frac{d\vec{k}'}{(2\pi)^3}W_{\vec{k},\vec{k}'}[1-\hat{k}\cdot\hat{k}']$$

Does the Job!