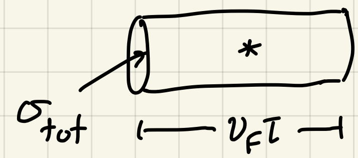
$$\delta f_{\mathbf{k}}(t) = \sum_{L,M} A_{LM}(t)\, Y_{LM}(\hat{k})$$

$(v_F \tau)(\sigma_{tot})(n_{imp}) \equiv 1$



we obtain

$$\frac{\partial A_{LM}}{\partial t} + (1-\nu_L)\, n_{imp}\, v_F\, \sigma_{tot}\, A_{LM} = 0$$

and

$$\tau_L^{-1} = (1-\nu_L)\, n_{imp}\, v_F\, \sigma_{tot}$$

$\nu_\infty = 0$

Note $\tau_{transport} = \tau_{L=1}$ and $\tau_{single\ particle} = \tau_{L=\infty}$. Thus,

$$A_{LM}(t) = A_{LM}(0)\, e^{-t/\tau_L}$$

- **Lecture 6 (Jan. 21)**

Screening: For a Coulomb impurity of charge $+Ze$,

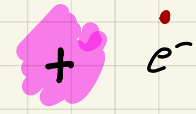
$$U(\vec{r}) = -\frac{Ze^2}{r} \quad \Rightarrow \quad \hat{U}(\vec{q}) = -\frac{4\pi Z e^2}{\vec{q}^{\,2}}$$

This results in the Rutherford differential cross section,

$$\sigma_F(\vartheta) = \left(\frac{Ze^2}{4\varepsilon_F \sin^2(\frac{1}{2}\vartheta)}\right)^2$$

for electrons at the Fermi level. There is a strong ϑ^{-4} divergence as $\vartheta \to 0$, and the expression for the transport lifetime diverges logarithmically. What went wrong?

The problem here is that we have not accounted for **screening**. There are many electrons, and they rearrange themselves so as to screen an impurity charge. The resulting potential arising from the impurity and the rearranged electrons is of the Yukawa form,



$$U(\vec{r}) = -\frac{Ze^2}{r}\, e^{-r/\lambda} \quad \Rightarrow \quad \hat{U}(\vec{q}) = -\frac{4\pi Z e^2}{\vec{q}^{\,2} + \lambda^{-2}}$$

where λ is the **screening length**. The resulting differential scattering cross section is

$$\sigma_F(\vartheta) = \left(\frac{Ze^2}{4\varepsilon_F} \cdot \frac{1}{\sin^2(\frac{1}{2}\vartheta) + (2k_F\lambda)^{-2}} \right)^2$$

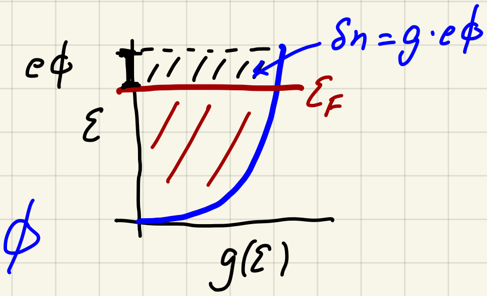
The nasty ϑ^{-4} divergence is thus cut off, and the transport lifetime is finite:

$$\frac{1}{\tau_F} = 2\pi n_{imp} v_F \left(\frac{Ze^2}{4\varepsilon_F}\right)^2 \int_0^\pi d\vartheta \, \sin\vartheta \,(1-\cos\vartheta) \left(\frac{1}{\sin^2(\frac{1}{2}\vartheta) + (2k_F\lambda)^{-2}} \right)^2$$

$$= 2\pi n_{imp} v_F \left(\frac{Ze^2}{4\varepsilon_F}\right)^2 \left\{ \ln(1+\alpha) - \frac{\alpha}{1+\alpha} \right\}$$

where $\alpha = 4k_F^2\lambda^2$.

The main theory for (static) screening in metals is called **Thomas-Fermi theory**. A weak electrostatic potential $\phi(\vec{r})$ induces a change in the local electron density $\delta n(\vec{r}) = g(\varepsilon_F)\, e\phi(\vec{r})$, where $g(\varepsilon_F)$ is the DOS at the Fermi level. In $d=3$, we have $g(\varepsilon_F) = \frac{m^* k_F}{\pi^2 \hbar^2}$ for ballistic dispersion. This imbalance is in turn related to $\phi(\vec{r})$ through Poisson's equation:



$$\nabla^2 \phi = 4\pi e\, \delta n$$
$$= 4\pi e^2 g(\varepsilon_F)\, \phi \equiv \lambda_{TF}^{-2}\, \phi$$

where $\lambda_{TF} = \left(4\pi e^2 g(\varepsilon_F)\right)^{-1/2}$. With an impurity test charge $Q = +Ze$ at the origin,

$$\nabla^2 \phi = \lambda_{TF}^{-2}\, \phi - 4\pi Z e\, \delta(\vec{r}) \quad \Rightarrow \quad (\vec{q}^{\,2} + \lambda_{TF}^{-2})\, \hat{\phi}(\vec{q}) = 4\pi Z e$$

Thus, $\hat{U}(\vec{q}) = -e\hat{\phi}(\vec{q}) = -\dfrac{4\pi Z e^2}{\vec{q}^{\,2} + \lambda_{TF}^{-2}} \Rightarrow U(\vec{r}) = -\dfrac{Ze^2}{r}\, e^{-r/\lambda_{TF}}$

The electrical resistivity is then

$$\rho = \frac{m^*}{n e^2 \tau_F} = \frac{h}{e^2} \cdot Z^2 a_B^* \cdot (n_{imp}/n) \cdot F(\pi k_F a_B^*)$$

where

$$a_B^* = \frac{\epsilon_\infty \hbar^2}{m^* e^2} = \epsilon_\infty \frac{m_e}{m^*}\, a_B \quad , \quad F(\alpha) = \left(\frac{\pi}{\alpha}\right)^3 \left[\ln(1+\alpha) - \frac{\alpha}{1+\alpha}\right]$$

With $h/e^2 = 25.8128\ \text{k}\Omega$ and for $a_B^* \approx a_B = 0.529\ \text{Å}$,

$$\rho = 1.37 \times 10^{-4}\ \Omega \cdot \text{cm} \times Z^2 (n_{imp}/n)\, F(\pi k_F a_B)$$

- **Boltzmann equation for holes**

Filled bands carry no current! For each band n,

$$\vec{j}(\vec{r},t) = -2e\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, f_n(\vec{r},\vec{k},t)\,\vec{v}_n(\vec{k}) = +2e\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, \bar{f}(\vec{r},\vec{k},t)\,\vec{v}_n(\vec{k})$$

where

$$\bar{f}_n(\vec{r},\vec{k},t) = 1 - f_n(\vec{r},\vec{k},t)$$

is the distribution function for **holes**. A hole is a fictitious particle of charge $+e$, also fermionic. **Four Laws of Holes**:

1. Under the influence of an applied electromagnetic field, the unoccupied levels of a band evolve as if they were occupied by real electrons of charge $q = -e$. The evolution of a Bloch wavepacket is thus described by the same semiclassical dynamics.

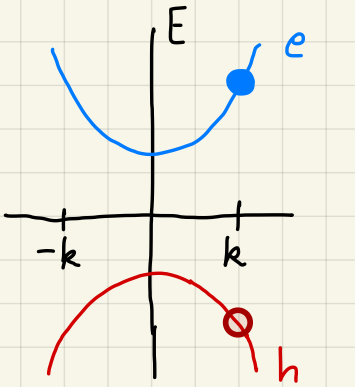
2. The current density due to a hole at wavevector $\vec{k}$ is given by $+e\,\vec{v}_n(\vec{k})/V$.

3. The crystal momentum of a hole at wavevector $\vec{k}$ is $\vec{P} = -\hbar\vec{k}$.

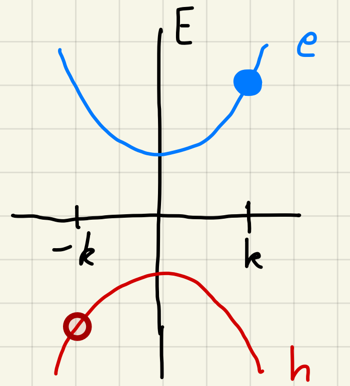
4. Any given band can be described in terms of either electrons or holes, but not both. It is often convenient to treat bands lying below or mostly below the Fermi level using the hole description

(e.g., for core or valence bands), and bands lying above or mostly above the Fermi level using the electron (particle) description.

<u>Example</u> :



$|\Psi_A\rangle = e^{+}_{k} h^{+}_{k} |0\rangle$



$|\Psi_B\rangle = e^{+}_{k} h^{+}_{-k} |0\rangle$

Conduction band : $\mathcal{E}_c(k) = \mathcal{E}_c(0) + \dfrac{\hbar^2 k^2}{2m_c^*}$, $v_c(k) = \dfrac{\hbar k}{m_c^*}$, $P_c(k) = \hbar k$

Valence band : $\mathcal{E}_v(k) = \mathcal{E}_v(0) - \dfrac{\hbar^2 k^2}{2m_v^*}$, $v_v(k) = -\dfrac{\hbar k}{m_v^*}$, $P_v(k) = -\hbar k$

Band gap : $E_g = \mathcal{E}_c(0) - \mathcal{E}_v(0)$

- State $|\Psi_A\rangle$: $j = -e\,v_c(k)/V + e\,v_h(k)/V = -\dfrac{e}{V}\left(\dfrac{\hbar}{m_c^*} + \dfrac{\hbar}{m_v^*}\right)k$

  $P = P_c(k) + P_e(k) = 0$

- State $|\Psi_B\rangle$: $j = -e\,v_c(k)/V + e\,v_h(-k)/V = -\dfrac{e}{V}\left(\dfrac{\hbar}{m_c^*} - \dfrac{\hbar}{m_v^*}\right)$

  $P = P_c(k) + P_e(-k) = 2\hbar k$

In $d=3$ dimensions, expanding about the valence and conduction band extrema,

$$\varepsilon_v(\vec{k}) = \varepsilon_v(\vec{K}_v) - \frac{\hbar^2}{2}(m_v^*)^{-1}_{\alpha\beta}(k^\alpha - K_v^\alpha)(k^\beta - K_v^\beta) + \dots$$
$$v_v^\alpha(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_v}{\partial k^\alpha} = -(m_v^*)^{-1}_{\alpha\beta}(k^\beta - K_v^\beta) + \dots$$

$$\varepsilon_c(\vec{k}) = \varepsilon_v(\vec{K}_v) + \frac{\hbar^2}{2}(m_c^*)^{-1}_{\alpha\beta}(k^\alpha - K_c^\alpha)(k^\beta - K_c^\beta) + \dots$$
$$v_c^\alpha(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_c}{\partial k^\alpha} = +(m_c^*)^{-1}_{\alpha\beta}(k^\beta - K_c^\beta) + \dots$$

Boltzmann equation for holes:

We recast the BE for particles,

$$\frac{\partial f}{\partial t} + \dot{\vec{r}}\cdot\frac{\partial f}{\partial \vec{r}} + \dot{\vec{k}}\cdot\frac{\partial f}{\partial \vec{k}} = I_{\vec{k}}[f]$$

in terms of the hole distribution $\bar{f} = 1 - f$:

$$\frac{\partial \bar{f}}{\partial t} + \dot{\vec{r}}\cdot\frac{\partial \bar{f}}{\partial \vec{r}} + \dot{\vec{k}}\cdot\frac{\partial \bar{f}}{\partial \vec{k}} = -I_{\vec{k}}[1-\bar{f}]$$

Now we linearize, writing $f = f^0 + \delta f$ and $\bar{f} = \bar{f}^0 + \delta\bar{f}$, where $\bar{f}^0$ is the local equilibrium distribution for holes:

$$f^0 = \frac{1}{\exp\left(\frac{\varepsilon_{\vec{k}} - \mu}{k_B T}\right) + 1} \quad \Rightarrow \quad \bar{f}^0 = \frac{1}{\exp\left(\frac{\mu - \varepsilon_{\vec{k}}}{k_B T}\right) + 1} = 1 - f^0$$

Thus we have $\delta\bar{f} = -\delta f$, hence

$$-I_k[1-\bar{f}] = -I_k[f^0 - \delta\bar{f}] = -\mathcal{L}(-\delta\bar{f}) = \mathcal{L}\,\delta\bar{f}$$

Thus, the Boltzmann equation for holes is

$$\frac{\partial \delta \bar{f}}{\partial t} - \frac{e}{\hbar c}\vec{v}\times\vec{B}\cdot\frac{\partial \delta \bar{f}}{\partial \boldsymbol{k}} + \vec{v}\cdot\left[e\vec{\mathcal{E}} + \frac{\varepsilon-\mu}{T}\vec{\nabla}T\right]\left(-\frac{\partial \bar{f}^{\circ}}{\partial \varepsilon}\right) = \mathcal{L}\,\delta\bar{f}^{\circ}$$

which is of the same form as for particles, with the important difference that $\bar{f}^{\circ} = 1 - f^{\circ}$, hence $-\frac{\partial \bar{f}^{\circ}}{\partial \varepsilon} \approx -\delta(\varepsilon-\varepsilon_F)$. N.B. In addition, the relation between $\vec{v}(\boldsymbol{k})$ and $\boldsymbol{k}$, as we have seen, is reversed for holes vis-a-vis particles.

- **Magnetoresistance and Hall effect**

The Boltzmann equn. reads [for holes, $f^{\circ} \to \bar{f}^{\circ}$, $\delta f \to \delta\bar{f}$]

$$\frac{\partial \delta f}{\partial t} - e\vec{v}\cdot\vec{\mathcal{E}}\,\frac{\partial f^{\circ}}{\partial \varepsilon} - \frac{e}{\hbar c}\vec{v}\times\vec{B}\cdot\frac{\partial \delta f}{\partial \boldsymbol{k}} = \mathcal{L}\,\delta f$$

Approximations : (i) $\mathcal{L}\,\delta f = -\delta f/\tau$, (ii) $\varepsilon(\boldsymbol{k}) = \pm\frac{\hbar^2}{2}m^{-1}_{\alpha\beta}k^{\alpha}k^{\beta}$.

Electric field : $\vec{\mathcal{E}}(t) = \vec{\mathcal{E}}e^{-i\omega t}$. Let's try a solution of the form

$$\delta f(\boldsymbol{k},t) = \boldsymbol{k}\cdot\vec{A}(\varepsilon(\boldsymbol{k}))\,e^{-i\omega t} \equiv \delta f(\boldsymbol{k})\,e^{-i\omega t}$$

From the BE, we obtain

$$(\tau^{-1} - i\omega)\,\boldsymbol{k}\cdot\vec{A} - \frac{e}{\hbar c}\epsilon_{\mu\nu\gamma}v^{\alpha}B^{\beta}\frac{\partial}{\partial k^{\gamma}}(\boldsymbol{k}\cdot\vec{A}) = e\vec{v}\cdot\vec{\mathcal{E}}\,\frac{\partial f^{\circ}}{\partial \varepsilon}$$

Now we may easily show that (Eqn. 5.251)

$$\epsilon_{\alpha\beta\gamma}v^{\alpha}B^{\beta}\frac{\partial}{\partial k^{\gamma}}(\boldsymbol{k}\cdot\vec{A}) = \epsilon_{\alpha\beta\gamma}v^{\alpha}B^{\beta}A^{\gamma}$$

whence

$$\Gamma_{\alpha\beta}\, A^{\beta} = \pm\hbar e \frac{\partial f^{0}}{\partial \varepsilon}\, \mathcal{E}^{\alpha}$$

with

$$\Gamma_{\alpha\beta} \equiv (\tau^{-1} - i\omega)\, m_{\alpha\beta} \pm \frac{e}{c}\, \epsilon_{\alpha\beta\gamma} B^{\gamma}$$

Therefore,

$$\delta f = \vec{k}\cdot\vec{A} = \pm\hbar e \frac{\partial f^{0}}{\partial \varepsilon}\, k_{\alpha}\, \Gamma^{-1}_{\alpha\beta}\, \mathcal{E}^{\beta}$$

$$= \pm\, e v^{\alpha} m_{\alpha\beta}\, \Gamma^{-1}_{\beta\gamma}\, \mathcal{E}^{\gamma} \frac{\partial f^{0}}{\partial \varepsilon}$$

The current density is

$$j^{\alpha} = \mp 2e \int_{\hat{\Omega}} \frac{d^{3}k}{(2\pi)^{3}}\, v^{\alpha}\, \delta f$$

$$= \underbrace{+\, 2e^{2} \int_{\hat{\Omega}} \frac{d^{3}k}{(2\pi)^{3}}\, v^{\alpha} v^{\beta} m_{\beta\gamma}\, \Gamma^{-1}_{\gamma\mu} \left(-\frac{\partial f^{0}}{\partial \varepsilon}\right)}_{\sigma_{\alpha\mu}} \mathcal{E}^{\mu}$$

We may further simplify to obtain

$$\sigma_{\alpha\beta}(\omega, \vec{B}) = \frac{2}{3} e^{2} \int_{-\infty}^{\infty} d\varepsilon\, \varepsilon\, g(\varepsilon)\, \Gamma^{-1}_{\alpha\beta}(\varepsilon) \left(-\frac{\partial f^{0}}{\partial \varepsilon}\right)$$

$$= n e^{2} \langle \Gamma^{-1}_{\alpha\beta} \rangle$$

Here $\Gamma_{\alpha\beta}(\varepsilon)$ gets its ε-dependence through $\tau(\varepsilon)$. We have

$$\langle \Gamma^{-1}_{\alpha\beta} \rangle \equiv \frac{\int_{-\infty}^{\infty} d\varepsilon\, \varepsilon\, g(\varepsilon)\, \Gamma^{-1}_{\alpha\beta}(\varepsilon) \left(-\frac{\partial f^{0}}{\partial \varepsilon}\right)}{\int_{-\infty}^{\infty} d\varepsilon\, \varepsilon\, g(\varepsilon) \left(-\frac{\partial f^{0}}{\partial \varepsilon}\right)}$$

The carrier density is

$$n = \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon) \times \begin{cases} f^{0}(\varepsilon) & \text{electrons} \\ 1 - f^{0}(\varepsilon) & \text{holes} \end{cases}$$

- **High field Hall effect**

Take $\omega = 0$. Then the BE is

$$-e\vec{v}\cdot\vec{\mathcal{E}}\,\frac{\partial f^{0}}{\partial \varepsilon} - \frac{e}{\hbar c}\,\vec{v}\times\vec{B}\cdot\frac{\partial \delta f}{\partial \vec{k}} = \cancel{-\frac{\delta f}{\tau}}$$

negligible if $\omega_c \tau >> 1$; $\omega_c = \frac{eB}{mc}$ (cyclotron frequency)

Take $\vec{\mathcal{E}} = \mathcal{E}_y \hat{y}$ and $\vec{B} = B_z \hat{z}$. Then the solution is

$$\delta f = \frac{\hbar c \mathcal{E}_y}{B_z}\, k_x\, \frac{\partial f^{0}}{\partial \varepsilon}$$

This should alarm us since $\vec{k}$ is only defined modulo a RLV. However, if $T \ll T_F$, the $\partial f^{0}/\partial \varepsilon \approx -\delta(\varepsilon - \varepsilon_F)$ factor confines $\vec{k}$ to the Fermi surface, which we presume lies completely within the first Brillouin zone. Then

$$j_x = 2ec\,\frac{\mathcal{E}_y}{B_z}\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, k_x\, \frac{\partial \varepsilon}{\partial k_x}\,\frac{\partial f^{0}}{\partial \varepsilon} = 2ec\,\frac{\mathcal{E}_y}{B_z}\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, k_x\, \frac{\partial f^{0}}{\partial k_x}$$

Integrate by parts, assuming $f^{0} \approx 0$ on the surface of the BZ. This yields

$$j_x = -\frac{2ec\mathcal{E}_y}{B_z}\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, f^{0} = -\frac{nec}{B_z}$$

Thus we obtain $\sigma^{e}_{xy} = -\sigma^{e}_{yx} = -\dfrac{nec}{B_z}$, completely independent of the details of the band structure (other than the requirement that there be no **open orbits** on the FS, which in general result in **non-saturating magneto-resistance**. [Recall $\rho_{xx}(\omega, B_z) = \frac{m^*}{ne^2\tau}(1 - i\omega\tau)$ which is field-independent.] For holes, we have

$$\sigma^h_{xy} = -\sigma^h_{yx} = +\frac{nec}{B_z}$$

We define the **Hall coefficient** $R_H = -\rho_{xy}/B_z$ and the **Hall number** $z_H = -1/n_{ion}ecR_H$. At high fields where $\omega_c\tau \gg 1$, the conductivity tensor is almost diagonal, i.e.

$$\sigma \approx \begin{pmatrix} 0 & \sigma_{xy} \\ -\sigma_{xy} & 0 \end{pmatrix} \Rightarrow \rho = \sigma^{-1} \approx \begin{pmatrix} 0 & -1/\sigma_{xy} \\ 1/\sigma_{xy} & 0 \end{pmatrix}$$

Thus $R_H \approx \mp 1/nec$ and $z_H \approx \pm n/n_{ion}$. The high field Hall effect tells us about the number density and the sign of the charge carriers. The Hall number is then a measure of valency.

- **Thermal transport**

  Consider a small region ΔV in thermodynamic equilibrium at temperature T and chemical potential μ. The first law says $T\Delta S = \Delta E - \mu\Delta N$. Divide by ΔV to get

$$dq \equiv T\,ds = d\varepsilon - \mu\, dn$$

with s, ε, n the densities of entropy, energy, and number. Thus, for the corresponding currents, we must have (continuity!)

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

where, assuming spin degeneracy,

$$\vec{j}_n = 2\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, \vec{v}\,\delta f = \vec{j}/(-e)$$

$$\vec{j}_\varepsilon = 2\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, \varepsilon\, \vec{v}\,\delta f$$

$$\vec{j}_q = \vec{j}_\varepsilon - \mu \vec{j}_n = 2\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, (\varepsilon - \mu)\, \vec{v}\,\delta f$$

The linearized Boltzmann equation, in the presence of an electric field and a temperature gradient, has the following time-independent solution:

$$\delta f = -\tau(\varepsilon)\, \vec{v} \cdot \left(e\vec{\mathcal{E}} + \frac{\varepsilon - \mu}{T} \vec{\nabla} T \right) \left(-\frac{\partial f^\circ}{\partial \varepsilon} \right)$$

(As before, for hole transport replace $f^\circ \to \bar{f}^\circ$ and $\delta f \to \delta \bar{f}$.) We then have

$$\vec{j} = -2e\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, \vec{v}\,\delta f \equiv L_{11}\vec{\mathcal{E}} - L_{12}\vec{\nabla} T$$

$$\vec{j}_q = 2\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, (\varepsilon - \mu)\, \vec{v}\,\delta f \equiv L_{21}\vec{\mathcal{E}} - L_{22}\vec{\nabla} T$$

where L_{11}, L_{12}, L_{21}, and L_{22} are each 3x3 matrices:

$$L_{11}^{\alpha\beta} = \frac{e^2}{4\pi^3\hbar}\int_{-\infty}^{\infty} d\varepsilon\ \tau(\varepsilon)\left(-\frac{\partial f^0}{\partial \varepsilon}\right)\int dS_\varepsilon\ \frac{v^\alpha v^\beta}{|\vec{v}|}$$

$$L_{21}^{\alpha\beta} = T L_{12}^{\alpha\beta} = -\frac{e}{4\pi^3\hbar}\int_{-\infty}^{\infty} d\varepsilon\ \tau(\varepsilon)(\varepsilon-\mu)\left(-\frac{\partial f^0}{\partial \varepsilon}\right)\int dS_\varepsilon\ \frac{v^\alpha v^\beta}{|\vec{v}|}$$

$$L_{22}^{\alpha\beta} = \frac{1}{4\pi^3\hbar T}\int_{-\infty}^{\infty} d\varepsilon\ \tau(\varepsilon)(\varepsilon-\mu)^2\left(-\frac{\partial f^0}{\partial \varepsilon}\right)\int dS_\varepsilon\ \frac{v^\alpha v^\beta}{|\vec{v}|}$$

We define the integrals

$$J_n^{\alpha\beta} \equiv \frac{1}{4\pi^3\hbar}\int_{-\infty}^{\infty} d\varepsilon\ \tau(\varepsilon)(\varepsilon-\mu)^n\left(-\frac{\partial f^0}{\partial \varepsilon}\right)\int dS_\varepsilon\ \frac{v^\alpha v^\beta}{|\vec{v}|}$$

in which case

$$L_{11}^{\alpha\beta} = e^2 J_0^{\alpha\beta} \quad , \quad L_{21}^{\alpha\beta} = T L_{12}^{\alpha\beta} = -e J_1^{\alpha\beta} \quad , \quad L_{22}^{\alpha\beta} = \frac{1}{T} J_2^{\alpha\beta}$$

The linear relations

$$\vec{j} = L_{11}\vec{\mathcal{E}} - L_{12}\vec{\nabla}T \quad , \quad \vec{j}_q = L_{21}\vec{\mathcal{E}} - L_{22}\vec{\nabla}T$$

may now be recast as

$$\vec{\mathcal{E}} = \rho\vec{j} + Q\vec{\nabla}T \quad , \quad \vec{j}_q = \Pi\vec{j} - \kappa\vec{\nabla}T$$

where

$\rho = L_{11}^{-1}$ = resistivity , $Q = L_{11}^{-1}L_{12}$ = thermopower

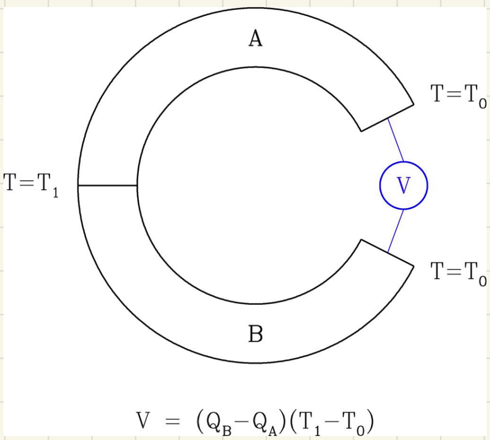
$\Pi = L_{21}L_{11}^{-1}$ = Peltier coefficient , $\kappa = L_{22} - L_{21}L_{11}^{-1}L_{12}$ = thermal conductivity

Note the following:

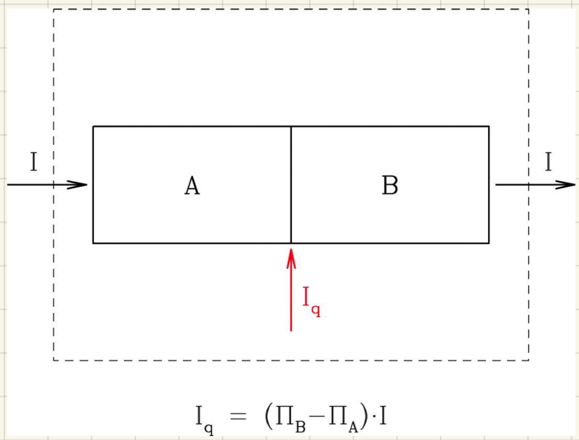
- $\vec{\nabla} T = 0 \Rightarrow \vec{\mathcal{E}} = \rho \vec{j}$ and $\vec{j}_q = \Pi \vec{j}$
- $\vec{j} = 0 \Rightarrow \vec{\mathcal{E}} = Q \vec{\nabla} T$ and $\vec{j}_q = -\kappa \vec{\nabla} T$

To measure the thermopower Q (also called the **Seebeck coefficient**), fashion a junction between two dissimilar metals A and B. Hold the junction at T_1 and the ends of the metals at T_0. A voltage develops:

$$V_A - V_B = -\int_A^B d\vec{l} \cdot \vec{\mathcal{E}} = (Q_B - Q_A)(T_1 - T_0)$$



thermocouple



Peltier effect device

Such a device is called a **thermocouple**. To elicit the Peltier effect, pass an electrical current I through a junction between two dissimilar metals. This results in a net heat flux into the junction of $I_q = (\Pi_A - \Pi_B) I$. Note that this effect is linear in I, as opposed to Joule heating which goes as I^2. If one forms an ABA bijunction, the heat absorbed at the first junction will be released at the second. Application: Peltier effect refrigerator.

- **Heat equation**

We start with the continuity equations for $\rho = -en$ and ε:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0 \quad , \quad \frac{\partial \varepsilon}{\partial t} + \vec{\nabla} \cdot \vec{j} = \vec{j} \cdot \vec{E}$$

NB not $\vec{\mathcal{E}}$!

Now invoke local thermodynamics: $\varepsilon = \varepsilon(n, T)$ from Gibbs–Duhem $\Rightarrow$

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial \varepsilon}{\partial n} \frac{\partial n}{\partial t} + \frac{\partial \varepsilon}{\partial T} \frac{\partial T}{\partial t}$$

$$= -\frac{\mu}{e} \frac{\partial \rho}{\partial t} + c_V \frac{\partial T}{\partial t}$$

Thus,

$$c_V \frac{\partial T}{\partial t} = \frac{\partial \varepsilon}{\partial T} + \frac{\mu}{e} \frac{\partial \rho}{\partial t}$$

$$= \vec{j} \cdot \vec{E} - \vec{\nabla} \cdot \vec{j}_\varepsilon - \frac{\mu}{e} \vec{\nabla} \cdot \vec{j}$$

$$= \vec{j} \cdot \vec{\mathcal{E}} - \vec{\nabla} \cdot \vec{j}_q$$

Now consider the case $\vec{j} = 0$. Since $\vec{j}_q = \Pi \vec{j} - \kappa \vec{\nabla} T = -\kappa \vec{\nabla} T$, we have

$$c_V \frac{\partial T}{\partial t} = \vec{\nabla} \cdot (\kappa \vec{\nabla} T) = \kappa_{\alpha\beta} \frac{\partial^2 T}{\partial x^\alpha \partial x^\beta} \qquad \text{(heat equation)}$$

assuming the thermal conductivity tensor is spatially nonvarying. This equation says that there is a time scale $\tau_T = C L^2 c_V / \kappa$

over which temperature relaxes exponentially in a system of characteristic linear dimension L (assuming κ isotropic). For a cube $C = 1/3\pi^2$.

- **Calculation of transport coefficients**

We have

$$\rho = \frac{1}{e^2} \mathcal{J}_0^{-1} \qquad Q = -\frac{1}{eT} \mathcal{J}_0^{-1} \mathcal{J}_1$$

$$\Pi = -\frac{1}{e} \mathcal{J}_1 \mathcal{J}_0^{-1} \qquad \kappa = \frac{1}{T}\left(\mathcal{J}_2 - \mathcal{J}_1 \mathcal{J}_0^{-1} \mathcal{J}_1\right)$$

with

$$\mathcal{J}_n^{\alpha\beta} \equiv \frac{1}{4\pi^3\hbar} \int_{-\infty}^{\infty} d\varepsilon\, \tau(\varepsilon)\, (\varepsilon-\mu)^n \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \int dS_\varepsilon\, \frac{v^\alpha v^\beta}{|\vec{v}|}$$

For isotropic systems, $\mathcal{J}_n^{\alpha\beta} = \mathcal{J}_n \delta^{\alpha\beta}$, with

$$\mathcal{J}_n = \frac{1}{12\pi^3\hbar} \int_{-\infty}^{\infty} d\varepsilon\, \tau(\varepsilon) \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \int dS_\varepsilon\, |\vec{v}|$$

To evaluate these expressions, use the Sommerfeld expansion,

$$\int_{-\infty}^{\infty} d\varepsilon\, H(\varepsilon) \left(-\frac{\partial f^0}{\partial \varepsilon}\right) = \pi D \csc(\pi D) H(\varepsilon)\Big|_{\varepsilon=\mu}$$

N.B.: $D \equiv k_B T \frac{\partial}{\partial \varepsilon}$

$$= H(\mu) + \frac{\pi^2}{6}(k_B T)^2 H''(\mu) + \mathcal{O}(T^4)$$

For a parabolic band with energy-independent scattering time τ, we have

$$\mathcal{J}_n = \frac{\sigma_0}{e^2} \varepsilon_F^{-3/2}\, \pi D \csc(\pi D) \left\{ \varepsilon^{3/2} (\varepsilon-\mu)^n \right\}\Big|_{\varepsilon=\mu}$$

with $\sigma_0 = ne^2\tau/m^*$ and

$$\varepsilon_F^{3/2} = \pi D \csc(\pi D)\, \varepsilon^{3/2} \Big|_{\varepsilon=\mu}$$

implicitly yields $\mu(\varepsilon_F, T)$. We obtain the following:

$$\mathcal{J}_0 = \frac{\sigma_0}{e^2} \quad , \quad \mathcal{J}_1 = \frac{\sigma_0}{e^2}\frac{\pi^2}{2}\frac{(k_B T)^2}{\varepsilon_F} \quad , \quad \mathcal{J}_2 = \frac{\sigma_0}{e^2}\frac{\pi^2}{3}(k_B T)^2$$

with $\sigma_0 = \frac{ne^2\tau}{m^*}$, whence, to lowest nontrivial order in T,

$$\rho = \frac{1}{\sigma_0} \quad , \quad Q = -\frac{\pi^2}{2}\frac{k_B^2 T}{e\varepsilon_F} \quad , \quad \kappa = \frac{\pi^2}{3}\frac{n\tau}{m^*}k_B^2 T$$

and $\Pi = QT$. The prediction of a universal ratio,

$$\frac{\kappa}{\sigma T} = \frac{\pi^2}{3}(k_B/e)^2 = 2.45 \times 10^{-8}\, V^2/K^2$$

is known as the **Wiedemann-Franz law**. Note that $Q < 0$ here is predicted to be negative. In fact, several nearly free electron metals such as Cs and Li have positive low-T thermopowers. What went wrong? We have neglected electron-phonon scattering.

- **Onsager relations**: $J_i = L_{ij} F_j$; J_i = current F_j = flux

Then $L_{ij}(\vec{B}) = \eta_i \eta_j L_{ji}(-\vec{B})$ where $\eta_i = \pm 1$ describes the parity of the current J_i under time reversal $\hat{T}$, i.e.

$$\hat{T} J_i = \eta_i J_i$$

Consequences: for $\vec{B}=0$, $K = K^t$ regardless of crystal structure!

When $\vec{B} \neq 0$,

$$\rho_{\alpha\beta}(\vec{B}) = \rho_{\beta\alpha}(-\vec{B}) \quad , \quad K_{\alpha\beta}(\vec{B}) = K_{\beta\alpha}(-\vec{B}) \quad , \quad \Pi_{\alpha\beta}(\vec{B}) = T\mathcal{Q}_{\beta\alpha}(-\vec{B})$$

- **Weak magnetic fields** in isotropic systems

  Expand to first order in $\vec{B}$:

$$\rho_{\alpha\beta}(\vec{B}) = \rho\,\delta_{\alpha\beta} + a\,\epsilon_{\alpha\beta\gamma} B^\gamma$$

$$K_{\alpha\beta}(\vec{B}) = K\,\delta_{\alpha\beta} + b\,\epsilon_{\alpha\beta\gamma} B^\gamma$$

$$\mathcal{Q}_{\alpha\beta}(\vec{B}) = \mathcal{Q}\,\delta_{\alpha\beta} + c\,\epsilon_{\alpha\beta\gamma} B^\gamma$$

$$\Pi_{\alpha\beta}(\vec{B}) = \Pi\,\delta_{\alpha\beta} + d\,\epsilon_{\alpha\beta\gamma} B^\gamma$$

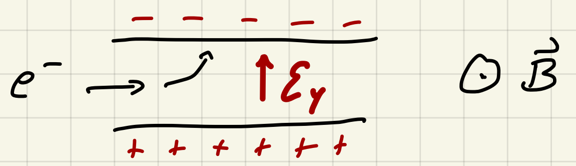
Onsager reciprocity entails $\Pi = T\mathcal{Q}$ and $d = Tc$.

We now have

$$\vec{\mathcal{E}} = \rho\vec{j} + a\,\vec{j}\times\vec{B} + \vec{\mathcal{Q}}\vec{\nabla}T + c\,\vec{\nabla}T\times\vec{B}$$

$$\vec{j}_q = \Pi\vec{j} + d\,\vec{j}\times\vec{B} - K\vec{\nabla}T - b\,\vec{\nabla}T\times\vec{B}$$

New phenomena!



- **Hall effect** $\quad \vec{\nabla}T = j_y = 0$

  $\vec{j} = j_x\hat{x}$ and $\vec{B} = B_z\hat{z} \Rightarrow \mathcal{E}_y = R_H\, j_x B_z$ with $R_H = -a$

- **Ettingshausen effect** $\quad \partial_x T = j_y = j_{q,y} = 0$

  $\vec{j} = j_x\hat{x}$ and $\vec{B} = B_z\hat{z} \Rightarrow \dfrac{\partial T}{\partial y} = P\, j_x B_z$ with $P = -d/K$

- Nernst effect $\vec{j} = \partial_y T = 0$

  $\vec{\nabla} T = \partial_x T \, \hat{x}$ and $\vec{B} = B_z \hat{z} \Rightarrow \mathcal{E}_y = \Lambda \, \partial_x T \, B_z$ with $\Lambda = -c$

- Righi-Leduc effect $\vec{j} = \mathcal{E}_y = 0$

  $\vec{\nabla} T = \partial_x T \, \hat{x}$ and $\vec{B} = B_z \hat{z} \Rightarrow \partial_y T = \mathcal{L} \, \partial_x T \, B_z$ with $\mathcal{L} = c/Q$