Lecture 20 | Diffusion, thermal conductivity, thermo-electric phenomena.

Diffusion

If particle density varies in space then particle flow appears. Diffusion coefficient is defined as

$$\vec{j}_D = -D\nabla n$$

We can view electrical current as diffusion of electrons under the action of electric field. Then

$$\vec{j} = -e\vec{j}_D = eD\nabla n$$

Substituting $n = 2\int f(\varepsilon + e\varphi)\frac{d^3k}{(2\pi)^3}$, $E = -\nabla\varphi$

we obtain $j = 2e^2 D\int \frac{\partial f}{\partial \varepsilon}\nabla\varphi \frac{d^3k}{(2\pi)^3}$

$$\vec{j} = -e^2 D\vec{E}\int \frac{\partial f}{\partial \varepsilon} N(\varepsilon)\, d\varepsilon$$

using $\frac{\partial f}{\partial \varepsilon} = -\delta(\varepsilon - \varepsilon_F)$ we obtain

$$j = e^2 D N(\varepsilon_F) E \equiv \sigma E \quad \text{thus}$$

The conductivity can be expressed through the diffusion coefficient $\underline{\sigma = e^2 D N(\varepsilon_F)}$

Thermal conductivity

In the presense of temperature gradient we can replace $v \frac{\partial f_0}{\partial \vec{r}}$ term in the Boltzmann equation by

$$\vec{v} \cdot \vec{\nabla} f_0 = \vec{v} \cdot \nabla T \frac{\partial f_0}{\partial T}$$

With $f_0 = \dfrac{1}{e^{\frac{\varepsilon - \mu}{T}} + 1}$

$$\frac{\partial f_0}{\partial T} = T \frac{\partial f_0}{\partial \varepsilon} \frac{\partial}{\partial T} \frac{(\varepsilon - \mu)}{T} = -\frac{(\varepsilon - \mu)}{T} \frac{\partial f_0}{\partial \varepsilon}$$

And the correction to the distribution function in the relaxation time approximation

$$f_1 = \tau \frac{\varepsilon - \mu}{T} (\vec{v} \cdot \vec{\nabla} T) \frac{\partial f_0}{\partial \varepsilon}$$

compare with

$$f_1 = e\tau (\vec{E} \cdot \vec{v}) \frac{\partial f_0}{\partial \varepsilon}$$

for calculation of conductivity

The heat current is

$$\vec{q} = 2\int \frac{d^3k}{(2\pi)^3} (\varepsilon_k - \mu)\, v_k f_1 \;\cdot$$

$$\vec{q} = \tau \int d\varepsilon \frac{d\Omega}{4\pi} N(\varepsilon)\, \vec{v}_k (\vec{v}_k \cdot \vec{\nabla} T) \frac{(\varepsilon - \mu)^2}{T} \frac{\partial f_0}{\partial \varepsilon}$$

angular integration gives again $\frac{1}{3}$ factor

$$\vec{q} = \frac{\tau}{3} \vec{\nabla} T \int d\varepsilon\, N(\varepsilon)\, v_k^2 \frac{(\varepsilon - \mu)^2}{T} \frac{\partial f_0}{\partial \varepsilon}$$

In this integral we cannot replace $\frac{\partial f_0}{\partial \varepsilon}$ by delta function and should use

$$\frac{\partial f_0}{\partial \varepsilon} = -\frac{1}{4T \cosh^2\left(\frac{\varepsilon - \mu}{2T}\right)}$$

Such integrals we discussed in the lecture 6 calculating specific heat

$$\int (\varepsilon - \mu)^2 \frac{\partial f_0}{\partial \varepsilon} = -\frac{1}{4T} \int_{-\infty}^{\infty} \frac{z^2 dz}{\cosh^2 \frac{z}{2T}} = -\frac{\pi^2 T^2}{3}$$

As a result we obtain

$$\vec{q} = -\frac{\pi^2}{9} T\, v_F^2 \tau N(\varepsilon_F)\, \vec{\nabla} T$$

Using definition of the thermal conductivity

$$\vec{q} = -\varkappa \vec{\nabla} T$$ we obtain

$$\varkappa = \frac{\pi^2}{9} T\, v_F^2 N(\varepsilon_F)\tau$$

And comparing it to the conductivity

$$\sigma = \frac{e^2 v_F^2 N(\varepsilon_F)\tau}{3}$$ we arrive at

the <u>Wiedemann-Franz law</u>

$$\underline{\frac{\varkappa}{\sigma T} = \frac{\pi^2}{3e^2}}$$

This law is derived within the relaxation type approximation, hence for elastic scattering. For inelastic scattering (phonons at low temperatures) it is not valid. Low angle scattering has the same effect on heat transport as back scattering. As a result there $\frac{\varkappa}{\sigma T} \propto \left(\frac{T}{\Theta_D}\right)^2$

see J.M. Ziman book.

General transport coefficients

Suppose now that we have both $\vec{\nabla} T$ and $\vec{E}$ in the sample. Then the Boltzmann equation is

$$-\frac{\partial f^0}{\partial \varepsilon} \vec{v}_k \cdot \left(\frac{\varepsilon_k - \mu}{T} \vec{\nabla} T - \vec{E} \right) = I(f)$$

We include gradient of chemical potential in $\vec{E} = -\vec{\nabla}\varphi - \frac{\vec{\nabla}\mu}{e}$.

In the relaxation time approximation

$$f_1(k) = -\frac{\partial f_0}{\partial \varepsilon_k} \tau \cdot \vec{v}_k \left(\vec{E} - \frac{\varepsilon_k - \mu}{T} \vec{\nabla} T \right)$$

Then both electric and heat current will be present

$$\vec{j} = e^2 K_0 \cdot \vec{E} - \frac{e}{T} K_1 (-\vec{\nabla} T)$$

$$\vec{q} = -e K_1 \cdot \vec{E} + \frac{1}{T} K_2 (-\vec{\nabla} T)$$

where transport coefficients are

$$K_n = \frac{-1}{3\pi^2} \tau \int d\varepsilon \frac{d\Omega}{4\pi} \frac{v_x^2}{|v|} (\varepsilon - \mu)^n \frac{\partial f_0}{\partial \varepsilon} =$$

$$= -\frac{n}{m} \tau \int d\varepsilon \frac{\partial f_0}{\partial \varepsilon} (\varepsilon - \mu)^n$$

which gives for low temperatures

$$K_0 = \frac{v_F^2 \tau N(\varepsilon_F)}{3} = \frac{n \tau}{m}$$

$$K_1 = \frac{\pi^2}{9} T^2 \frac{\partial \left[v^2 \tau N(\varepsilon_F) \right]}{\partial \varepsilon_F}$$

$$K_2 = \frac{\pi^2}{3} T^2 K_0$$

To determine the thermal conductivity we should solve the general transport equations with $j = 0$

Then we obtain

$$\vec{E} = -\frac{K_1}{T K_0} \vec{\nabla} T$$

and $\vec{q} = -\frac{K_2}{T}\left(1 - \frac{K_1^2}{K_0 K_2}\right)\vec{\nabla} T$

With K_n presented above, the second term $\frac{K_1^2}{K_0 K_2} \sim \frac{T^2}{\mathcal{E}_F^2} \ll 1$ and

we obtain $\quad \varkappa = \frac{K_2}{T}$.

Thermoelectric effect

If the temperature gradient is present then an electric field is induced wi

$$\vec{E} = Q\,\vec{\nabla} T = -\frac{K_1}{eTK_0}\vec{\nabla} T$$

with the Seebeck coefficient

$$Q = -\frac{\pi^2 T}{3e}\frac{d}{d\mathcal{E}_F}\ln\left(v_F^2 \tau N(\mathcal{E}_F)\right) = -\frac{\pi^2 T}{3e}\frac{d\sigma}{\sigma\, d\mathcal{E}_F}$$

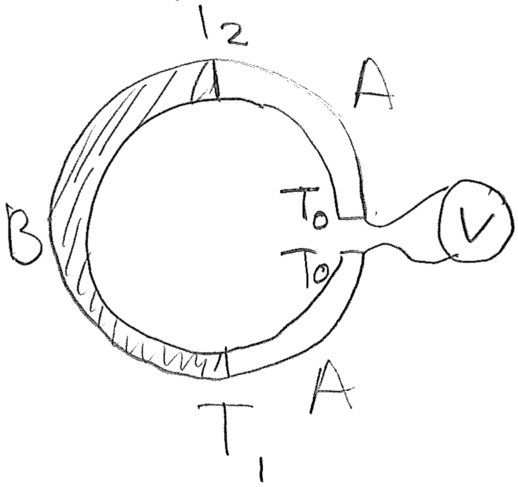
For free electrons that scatter on impurities

$$Q = -\frac{\pi^2}{3e}\frac{T}{\mathcal{E}_F} \qquad \text{we use } \tau \sim \frac{\ell}{v_F}$$

If $\tau(\mathcal{E})$ has strong energy dependence near the Fermi surface (Kondo effect) Seebeck coefficient is enhanced

The Seebeck effect

One takes bimetal sircuit



The electromotive force

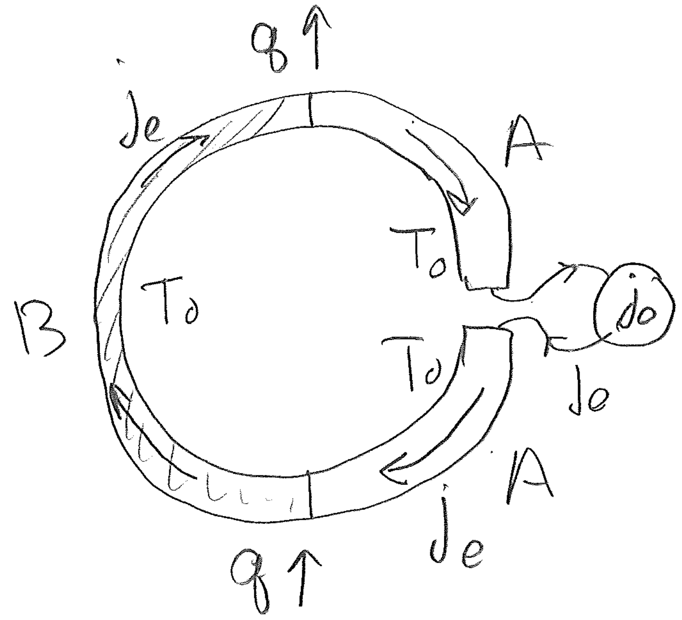
$$\int \vec{E}\cdot dl = Q_A \int_{T_0}^{T_1} dl\cdot\vec{\nabla}T + Q_B \int_{T_1}^{T_2} dl\cdot\vec{\nabla}T +$$

$$+ Q_A \int_{T_2}^{T_0} dl\cdot\vec{\nabla}T = Q_A(T_1 - T_2) + Q_B(T_2 - T_1)$$

$$= (Q_A - Q_B)(T_2 - T_1)$$

This produces voltage between the two ends of metal A

Peltier effect



Here one keeps the temperature the same everywhere and drives the current through the ring. In this case one generates the heat current

$$q^{A,B} = e\,K_1^{A,B} \cdot E \,, \quad j = e^2 K_0 E \quad \text{and}$$

$$q^{A,B} = \frac{K_1^{A,B}}{e\,K_0^{A,B}}\, j = \Pi^{A,B} j\,; \quad q = (\Pi_A - \Pi_B)\, j = \Pi j$$

with the Peltier coefficient

$$\Pi = (Q_A - Q_B)\, T.$$