Electrical & Thermal Conduction

- Thermal conductivity
- Electron dynamics
- Fermi-Dirac distribution
- Electronic heat capacity
- Boltzmann transport theory
- Relaxation-time approximation
- Electron mobility
- Hall Effect

Thermal conductivity

$\mathbf{J}_u = -K\Delta T$, where ΔT is the temperature gradient.

$\mathbf{J}_u$ = flux of thermal energy

$$\mathbf{J}_A = \text{flux of } (A) = \frac{\Delta A}{\Delta t} / \text{ unit area} = \rho_A \cdot \mathbf{v}.$$

Thermal energy density gained due to particle flow between t and $t+\tau$.

$$u = -nc\Delta T = -C\Delta T, \;\; C = \text{heat capacity /volume} = -C(\frac{dT}{dx})v_x\tau.$$

$v_x\tau$ = distance travelled within time τ. τ = mean free time.

$$J_u =< ncx >= -c(\frac{dT}{dx}) < v_x^2 > \tau = -\frac{1}{3}c < v^2 > \tau(\frac{dT}{dx}) = -\frac{1}{3}Cvl(\frac{dT}{dx}),$$

where $v = \sqrt{< v^2 >}$ = average particle velocity, $l = v\tau$ = mean free path

$$\Rightarrow K = \frac{1}{3}Cvl \;\; \ldots \text{ valid for both phonons and electrons.}$$

Phonon mean free path is determined by phonon-defect scattering or phonon-phonon scattering.

$l^{-1} \propto$ scattering rate $\propto$ number of phonons available

$$<n>= (e^{\hbar\omega/k_BT} - 1)^{-1} = k_BT/\hbar\omega \text{ for } k_BT \gg \hbar\omega.$$

So, at high tempereature ($k_BT \gg \hbar\omega$) number of phonons $\propto T$ and $l \propto 1/T$ due to phonon-phonon scattering.

Note: Any momentum-conserving scattering ($\mathbf{k}_1+\mathbf{k}_2 = \mathbf{k}_3$) (N-process) will lead to no change in thermal current. Only the Umbklapp process (U-rocess), in which $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{G}, \mathbf{G} =$ a nonzero reciprocal lattice vector, can change the thermal current and establish thermal equilibrium.

⋆ Geometric effect (phonon-scattering due to boundaries)

l is limited by the width of the sample (D). When phonon-phonon scattering becomes negligible at the low temperatures, the geometric effect prevails, and we have $K \sim CvD$. Thus,

$$K \sim \begin{cases} T^3 \text{ as } T \to 0 \\ T^{-1} \text{ as } T > \Theta_D \end{cases}$$

Electron dynamics

Electron velocity:

$\langle p \rangle = -i\hbar \int d^3 r \psi^*(r) \nabla \psi(r)$,

where

$$\psi(k,r) = e^{ik.r} u(k,r)$$

$\langle \mathbf{p} \rangle = \hbar \mathbf{k} - i\hbar \int d^3\mathbf{r}\, u^*(\mathbf{r}) \nabla u(\mathbf{r}) = \hbar \mathbf{k} + \langle \mathbf{p} \rangle_u$

Now consider the S.E. for u

$$Hu(k,r) = [\frac{-\hbar^2}{2m}\nabla^2 + \frac{\hbar}{m}\vec{k}\cdot\vec{p} + V_0(r)]u(k,r) = [E(k) - \frac{\hbar^2 k^2}{2m}]u(k,r)$$

$\langle \mathbf{p} \rangle_u = (m/\hbar)\langle \partial H/\partial \mathbf{k} \rangle_u = = (m/\hbar)\partial E(\mathbf{k})/\partial \mathbf{k} - \hbar \mathbf{k}$ ……Feynnman-Hellman Thm.

So, we obtain the group velocity for electron in solids

$\mathbf{v}_\mathbf{k} = \langle \mathbf{p} \rangle / m = (1/\hbar)\partial E(\mathbf{k})/\partial \mathbf{k}$

Free Electron Gas

Electrons in the conduction band of a semiconductor or metal behave like free moving particles with effective mass m, which is usually smaller than the bare electron mass. A free particle satisfies the Shrödinger equation

$$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\psi(\mathbf{r})=\epsilon\psi(\mathbf{r})$$

[Note: $\mathbf{p}=\hbar\mathbf{k}=i\hbar\nabla$ in QM]

Solution: $\psi(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}$ subject to periodic boundary conditions $\psi(0)=\psi(L)$

$$\Rightarrow k_x=n_x(\frac{2\pi}{L}),\ k_y=n_y(\frac{2\pi}{L}),\ k_z=n_z(\frac{2\pi}{L}),$$

$$n_x,n_y,n_z \text{ are integers} \quad \Rightarrow \sum_{\mathbf{k}}=\frac{V}{(2\pi)^3}\int d^3k.$$

Dispersion relation: $\epsilon(\mathbf{k})=\frac{\hbar^2}{2m}k^2$.

DOS: $D(\epsilon)=\sum_{\mathbf{k}}\delta(\epsilon-\epsilon(\mathbf{k}))$

$$N(\epsilon)=\sum_{\mathbf{k}}\theta(\epsilon-\epsilon(\mathbf{k}))=\sum_{\mathbf{k}}\theta(\bar{k}-|k|)|_{\bar{k}=\sqrt{2mE}/\hbar}=\frac{V}{(2\pi)^3}\frac{4\pi}{3}\bar{k}^3=\frac{V}{2\pi^2}\frac{1}{3}(\frac{2mE}{\hbar^2})^{3/2}.$$

$$D(\epsilon)\frac{dN}{d\epsilon}=\frac{V}{4\pi^2}(\frac{2m}{\hbar^2})^{3/2}\epsilon^{1/2}.$$

Spin degeneracy: Each electron has two internal degrees of freedom, which [Cf: each phonon has three internal degrees of freedom] are described by spin-1/2 (up and down).

Fermi-Dirac distribution

Average occupancy of a state with energy ϵ in a system maintained at constant temperature ($\tau = k_B T$) and chemical potential (μ) is

$$f(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/\tau} + 1}.$$

Gibbs factor: The relative probability of finding a system with N particles and energy ϵ_N in thermal and diffusive contact with a reservoir with temperature τ and chemical potential μ is

$$G(\epsilon) = \frac{1}{\mathcal{Z}} e^{-(\epsilon_N - \mu N)/\tau};\ \mathcal{Z} = \sum_N e^{-(\epsilon_N - \mu N)/\tau}$$

$$\Rightarrow < n >_\epsilon = \frac{1}{\mathcal{Z}} e^{-(\epsilon-\mu)/\tau} \equiv f(\epsilon)$$

for fermions, where $\mathcal{Z} = 1 + e^{-(\epsilon-\mu)/\tau}$.

Meaning of Chemical potential for fermions: At $\tau = 0, \mu(0) = \epsilon_F$ is the energy (Fermi energy) below which all states are occupied and above which all states are empty. At finite τ, the states with energy near $\mu(\tau)$ are partially occupied, and the level $\mu(\tau)$ is determined by either the reservoir in contact or the total number of particles in the system, $N (N \ll 1)$.

$$N = 2\sum_{\mathbf{k}} f(\epsilon(k)) = \int D(\epsilon) f(\epsilon) d\epsilon = 2\frac{V}{4\pi^2}(\frac{2m}{\hbar^2})^{3/2}\int^{\infty}\epsilon^{1/2}\frac{1}{e^{(\epsilon-\mu)/\tau}+1}d\epsilon.$$

The factor 2 is due to spin degeneracy. At $\tau \to 0, \mu \to \epsilon_F$

$$N = \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\int_0^{\epsilon_F}\epsilon^{1/2}d\epsilon = \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}(\frac{2}{3}\epsilon_F^{3/2})$$

$$= \frac{V}{3\pi^2}(\frac{2m}{\hbar^2})^{3/2}\epsilon_F^{3/2} \Rightarrow D(\epsilon) = (\frac{3N}{2\epsilon_F})(\frac{\epsilon}{\epsilon_F})^{1/2}.$$

Fermi wave vector k_F is related to ϵ_F via

$$\epsilon_F = \frac{\hbar^2}{2m}k_F^2 \quad \text{or} \quad k_F = \sqrt{2m\epsilon_F}/\hbar.$$

It is related to N via

$$N = 2\sum_{\mathbf{k}} f(\epsilon(k)) = 2\sum_{\mathbf{k}}\theta(k_F - |k|) = 2\frac{V}{(2\pi)^3}\int d^3k\theta(k_F - |k|) = \frac{V}{3\pi^2}k_F^3$$

or $k_F = (3\pi^2 N/V)^{1/3}$

Fermi velocity, v_F

$$v_F = p_F/m = \hbar k_F/m = (\frac{\hbar}{m})(3\pi^2 N/V)^{1/3}$$

Electronic Heat Capacity

Total electron energy at temperature τ is

$$U(\tau) = \int D(\epsilon)\epsilon f(\epsilon)d\epsilon = (\frac{3N}{2\epsilon_F^{3/2}})\int \epsilon^{3/2} f(\epsilon)d\epsilon = (\frac{3N}{2\epsilon_F^{3/2}})\frac{2}{5}\epsilon_F^{5/2}$$

$$= \frac{3}{5}\epsilon_F \quad \text{as} \quad \tau \to 0.$$

$$C_{el} = \frac{\partial U}{\partial T} = (\frac{\partial U}{\partial \tau})k_B.$$

$$(\frac{\partial U}{\partial \tau}) = \int_0^\infty \epsilon D(\epsilon)\frac{\partial f}{\partial \tau}d\epsilon$$

$$\text{and since } \epsilon_F \frac{\partial N}{\partial \tau} = 0 = \int_0^\infty \epsilon_F D(\epsilon)(\frac{\partial f}{\partial \tau})d\epsilon$$

$$\Rightarrow C_{el}/k_B = \int_0^\infty (\epsilon - \epsilon_F)D(\epsilon)(\frac{\partial f}{\partial \tau})d\epsilon$$

$$\frac{\partial f}{\partial \tau} = \frac{\partial}{\partial \tau}[\frac{1}{e^{(\epsilon-\mu)/\tau}+1}] = \frac{\partial}{\partial x}(\frac{1}{e^x+1})\frac{\partial x}{\partial \tau} = \frac{e^x}{(e^x+1)^2}\frac{x}{\tau},$$

$$\text{where } \mu(\tau) = \epsilon_F + \frac{\partial \mu}{\partial \tau}\tau \; ; x \equiv (\epsilon - \epsilon_F)/\tau.$$

$\partial f/\partial \tau$ is sharply peaked at $x = 0$ (or $\epsilon = \epsilon_F$).

$$\Rightarrow C_{el} = D(\epsilon_F)\int_{-\epsilon_F/\tau}^\infty \frac{x^2 e^x}{(e^x+1)^2}(\tau dx) = \tau(\frac{3N}{2\epsilon_F})\int_{-\infty}^\infty \frac{x^2 e^x}{(e^x+1)^2}dx \;(\text{ for } \tau \ll \epsilon_F) = \frac{1}{2}\pi^2 N(\tau/\epsilon_F).$$

Heat capacity in metals:

$$C_v = C_{el} + C_{ph} = \gamma T + AT^3 \text{ for low temperatures .}$$

$\gamma = \frac{1}{2}\pi^2 N k_B/\epsilon_F$, $A = \frac{3}{5}\pi^4 N_a k_B/\Theta^3$.

Electrical conductivity:

$$\mathbf{F} = m\frac{d\mathbf{v}}{dt} = \hbar\frac{d\mathbf{k}}{dt} = -e\mathbf{E},$$

$$\Delta\mathbf{k} = -(e\mathbf{E}/\hbar)\Delta t \text{ or } \Delta\mathbf{v} = -(\frac{e\mathbf{E}}{m})\Delta t$$

Let $\Delta t = \tau$ ... mean free time (due to scattering)

$$\mathbf{J} = n(-e) < \mathbf{v} >= n(-e)\Delta\mathbf{v} = (ne^2\tau/m)\mathbf{E} = \sigma\mathbf{E}$$

$\sigma = (ne^2\tau/m)$ is called the conductivity.

Relation between thermal and electrical conductivity

Note: At $\mathbf{E} = 0$, Fermi sphere is centered at 0 and we have $< \mathbf{v} >= 0$, whereas as finite $\mathbf{E}$,

Fermi sphere is displaced and $< \mathbf{v} >= \Delta v = -eE\tau/m$.

Resistivity $\rho = 1/\sigma = m/(ne^2\tau)$.

Mean free path $l = v_F\tau$ (not $< v > \tau$ here).

In Cu, $v_F \approx 1.6 \times 10^{-8} cm/s, \tau \approx 2 \times 10^{-9} s$ (at 4K) and $\approx 2 \times 10^{-14} s$ (at 300K)

$l \approx 0.3cm$ (at 4K) and 10^{-6} cm (at 300K).

Thermal conductivity:

$$K = \frac{1}{3} cvl \; ; c = C_{el}/\text{volume} = \frac{1}{2}\pi^2 n (\frac{k_B T}{\epsilon_F})$$

$v \sim v_F$ and $l \approx v_F\tau$.

$$\Rightarrow K = \frac{1}{3}\frac{1}{2}\pi^2 n (\frac{k_B T}{\frac{1}{2} m v_F^2}) \cdot v_F^2 \tau = \frac{\tau\pi^2 n k_B^2 T}{3m}$$

$$\frac{K}{\sigma} = K/(ne^2\tau/m) = \frac{\pi^2}{3}(\frac{k_B}{\sigma})^2 T \equiv L \cdot T.$$

Scattering mechanisms

1. Electron-phonon scattering ($\frac{1}{\tau_L}$)

2. Electron-defect scattering ($\frac{1}{\tau_i}$) (insensitive to temperature).

Defects include impurities and lattice imperfections.

3. Electron-electron scattering. ($\frac{1}{\tau_e}$).

$$\frac{1}{\tau} = \frac{1}{\tau_L} + \frac{1}{\tau_i} + \frac{1}{\tau_e}$$

or, $\rho = \rho_L + \rho_i + \rho_e$.

$\rho_L \sim T^5$ at low temperatures (mostly due to normal electron-phonon scattering). In transport theory, we have $< A >= \frac{1}{N}\sum_{\mathbf{k}} f(\mathbf{k})A(\mathbf{k})$, where $f(k)$ is the non-equilibrium electron distribution.

$N = \sum_{\mathbf{k}} f(\mathbf{k})$ is the number of electrons

$$f(k) \rightarrow f_0(k) = \{e^{[\epsilon(k)-\mu]/\tau} + 1\}^{-1}$$

when thermal equilibrium is reached.

$$\mathbf{J} = n(-e) < \mathbf{v} >= (-e)\frac{1}{V}\sum_{\mathbf{k}} f(k)(\frac{\hbar\mathbf{k}}{m}).$$

$f(k)$ is determined by the Boltzmann transport equation. In its simplest form, we have

Boltzmann transport theory

We assume that there exists a distribution function $f((\mathbf{k},\mathbf{r},t)$, which measures the number of carriers in state $\mathbf{k}$ in the neighbor of $\mathbf{r}$ at time t. The values of $\mathbf{k}$ and $\mathbf{r}$ are somewhat vague, subject to the uncertainty $\Delta k \Delta r = \hbar$. The "Average" of a physical quantity $A(\mathbf{r},\mathbf{k},t)$ is given by

$$< A(\mathbf{r},t) >= \int f(\mathbf{k},\mathbf{r},t) A(\mathbf{r},\mathbf{k},t)\frac{d^3k}{4\pi^3}, \ (n_0(\mathbf{r}) = \int f(\mathbf{k},\mathbf{r},t)\frac{d^3k}{4\pi^3})$$

$$e.g. \ \ J = e\int \mathbf{v}(\mathbf{k}) f(\mathbf{k},\mathbf{r},t)\frac{d^3k}{4\pi^3} \ \cdots \ \text{electric current.}$$

The dynamics of carriers in solid is described by

$$\dot{\mathbf{k}} = -e[\mathbf{E} + \frac{1}{c}\mathbf{v}_k \times \mathbf{H}] = \mathbf{F}; \ \mathbf{k} = \text{ crystal momentum.}$$

$$\dot{\mathbf{r}} = \mathbf{v}_k = \partial\epsilon(\mathbf{k})/\partial\mathbf{k}; \ \epsilon(\mathbf{k}) = \text{ band energy .}$$

If no collision occurs, the number of particles is conserved, i.e.

$$f(\mathbf{r} + \mathbf{v}dt, \mathbf{k} + \mathbf{f}dt, t + dt) = f(\mathbf{r},\mathbf{k},t).$$

$$\frac{dt}{dt} = \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{F}\cdot\frac{\partial f}{\partial \mathbf{k}} + \frac{\partial f}{\partial t} = 0.$$

with collisions:

$$\frac{df}{dt} = (\frac{\partial f}{\partial t})_{coll} = \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{F}\cdot\frac{\partial f}{\partial \mathbf{k}} + \frac{\partial f}{\partial t}$$

$$= -(\frac{\partial f}{\partial t})_{diff} - (\frac{\partial f}{\partial t})_{field} + \frac{\partial f}{\partial t} \ \cdots \ \text{Boltzmann's equation.}$$

$$\Rightarrow \frac{\partial f}{\partial t} = (\frac{\partial f}{\partial t})_{diff} + (\frac{\partial f}{\partial t})_{field} + (\frac{\partial f}{\partial t})_{coll}$$

total rate of change of distribution at $(\mathbf{u},\mathbf{r},t)$. At steady state, $\frac{\partial f}{\partial t} = 0$.

Scattering rate

$$(\frac{\partial f}{\partial t})_{coll} = -(\text{out-scattering rate}) + (\text{in-scattering rate})$$

$$= -\sum_{k'} f_k(1 - f_{k'})S_{kk'} + \sum_{k'} f_{k'}(1 - f_k)S_{kk'}.$$

$S_{kk'}$ = scattering rate from state $\mathbf{k}$ to state $\mathbf{k}'$. e.g.

(i) Electron-LA phonon scattering

$$S_{kk'} = 2\pi|M_q|^2[\delta(\epsilon_k - \epsilon_{k'} - \omega_q)(N_q + 1) + \delta(\epsilon_k - \epsilon_{k'} + \omega_q)N_q]_{q=k-k'}$$

$$= 2\pi|M_{k-k'}|^2(2N_{k-k'} + 1)\delta(\epsilon_k - \epsilon_{k'}) \text{ (ignore } \omega_q). \quad \text{(nearly elastic scattering)}$$

(ii) Electron-LO phonon scattering (inelastic)

$$S_{kk'} = 2\pi|M_{k-k'}|^2[\delta(\epsilon_k - \epsilon_{k'} - \omega_0)(N_0 + 1) + \delta(\epsilon_k - e_{k'} + \omega_0)N_0]$$

(iii) Electron-impurity scattering (elastic)

$$S_{kk'} = 2\pi|< k|V_{imp}|k' >|^2\delta(\epsilon_k - e_{k'}),$$

where V is the impurity potential. Microscopic reversibility (for elastic scattering)

$$S_{kk'} = S_{k'k}.$$

Linearized Boltzmann equation: (valid in low-field case)
Use $S_{kk'} = S_{k'k}$ (elastic scattering), We have

$$(\frac{\partial f}{\partial t})_{coll} = \int (f_k - f_{k'}) S_{kk'} d^3k' = -\int [(f_k - f_k^0) - (f_{k'} - f_{k'}^0)] S_{kk'} d^3k'$$

$$\text{since} \quad f_{k'}^0 = f_k^0 = [e^{\beta(\epsilon_k - \mu)} + 1]^{-1}.$$

Assume a constant temperature gradient and electrostatic field,

$$\mathbf{v}_k \cdot \frac{\partial f}{\partial \mathbf{r}} = \mathbf{v}_k \cdot \frac{\partial f_k^0}{\partial T} \nabla T, \ \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{k}} = -e\mathbf{E} \cdot \mathbf{v}_k \frac{\partial f_k^0}{\partial \epsilon_k}$$

$$\Rightarrow \mathbf{v}_k \cdot \frac{\partial f_k^0}{\partial T} \nabla T - e\mathbf{E} \cdot \mathbf{v}_k \frac{\partial f_k^0}{\partial \epsilon_k} = \sum_k [(f_k - f_k^0) - (f_{k'} - f_{k'}^0)] S_{kk'}.$$

For spherical energy band, $\epsilon_{\mathbf{k}} = \epsilon(k) = \epsilon(k')$

$$\Rightarrow k = k', \ \mathbf{v}_k = \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} = v_k \hat{k}.$$

Try the solution $f_k - f_k^0 = \mathbf{a}(k) \cdot \hat{k}$

$$\Rightarrow (\frac{\partial f}{\partial t})_{coll} = -\mathbf{a}(k) \cdot \sum_{k'} S_{kk'} (\hat{k} - \hat{k}')$$

$$= -\mathbf{a}(k) \cdot \hat{k} \sum_{k'} S(k, \hat{k} \cdot \hat{k}')(1 - \hat{k} \cdot \hat{k}') = -(\mathbf{a}(k) \cdot \hat{k})/\tau(k).$$

(*Note: $S_{kk'}$ is a function of $k = k'$ and $|\mathbf{k} - \mathbf{k}'|$ only, or $S_{kk'} = S(k, \hat{k} \cdot \hat{k}')$)

$$\text{and} \quad \mathbf{a}(k) = -v_k (\frac{\partial f_k^0}{\partial T} \nabla T - e\mathbf{E} \frac{\partial f_k^0}{\partial \epsilon_k}) \tau(k) \ \cdots \ \text{exact solution.}$$

Relaxation-time approximation

$$(\frac{\partial f}{\partial t})_{coll} = -(f_k - f_k^0)/\tau(k)$$

$$\frac{1}{\tau(k)} = \int d^3k' S(k,\theta')(1 - cos\theta').$$

In the absence of field and with constant relaxation time, τ, we have

$$(\frac{\partial f_k}{\partial t}) = -(f_k - f_k^0)/\tau.$$

with solution

$$f_k(t) = f_k^0 + (f_k(0) - f_k^0)e^{-t/\tau}.$$

In the low field limit, we have

$$(\frac{\partial f_k}{\partial t}) = e\mathbf{E} \cdot \mathbf{v}_k \frac{\partial f_k^0}{\partial \epsilon_k} - (f_k - f_k^0)/\tau.$$

or (let $g_k = f_k - f_k^0$)

$$(\frac{\partial g_k}{\partial t}) = e\mathbf{E} \cdot \mathbf{v}_k \frac{\partial f_k^0}{\partial \epsilon_k} - g_k/\tau.$$

with solution

$$g_k(t) = e\mathbf{E} \cdot \mathbf{v}_k \frac{\partial f_k^0}{\partial \epsilon_k}[1 - e^{-t/\tau}].$$

DC conductivity

Consider the case $\nabla T = 0$ and $\mathbf{E} =$ constant .

$$f_k = f_k^0 + e\mathbf{E}\cdot\mathbf{v}_k(\frac{\partial f_k^0}{\partial \epsilon_k})\tau(k)$$

$$J_i = -e\int \frac{d^3k}{4\pi^3} v_i(\mathbf{k}) f(\mathbf{k}) = e^2\sum_j E_j \int \frac{d^3k}{4\pi^3} v_i(\mathbf{k}) v_j(\mathbf{k})(-\frac{\partial f_k^0}{\partial \epsilon_k})\tau(k) = \sum_j \sigma_{ij}E_j.$$

$$\sigma_{ij} = e^2\int \frac{d^3k}{4\pi^3} v_i(\mathbf{k}) v_j(\mathbf{k})(-\frac{\partial f_k^0}{\partial \epsilon_k})\tau(k) \cdots \text{ conductivity tensor}$$

Good approx. for metals

NOTE: $\mathbf{v}(\mathbf{k})\frac{\partial f_k^0}{\partial \epsilon_k} = \frac{\partial f_k^0}{\partial \epsilon_k}\frac{\partial \epsilon_k}{\partial \mathbf{k}} = \frac{\partial f_k^0}{\partial \mathbf{k}}$

So, $\sigma_{ij} = e^2\tau(k_F)\int \frac{d^3k}{4\pi^3}\frac{\partial}{\partial k_j}(v_i(\mathbf{k}))f_k^0$ (integration by parts)

$= e^2\tau(k_f)\int \frac{d^3k}{4\pi^3} f^0(\epsilon_k) m_{ij}^{-1}(\mathbf{k}) \cdots$ effective mass tensor

$= [ne\tau(k_F)/m^*]\delta_{ij}$ (for spherical nondegenerate bands).

Electron mobility

- Temperature dependence of electron mobility in semiconductors:

$$\mathbf{J} = -en_0 < v > = -e^2 \int \frac{d^3k}{4\pi^3} \tau(k) \mathbf{v}_k (\mathbf{v}_k \cdot \mathbf{E}) \frac{\partial}{\partial E_k} f^0(E_k)$$

(in effective-mass approximation)

$$= [-\frac{2}{3}\frac{e^2}{m^*} \int \frac{d^3k}{4\pi^3} \tau(k) \epsilon_k \frac{\partial f^0}{\partial \epsilon_k}]\mathbf{E} = \frac{n_0 e^2}{m^*} < \tau > \mathbf{E} = \sigma \mathbf{E} = e n_0 \mu \mathbf{E}.$$

$$< \tau > = \frac{2}{3n_0} \int \frac{d^3k}{4\pi^3} \tau(k) \epsilon_k (-\frac{\partial f^0}{\partial \epsilon_k}) = \frac{1}{n_0} \int \frac{d^3k}{4\pi^3} \tau(k) v_z(k) (-\frac{\partial f^0}{\partial v_z}) \cdots \text{ relaxation time}$$

$$\sigma = n_0 e^2 < \tau > /m^* \cdots \text{ DC conductivity} ; \mu = e < \tau > /m^* \cdots \text{ mobility}$$

$$< \tau > \propto T^r \text{ for non-degenerate electron gas } (T > 100K).$$

$r = -3/2, -1/2, 0, 3/2$ for LA-deformation potential, piezoelectric, neutral impurity, and ionized impurity scattering, respectively.

AC conductivity

Use the relaxation-time approximation:

$$\frac{\partial f}{\partial t} + e\mathbf{E}(t) \cdot \frac{\partial f}{\partial \mathbf{k}} = \frac{f - f^0}{\tau(k)}$$

Define $f = f^0 + g(t)$ and linearize to get

$$\frac{\partial g(t)}{\partial t} + e\mathbf{E}(t) \cdot \frac{\partial f^0}{\partial \mathbf{k}} = -\frac{g(t)}{\tau(k)}.$$

Assign $e^{i\omega t}$ dependence to $g(t)$ and $\mathbf{E}(t)$

$$\Rightarrow [i\omega + \frac{1}{\tau(k)}]g(\omega) = -e\mathbf{E}(\omega)\frac{\partial f^0}{\partial \mathbf{k}}.$$

$$\text{So,}\ \ \mathbf{j}(\omega) = e^2 \int \frac{d^3k}{4\pi^3}[i\omega + \frac{1}{\tau_k}]^{-1}\mathbf{v}_k\mathbf{v}_k \cdot \mathbf{E}(\omega)(-\frac{\partial f^0}{\partial \epsilon_k}) = \sigma(\omega) \cdot \mathbf{E}$$

$$\text{or}\ \ \sigma_{ij}(\omega) = e^2 \int \frac{d^3k}{4\pi^3}[i\omega + \frac{1}{\tau(k)}]^{-1}v_i v_j(-\frac{\partial f^0}{\partial \epsilon_k})$$

NOTE: as $\omega \to \infty$, we have

$$\frac{e^2}{i\omega}\int \frac{d^3k}{4\pi^3}v_i(k)(-\frac{\partial}{\partial k_j}f^0) = \frac{e^2}{i\omega}\int \frac{d^3k}{4\pi^3}f^0(\epsilon_k)\frac{\partial^2 \epsilon}{\partial k_i \partial k_j} = \frac{n_0 e^2}{i\omega} < m_{ij}^{*-1} >_0 .$$

$$R_e\sigma_{ij}(\omega) = e^2 \int \frac{d^3k}{4\pi^3}\frac{\tau(k)}{1 + w^2\tau^2(k)}v_i(k)v_j(k)(-\frac{\partial f^0}{\partial \epsilon_k})$$

$$I_m\sigma_{ij}(\omega) = e^2 \int \frac{d^3k}{4\pi^3}\frac{\omega\tau^2(k)}{1 + w^2\tau^2(k)}v_i(k)v_j(k)(-\frac{\partial f^0}{\partial \epsilon_k}).$$

Electron conduction in metals

Electron distribution is degenerate in metals,

$$-\frac{\partial f^0}{\partial \epsilon_k} \approx \delta(\epsilon_{k'} - \epsilon_F)$$

$$\text{So,}\ \ \sigma = n_0 e^2 < \tau > /m^* with < \tau > = \frac{2}{3}\int \frac{d^3k}{4\pi^3}\tau(k)\epsilon_k(-\frac{\partial f^0}{\partial \epsilon_k}) \approx \tau(\epsilon_F).$$

Resistivity, $\rho = \sigma^{-1} = \sum_i \rho_i$ (from various mechanisms) ... Mathiessen's rule. [since $\tau^{-1} = \sum_i \tau_i^{-1}$]

(i) impurity scatterings: $\tau(\epsilon_F)$ is independent of T, so is ρ_I.

(ii) Acoustic-phonon deformation:

$$\tau(\epsilon_F)^{-1} \propto T \ \Rightarrow\ \rho_{ac} \propto T\ (\text{ for }\ T \ll \theta_D)$$

For $T < \Theta_D$, we cannot use the approximation $N_q = \frac{k_B T}{\omega_q} - \frac{1}{2}$. In this case, we cannot use the relaxation-time approximation since $S_{kk'} \neq S_{kk'}$ when N_q and $(N_q + 1)$ are substantially different. Here, we have to consider large-angle scattering with $q = |\mathbf{k} - \mathbf{k}'|\ k_F$; hence the maximum acoustic phonon frequency is close to Θ_D.

Electron motion in B field

$$\frac{d}{dt} < A >= -\frac{1}{\tau} < A > + \text{ driving term} \quad \text{... equation of motion due to collision.}$$

$$\text{Let } A = \mathbf{v} \Rightarrow \frac{d}{dt} < \mathbf{v} >= -\frac{1}{\tau} < \mathbf{v} > + \frac{1}{m}\mathbf{F} \text{ ... external force}$$

$$\mathbf{F} = -e[\mathbf{E} + \frac{1}{c} < \mathbf{v} > \times \mathbf{B}] \text{ ... Lorentz force.}$$

Let $\mathbf{B} = B_z \hat{z}$

$$\Rightarrow m(\frac{d}{dt} + \frac{1}{\tau})v_x = -e(E_x + \frac{B}{c}v_y)$$

$$m(\frac{d}{dt} + \frac{1}{\tau})v_y = -e(E_z - \frac{B}{c}v_x)$$

$$m(\frac{d}{dt} + \frac{1}{\tau})v_z = -eE_z.$$

In steady state $\frac{d}{dt} < \mathbf{v} >= 0$

$$\Rightarrow v_x = -\frac{e\tau}{m}E_x - \omega_c \tau v_y, \; v_y = -\frac{e\tau}{m}E_y + \omega_c \tau v_y, \; v_z = -\frac{e}{\tau}mE_z$$

$$\text{or } \mathbf{v} = -\frac{e\tau}{m}\mathbf{E} - t\mathbf{v} \times \vec{\omega}_c,$$

where $\omega_c = eB/mc$ is the "cyclotron frequency".

Let $\mathbf{E} = \mathbf{E}_l + \mathbf{E}_t$, where $\mathbf{E}_e || \mathbf{v}$ and $\mathbf{E}_t \perp \mathbf{v}$

$$\Rightarrow \mathbf{v} = -\frac{e\tau}{m}\mathbf{E}_l \text{ and } \frac{e\tau}{m}\mathbf{E}_t = -\tau\mathbf{v} \times \vec{\omega}_c.$$

Hall Effect

For an applied $\mathbf{E}$ field along x, we expect $v_x = -\frac{e\tau}{m}E_x$.

Current $J_x = n(-e)v_x = \dfrac{ne^2\tau}{m}E_x$ independent of sign of charge .

$$\mathbf{E}_t = (\frac{m}{e})\mathbf{v} \times \vec{\omega}_c = (\frac{m}{e})v_x(\frac{eB}{mc})\hat{y} = -(\frac{\tau eB}{mc})E_x\hat{y}.$$

Define $R_H = \dfrac{E_y}{J_x B} = (\dfrac{m}{ne^2\tau B})\dfrac{E_y}{E_x} = -\dfrac{1}{nec}$ ... Hall coefficient,

which depends on the sign of charge.

$\rho_H = \dfrac{E_y}{J_x} = -\dfrac{B}{nec}$ is the Hall resistance.