Exam. 7th Dec
MTW [illegible] Th

(T1)

# Transport in Solids

## Topics

1) Theory of electrical conduction in metals.
   - a) Impurity scattering
   - b) Phonon scattering.

2 methods: a) Semi-classical treatment based on Boltzmann's equation

b) Green's function formalism, based on Kubo formula and multiple-scattering theory.

[ Second formalism will be worked out for the problem of impurity scattering. ]

2) Effects of magnetic field on electrical conduction.
   - a) Hall effect
   - b) Magnetoresistance.

3) Transport of energy. Thermal conduction.
   - a) Thermal conductivity due to conduction electrons
   - b) " " due to phonons.

4) Thermoelectric effects (Transport of both charge and energy).

## I) Electrical conduction in metals

In several previous calculations, we saw that the d.c. ~~cond~~ conductivity of a metal is zero if no scattering is present. In the band theory of electrons, we found that the trajectory of a Bloch electron in a uniform external electric field is periodic in time, so that it does not carry any net dc current. When discussing the Kubo formula for the conductivity, we again found that in the absence of any scattering, the real part of the conductivity of the conduction electron is zero. There, this result was explained by showing that a free electron can not absorb a photon, and conserve both energy & momentum in the process. Thus, we need some scattering events in which the extra energy/momentum can be absorbed. In a metal, two different types of scattering are important.

1) Impurity scattering. In discussing these processes, we will assume that the impurities do not have any internal structure. Thus, the energy of an electron does not change as it scatters from an impurity ⇒ Elastic scattering. The momentum, of course, changes. The change in momentum is absorbed by the impurity without any recoil, which means that we are assuming that the impurities have infinite mass.

2) Scattering by phonons: This comes from the el-phonon interaction considered before. ~~E~~ Both the energy & the momentum of an electron changes in either emission or absorption of a phonon. ⇒ Inelastic scattering. Strongly temperature dependent.

Here, we'll try to understand the effects of both types of scattering. This problem is of great practical importance. There are also some intriguing theoretical questions raised by this problem. These questions are about the basic nature of irreversible processes. A system with a non-zero real part of the conductivity is dissipative. A dissipative system is, by definition, irreversible. On the other hand, we are trying to describe the behavior of the system in terms of the quantum mechanics of the ~~ca~~ microscopic constituents. The ~~qua~~ microscopic equations of motion are reversible. [Hamiltonian system is periodic]. So, it is an interesting question to ask how irreversible behavior on the ~~ma~~ macroscopic scale arises from a set of reversible microscopic equations. It turns out that the irreversibility arises from the presence of a *macroscopic* number of impurities, distributed at *random*.

G. V. Chester, Rep. Prog. Phys. *26*, 411 (1963)

I'll not go into the details. But let me remark that it is necessary to have a macroscopic number of impurities (number goes to infinity in the thermodynamic limit), and complete randomness in their positions, so that the scattering from them adds up incoherently. When these two conditions are satisfied, it can be shown that, although the microscopic description is reversible, the macroscopic response can be irreversible i.e. dissipative.

In describing the process of electrical conduction in metals, we'll make the following assumptions:

1) Consider only conduction electrons. Parabolic

* Also, the effects of el-el interaction can be included in a more detailed way in the GF formalism.

band, isotropic effective mass $m^*$ => plane waves.

2) Neglect electron-electron interaction, except for the ~~effe~~ screening effect, which is taken care of by a static dielectric function $\epsilon(\vec q)$. In particular, when we discuss the scattering of an electron by an impurity, we'll use the screened ~~pA~~ impurity potential. [It is possible to ~~stu~~ study a Boltzmann equation for the quasiparticles in ~~Fermi~~ Landau's Fermi liquid theory.] *

3) External perturbations (electromagnetic field, temperature gradient etc.) are time independent, and slowly varying in space (continuum description is valid). Also, these perturbations are small ~~(compared to the energies associated with unperturbed electrons i.e. the Fermi energy)~~, so that in the Boltzmann equation approach, we'll be able to linearize the equation, and in the GF approach, we'll be able to use linear response theory.

$$\frac{d\vec r}{dt} = \vec v = \frac{1}{\hbar}\frac{\partial E(\vec k)}{\partial \vec k}, \quad \frac{\partial}{\partial t}(\hbar \vec k) = \vec F$$

## Boltzmann Equation

This is a semi-classical description in which the electrons will be described by wave-packets. The time evolution of such a wave packet is described by a distribution function which is defined in the 6-dimensional phase space $(\vec p, \vec r) \to (\vec k, \vec r)$.

$$\frac{2}{(2\pi)^3} f(\vec k, \vec r, t)\, d^3k\, d^3r = \# \text{ of electrons}$$

centered at $\vec r$

in the volume element $d^3r$, with ~~momentum~~ $\vec k$ in the range $d^3k$ centered at $\vec k$, at time $t$. The meaning of $f$ is clear from this definition. First, note that $\frac{d^3k\, d^3r}{(2\pi)^3} = \frac{d^3p\, d^3r}{h^3}$ is the number of ~~particles~~ states allowed in the phase-space volume $d^3p\, d^3r$ by the uncertainty principle. The factor 2 comes from spin. Thus, the function $f(\vec{k},\vec{r},t)$ tells us about how many of these allowed states are occupied. It varies between 0 to 1, thus the Pauli principle is satisfied.

The transport equation deals with how this distribution function evolves in time in the presence of external fields. Here, I'll give a rather simple non-rigorous derivation of the Boltzmann equation. Let us consider a particular state $(\vec{k}_0, \vec{r}_0)$ which is occupied at $t=0$ i.e. $f(\vec{k}_0, \vec{r}_0, 0) = 1$.* At later times, ~~this state~~ wave packet representing the electron in this state will evolve will ~~move in phase space~~ according to the semi-classical equations of motion. This time evolution can be described by a trajectory in phase space, parametrized by two functions, $\vec{k}_0(t), \vec{r}(t)$, with $\vec{k}(0) = \vec{k}_0$, $\vec{r}(0) = \vec{r}_0$. If we follow this trajectory, then, at any time t, there is ~~an~~ always an electron in the state $\vec{k}(t), \vec{r}(t)$ at time t, unless ~~there are~~ the electron is scattered out of this state by some interaction which has not been included in our semiclassical Hamiltonian. Such scattering events ~~are~~ correspond to discontinuous jumps in phase space (the momentum changes discontinuously), and these jumps are not included in the semiclassical trajectory we are considering here ~~, and such processes can not be included in the semiclassical description~~. Also, some other electrons can be scattered into the state, which will increase $f(\vec{k}(t), r(t), t)$. If such scatterings are not present, then it is clear that

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* Actually, we mean that there is one occ. state in the volume $\sim h^3$ of phase space around $(\vec{k}_0, \vec{r}_0)$.

$$f\left(\vec{k}(t), \vec{r}(t), t\right) = 1$$

$$\Rightarrow \frac{df}{dt} = 0 \Rightarrow \frac{\partial \vec{k}}{\partial t} \cdot \frac{\partial f}{\partial \vec{k}} + \frac{\partial \vec{r}}{\partial t} \cdot \frac{\partial f}{\partial \vec{r}} + \frac{\partial f}{\partial t} = 0$$

$$\Rightarrow \frac{1}{\hbar} \vec{F} \cdot \vec{\nabla}_{\vec{k}} f + \vec{v} \cdot \vec{\nabla}_r f + \frac{\partial f}{\partial t} = 0.$$

$\vec{v}$: velocity of the wave packet, is a fn. of $\vec{k}$.

~~The third term arises from any explicit time-dependence of the temperature, external fields etc. We have assumed that such explicit time dependences are not present $\Rightarrow \frac{\partial f}{\partial t} = 0$. Then, in the absence of scatterings, we have~~ Thus, in the absence of scattering, we have

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar} \vec{F} \cdot \vec{\nabla}_k f - \vec{v} \cdot \vec{\nabla}_r f.$$

When scatterings are present, we must have

$$\frac{df}{dt} = \left.\frac{\partial f}{\partial t}\right|_{\text{scat.}}$$

$$\Rightarrow \frac{\partial f}{\partial t} = -\frac{1}{\hbar} \vec{F} \cdot \vec{\nabla}_k f - \vec{v} \cdot \vec{\nabla}_r f + \left.\frac{\partial f}{\partial t}\right|_{\text{scat.}}$$

This is the Boltzmann equation. Its interpretation is simple. The first term tells us about the change in momentum due to external fields. This means that points are moving in and out of the ~~phase space~~ volume element $d^3k$ in $\vec{k}$-space. If the distribution fn. depends upon the momentum, the # coming in will be different from the number going out, and $f$ will change with time. The second term is the drift or diffusion term. If $f$ depends on $\vec{r}$ (this will be the case when a temperature gradient is present, or if there are other macroscopic inhomogeneities), then the number of electrons entering a volume element $d^3r$ is real space will be different from the number going out. Finally, there is the scattering term. These three contributions add up to give the rate of change of $f$ with time. In a steady state situation, $f$ does not change with time, and we have the equation

$$-\frac{1}{\hbar}\vec{F}\cdot\vec{\nabla}_k f - \vec{v}\cdot\vec{\nabla}_r f + \left.\frac{\partial f}{\partial t}\right|_{\text{scat}} = 0$$

We have to solve this to find $f$. Then various currents can be calculated:

El. current density: $\vec{j}(\vec{r}) = -\frac{e}{4\pi^3}\int \vec{v}(\vec{k})\, f(\vec{k},\vec{r})\, d^3k$ Charge $(-e)$

Energy or heat current:

$$\vec{Q}(\vec{r}) = \frac{1}{4\pi^3}\int E(\vec{k})\,\vec{v}(\vec{k})\, f(\vec{k},\vec{r})\, d^3k \quad \text{etc.}$$

External fields

$$\vec{F} = -e\left(\vec{E} + \frac{1}{c}\,\vec{v}\times\vec{B}\right)$$

Temperature gradient

$$\vec{v}\cdot\vec{\nabla}_r f = \left(\vec{v}\cdot\vec{\nabla}_r T\right)\cdot\frac{\partial f}{\partial T}$$

The scattering term is difficult to obtain.

## Boltzmann Equation

$$+\frac{1}{\hbar}\vec{F}\cdot\frac{\partial f(\vec{k},\vec{r})}{\partial\vec{k}}+\vec{V}(\vec{k})\cdot\frac{\partial f(\vec{k},\vec{r})}{\partial\vec{r}}=\left.\frac{\partial f}{\partial t}\right]_{\text{scat}}$$

$\vec{F}$: External force. $\vec{V}$: velocity.

The main problem is to find a suitable form for the scattering term $\left.\frac{\partial f}{\partial t}\right]_{\text{scat}}$. We can write down a formal expression for this term. Let $W(\vec{k},\vec{k}')$ be the rate at which electrons are scattered from state $\vec{k}'$ to state $\vec{k}$. Similarly, $W(\vec{k}',\vec{k})$ be the rate of the reverse process. Now, an electron can be scattered into $\vec{k}$ from $\vec{k}'$ only if $\vec{k}'$ is occupied, and $\vec{k}$ is empty, because of the Pauli principle. Thus, the rate at which electrons are scattered out of the state $\vec{k}$ is given by

~~Assume that there is no temperature gradient~~

(assume that these rates are independent of $\vec{r}$)

~~Assume that these are independent of $\vec{r}$~~

$$\text{Loss}:\quad\sum_{\vec{k}'}W(\vec{k}',\vec{k})\,f(\vec{k},\vec{r})\left[1-f(\vec{k}',\vec{r})\right]$$

Rate of scattering into state $\vec{k}$ is given by

$$\text{gain}:\quad\sum_{\vec{k}'}W(\vec{k},\vec{k}')\,f(\vec{k}',\vec{r})\left[1-f(\vec{k},\vec{r})\right]$$

$$\Rightarrow\left.\frac{\partial f(\vec{k},\vec{r},t)}{\partial t}\right]_{\text{scat}}=\sum_{\vec{k}'}\Big\{W(\vec{k},\vec{k}')f(\vec{k}',\vec{r})\left[1-f(\vec{k},\vec{r})\right]-W(\vec{k}',\vec{k})f(\vec{k},\vec{r})\left[1-f(\vec{k}',\vec{r})\right]\Big\}$$

The sum over $\vec{k}'$ can be converted into an integral, and we end up with a nonlinear integro-differential equation, which is rather difficult to solve in general. The approximation most often used is to linearize this equation.

* this is independent of position because we have included the temperature gradient in the list of perturbations.

This is done by assuming that the external fields, ~~and~~ temperature gradients and other disturbances are small, so that the distribution function $f(\vec{k},\vec{r})$ is not very different from the equilibrium distribution for $f_0(\vec{k})^*$. One then writes the Boltzmann equation in terms of the difference between $f$ and $f_0$, and keeps only the ~~smallest~~ lowest order terms in this difference.

So, we write

$$f(\vec{k},\vec{r}) = f_0(\vec{k}) + f_1(\vec{k},\vec{r})$$

$f_1$ is small, $f_0(\vec{k})$ is just the Fermi distribution for

$$f_0(\vec{k}) = 1\Big/\left[1+e^{(E(\vec{k})-\mu)/k_BT}\right]$$

The left hand side of the Boltzmann equation now reads

$$\vec{F} = -e\left(\vec{E}+\frac{1}{c}\vec{V}\times\vec{B}\right)$$

$$\vec{V}\cdot\frac{\partial f}{\partial\vec{r}} = \left(\vec{V}\cdot\vec{\nabla}_r T\right)\frac{\partial f}{\partial T}$$

$$-\frac{e}{\hbar}\left(\vec{E}+\frac{1}{c}\vec{V}\times\vec{B}\right)\cdot\left(\frac{\partial f_0}{\partial\vec{k}}+\frac{\partial f_1}{\partial\vec{k}}\right) + \vec{V}\cdot\vec{\nabla}_r T\left(\frac{\partial f_0}{\partial T}+\frac{\partial f_1}{\partial T}\right)$$

We want to keep only the lowest order terms.

$$\frac{\partial f_0}{\partial\vec{k}} = \frac{\partial f_0}{\partial E}\frac{\partial E(\vec{k})}{\partial(\vec{k})} = \frac{\partial f_0}{\partial E}\hbar\vec{V}(\vec{k})$$

We keep only this term for the electric field.

$$\Rightarrow\quad -\frac{e}{\cancel{\hbar}}\vec{E}\cdot\vec{V}\cancel{\hbar}\frac{\partial f_0}{\partial E}$$

~~This~~ The corresponding term ~~to~~ for the magnetic field is zero. So we have to keep the next term.

$$\Rightarrow\quad -\frac{e}{\hbar c}\left(\vec{V}\times\vec{B}\right)\cdot\vec{\nabla}_k f_1$$

For the thermal gradient, we keep only the $f_0$ term.

$$\frac{\partial}{\partial T} f_0(\vec{k}) = -\left[f_0(\vec{k})\right]^2\left(-\frac{1}{k_B}\right)\left[\frac{\partial}{\partial T}\left(\mu/T\right) + \frac{E}{T^2}\right] e^{(E-\mu)/kT}$$

$$= -\frac{\partial f_0}{\partial E}\left[T\frac{\partial}{\partial T}\left(\frac{\mu}{T}\right) + \frac{E}{T}\right]$$

$$\Rightarrow \text{L.H.S} = -\vec{V}(\vec{k})\cdot\left[e\vec{E} + \left(T\frac{\partial}{\partial T}\left(\frac{\mu}{T}\right) + \frac{E(\vec{k})}{T}\right)\vec{\nabla}_r T\right]\frac{\partial f_0}{\partial E}$$

$$\boxed{\vec{E}\to\vec{\mathcal{E}}} \qquad - \frac{e}{\hbar c}\left(\vec{V}\times\vec{B}\right)\cdot\vec{\nabla}_k f_1$$

$$= -\vec{V}(\vec{k})\cdot\left[e\vec{E} + T\vec{\nabla}_r\left(\frac{\mu}{T}\right) + \frac{E(\vec{k})}{T}\vec{\nabla}_r T\right]\frac{\partial f_0}{\partial E}$$

$$- \frac{e}{\hbar c}\left(\vec{V}\times\vec{B}\right)\cdot\vec{\nabla}_k f_1.$$

Now, we want to linearize the right hand side. To do that, we note that if we replace $f(\vec{k},\vec{r})$ by $f_0(\vec{k})$ in the expression for $\left.\frac{\partial f}{\partial t}\right|_{\text{scat}}$, we must get zero. This is because the scatterings can not change the equilibrium distribution. At equilibrium, the average occupation of a particular state is determined only by the energy of that state, and nothing can change that. If anything, the scattering processes will help to obtain equilibrium if the initial state is a non-equilibrium one. Thus, we can write

$$\sum_{\vec{k}'}\left[W(\vec{k},\vec{k}')f_0(\vec{k}')\left[1-f_0(\vec{k})\right] - W(\vec{k}',\vec{k})f_0(\vec{k})\left(1-f_0(\vec{k}')\right)\right] = 0.$$

Note that this is just the detailed balance condition. If we define

$$P(\vec{k},\vec{k}') = W(\vec{k},\vec{k}')f_0(\vec{k}')\left(1-f_0(\vec{k})\right),$$

then the condition above implies That

$$P(\vec{k},\vec{k}') = P(\vec{k}',\vec{k})$$

Now,

$$P(\vec{k},\vec{k}') = W(\vec{k},\vec{k}')\, f_0(\vec{k}')\, f_0(\vec{k})\, e^{(E(\vec{k})-\mu)/k_BT}$$

$$P(\vec{k}',\vec{k}) = W(\vec{k}',\vec{k})\, f_0(\vec{k})\, f_0(\vec{k}')\, e^{(E(\vec{k}')-\mu)/k_BT}$$

$$\Rightarrow \quad \cancel{\boxed{\frac{P(\vec{k},\vec{k}')}{P(\vec{k}',\vec{k})}}} \quad \cancel{=} \quad \cancel{\boxed{\frac{e^{-\beta E(\vec{k}')}}{e^{-\beta E(\vec{k})}}}} \qquad W(\vec{k},\vec{k}')\, e^{-E(\vec{k}')/k_BT} = W(\vec{k}',\vec{k})\, e^{-E(\vec{k})/k_BT}$$

which means that, at equilibrium, the ratio of rate of transition from $\vec{k} \to \vec{k}'$ and that for $\vec{k}' \to \vec{k}$ must be equal to the ratio of the corresponding Boltzmann factors. This is the detailed balance condition which must be satisfied at thermal equilibrium. Now, if we write $f = f_0 + f_1$, The

$$\left.\frac{\partial f_1}{\partial t}\right]_{scat.} = \sum_{\vec{k}'} \Big\{ W(\vec{k},\vec{k}') \left[ f_0(\vec{k}') + f_1(\vec{k}') \right] \times \left[ 1 - f_0(\vec{k}) - f_1(\vec{k}) \right]$$

$$- W(\vec{k}',\vec{k}) \left[ f_0(\vec{k}) + f_1(\vec{k}) \right] \left[ 1 - f_0(\vec{k}') - f(\vec{k}') \right] \Big\}$$

$$\boxed{\text{keep terms linear in } f_1}$$

$$= \sum_{\vec{k}'} \Big\{ W(\vec{k},\vec{k}') \Big( f_1(\vec{k}') \left[ 1 - f_0(\vec{k}) \right] - f_1(\vec{k}) f_0(\vec{k}') \Big) - W(\vec{k}',\vec{k}) \Big[ f_1(\vec{k}) \times \left( 1 - f_0(\vec{k}') \right) - f_1(\vec{k}') f_0(\vec{k}) \Big] \Big\}$$

$$= \sum_{\vec{k}'} P(\vec{k},\vec{k}') \left[ \frac{f_1(\vec{k}')}{f_0(\vec{k}')\left(1 - f_0(\vec{k}')\right)} - \frac{f_1(\vec{k})}{f_0(\vec{k})\left(1 - f_0(\vec{k})\right)} \right]$$

This suggests That it may be useful to define a new function $\phi$, which includes this factor $f_0(1-f_0)$ that appears above.

So, we write

$$f_1(\vec{k},\vec{r},t) \equiv \phi(\vec{k},\vec{r},t)\,\frac{\partial f_0(\vec{k})}{\partial E(\vec{k})}$$

$$= \phi(\vec{k},\vec{r},t)\, f_0(\vec{k})\left(1-f_0(\vec{k})\right)\left(-\frac{1}{k_BT}\right)$$

$$\Rightarrow \left.\frac{\partial f_1}{\partial t}\right]_{scat.} = \sum_{\vec{k}'} P(\vec{k},\vec{k}')\left(-\frac{1}{k_BT}\right)\Big[\phi(\vec{k}',\vec{r}) - \phi(\vec{k},\vec{r})\Big]$$

Thus finally we get the linearized Boltzmann equation

$$\vec{V}(\vec{k})\cdot\left[e\vec{E} + T\,\vec{\nabla}_r(\mu/T) + \frac{E(\vec{k})}{T}\,\vec{\nabla}_r T\right]\frac{\partial f_0(\vec{k})}{\partial E}$$

$$= \sum_{\vec{k}'} P(\vec{k},\vec{k}')\,\frac{1}{k_BT}\Big[\phi(\vec{k}',\vec{r}) - \phi(\vec{k},\vec{r})\Big]$$

$$- \frac{e}{\hbar c}\left[\vec{V}(\vec{k})\times\vec{B}\right]\cdot\vec{\nabla}_k f_1(\vec{k},\vec{r})$$

This is a linear intego-differential equation, and we'll try to solve it in some special cases.

## Impurity Scattering

$\vec{B} = 0$, No temperature gradient.

$$e\,\vec{V}(\vec{k})\cdot\vec{E}\;\frac{\partial f_0(\vec{k})}{\partial E} = \frac{1}{k_BT}\sum_{\vec{k}'} P(\vec{k},\vec{k}')\Big[\phi(\vec{k}') - \phi(\vec{k})\Big]$$

Also, assume elastic scattering. $E(\vec{k}) = E(\vec{k}')$.

$$\downarrow$$

$$f_0(\vec{k}) = f_0(\vec{k}')$$

$$P(\vec{k},\vec{k}') = W(\vec{k},\vec{k}')\left(1-f_0(\vec{k})\right)f_0(\vec{k})$$

$$= W(\vec{k},\vec{k}')(-k_BT)\,\frac{\partial f_0(\vec{k})}{\partial E}$$

$$\Rightarrow e\,\vec{V}(\vec{k})\cdot\vec{E} = -\sum_{\vec{k}'} W(\vec{k},\vec{k}')\Big[\phi(\vec{k}') - \phi(\vec{k})\Big]$$

## Impurity scattering

Boltzmann Equation:

$$e\,\vec{V}(\vec{k})\cdot\vec{\mathcal{E}} = -\sum_{\vec{k}'} W(\vec{k},\vec{k}')\left[\phi(\vec{k}')-\phi(\vec{k})\right]$$

$$\phi(\vec{k}) = \left[\frac{\partial f_0(\vec{k})}{\partial E(\vec{k})}\right]^{-1} f_1(\vec{k})$$

$W(\vec{k},\vec{k}')$: Transition rate for state $\vec{k}'$ to $\vec{k}$

Elastic scattering: $W(\vec{k},\vec{k}') = W(\vec{k}',\vec{k})$

$$W(\vec{k},\vec{k}') = \frac{2\pi n_i}{\hbar}\left|T(\vec{k},\vec{k}')\right|^2 \delta\left[E(\vec{k})-E(\vec{k}')\right]$$

$$T(\vec{k},\vec{k}') = T(k,\cos\theta)\,, \quad \cos\theta = \hat{k}\cdot\hat{k}'$$ (spherically symmetric potential)

Here, we have put the volume $\Omega$ of the system equal to unity. The T-matrix describes the scattering properties of a single impurity. It is closely related to the scattering cross-sections. The total scattering cross section

$$\sigma(k) = \frac{1}{V(\vec{k})}\sum_{\vec{k}'} W(\vec{k}',\vec{k})/n_i$$

$$= \left(\frac{m^*}{2\pi\hbar^2}\right)^2 \int d\Omega \left|T(k,\cos\theta)\right|^2, \quad d\Omega = \sin\theta\, d\theta\, d\phi$$

$$\boxed{\frac{d\sigma(k)}{d\Omega} = \left(\frac{m^*}{2\pi\hbar^2}\right)^2 \left|T(k,\cos\theta)\right|^2}$$

$$T(\vec{k},\vec{k}') = \frac{-2\pi\hbar^2}{m^* k}\sum_{\ell}(2\ell+1)\,P_\ell(\cos\theta)\,e^{i\delta_\ell(k)}\sin\delta_\ell(k)$$

$\delta_\ell(k) \Rightarrow$ phase shift for $\ell$-wave scattering.

Solution $\quad \phi(\vec{k}) = C(k)\,\hat{k}\cdot\vec{E}$

$(\theta,\phi)$: Angular coordinates of $\vec{k}'$, with $\vec{k}$ along the z-axis

$(\theta',\phi')$: " " " $\vec{E}$, " " " "

$$\text{L.H.S} = e\,V(k)\,\varepsilon \cos\theta'$$

$$\text{R.H.S} = -\frac{2\pi n_i}{\hbar}\frac{1}{(2\pi)^3}\int k'^2\,dk'\,\sin\theta\,d\theta\,d\phi\,\left[T(k,\cos\theta)\right]^2$$

$$\times\ \delta\left[E(\vec{k})-E(\vec{k}')\right] C(k)\,\varepsilon\left(\hat{k}'\cdot\hat{E}-\cos\theta'\right)$$

$$= -\frac{2\pi n_i}{\hbar}\frac{1}{(2\pi)^3}\,k\,\frac{m^*}{\hbar^2}\,C(k)\,\varepsilon\int \sin\theta\,d\theta\,d\phi\,\left|T(k,\cos\theta)\right|^2$$

$$\times\left[\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi') - \cos\theta'\right]$$

The $\phi$ integration gives zero for the first term.

$$\Rightarrow\quad \frac{2\pi n_i}{\hbar}\frac{1}{(2\pi)^3}\,k\,\frac{m^*}{\hbar^2}\,C(k)\,\varepsilon\int d\Omega\,\left|T(k,\cos\theta)\right|^2\cos\theta'$$

$$\times\left[1-\cos\theta\right]$$

$$= \underset{\uparrow}{\overset{V(\vec{k})}{n_i}}\left(\frac{m^*}{2\pi\hbar^2}\right)^2\underbrace{C(k)\,\varepsilon\cos\theta'}_{\phi(\vec{k})}\int d\Omega\,\left|T(k,\cos\theta)\right|^2(1-\cos\theta)$$

Now, we can cancel out $\varepsilon\cos\theta'$ in both sides, and it is clear that if we properly choose $C(k)$, then both sides will be equal for all $k$. Thus, we have a solution. This can be put in a more familiar form by noting that the R.H.S is actually equal to

$$-\left[\frac{\partial f_0(\vec{k})}{\partial E(\vec{k})}\right]^{-1}\frac{\partial f_1}{\partial t}\Bigg]_{\text{scat}}.$$

The expression for the RHS obtd. above is

$$\left[\frac{\partial f_0(\vec{k})}{\partial E(\vec{k})}\right]^{-1} f_1(\vec{k})\,\frac{1}{\tau(k)}$$

where,

$$1/\tau(k) \equiv n_i\, V(k) \left(\frac{m^*}{2\pi\hbar^2}\right)^2 \int d\Omega\, \left|T(k,\cos\theta)\right|^2 (1-\cos\theta)$$

$$\Rightarrow \boxed{\left.\frac{\partial f(\vec{k})}{\partial t}\right|_{scat} = -\frac{f_1(\vec{k})}{\tau(\vec{k})}}$$

$\tau(k)$ is clearly a relaxation time.

$$1/\tau(k) = n_i\, V(k) \int d\Omega\, \frac{d\sigma(k)}{d\Omega}\,(1-\cos\theta)$$

Thus, in this case, the exact solution of the linearized Boltzmann equation leads to a well-defined relaxation time, which is a function of k i.e. of energy. Using the above form for $\left.\frac{\partial f_1}{\partial t}\right|_{scat}$ is known as the <u>relaxation time approximation</u>. In this particular case, this approximation is equivalent to the linearization approximation. However, not all linearized Boltzmann equations can be put in the relaxation time form. Here, we obtain this form because we have put B = 0, and assumed elastic scattering. In more complicated situations, we would not obtain such a simple form. However, when such a description is applicable, we can use it to check the validity of ~~justify, in some sense,~~ the linearization approximation. It is not difficult to see that the linearization approximation will be good if the relaxation time $\tau$ is small. One way of seeing this is to write the equation above as

$$f_1(\vec{k},t) \sim e^{-t/\tau(k)}$$

No external field

$$\frac{\partial f_1}{\partial t} = \left.\frac{\partial f_1}{\partial t}\right|_{scat}$$

i.e. $\tau(k)$ in some sense measures the time.

constant with which any departure from equilibrium due to the scattering decays. Thus, if the time of observation is large compared to $\tau$, and if the external disturbances are small, then the departure from equilibrium will also be small, and the linear order approximation is good. If, on the other hand, $\tau$ is comparable or longer than the time of observation, then any departure from equilibrium will not decay over the time of observation, and $f_1$ can be large even if the external fields are small. The importance of $\tau$ can be seen more clearly if we look at the solution for $\phi$ obtained above.

$$\left(\frac{\partial f_0}{\partial E}\right)^{-1} f_1 = \phi(\vec{k}) = C(k)\,\hat{k}\cdot\vec{\mathcal{E}} \qquad \underline{C(k) = e\,V(k)\,\tau(k)}$$

$$= e\,V(k)\,\tau(k)\,\hat{k}\cdot\vec{\mathcal{E}}$$

Thus, for $\phi(\vec{k})$ to be small, both $\mathcal{E}$ and $\tau(k)$ has to be small.

We note here that the relaxation time $\tau(k)$ that appears here is not the usual relaxation time defined ~~through the total transition probability~~ as the average time between scattering events. This time is given by

~~$\tau_0(k) = \frac{1}{\sum_{k'} W(k,k')} = \frac{1}{V(k)\,\sigma(k)}$~~

$$\frac{1}{\tau_0(k)} = \sum_{k'} W(k,k') = n_i\, V(\vec{k})\,\sigma(k)$$

$$= n_i\, V(k) \int d\Omega\, \frac{d\sigma(k)}{d\Omega}$$

$\tau(k)$ involves an extra factor $(1-\cos\theta)$. This is expected, because small angle scattering ($\theta \simeq 0$) does not impede the flow of electrons and contributes

$$\boxed{-\vec{V}(\vec{k})\cdot e\vec{E}\,\frac{\partial f_0}{\partial E} = -\frac{f_1(\vec{k},r,t)}{\tau(k)}}$$

little to the resistivity. The important scattering events are the large angle one, and in the expression for $\tau(k)$, these events are given larger weight.

We can now calculate the conductivity.

$$f_1(\vec{k}) = \frac{\partial f_0(\vec{k})}{\partial E}\,\phi(\vec{k}) = \frac{\partial f_0(\vec{k})}{\partial E}\,eV(k)\,\tau(k)\,\hat{k}\cdot\vec{\mathcal{E}}$$

$$= \frac{\partial f_0(\vec{k})}{\partial E}\,e\tau(\vec{k})\,\vec{V}(\vec{k})\cdot\vec{\mathcal{E}}$$

$$\vec{j} = -\frac{e}{4\pi^3}\int \vec{V}(\vec{k})\,f(\vec{k})\,d\vec{k}$$

<u>Current density</u>

$E(k) = \frac{\hbar^2k^2}{2m^*}$

$$= -\frac{e^2}{4\pi^3}\int \vec{V}(\vec{k})\cdot\vec{\mathcal{E}}\,\frac{\partial f_0(\vec{k})}{\partial E}\,\vec{V}(k)\,\tau(k)\,d^3k.$$

$\delta(E(k)-E_f)$

$= \delta(k-k_f)\,\frac{m^*}{\hbar^2 k_f}$

At low temperatures, $\frac{\partial f_0(\vec{k})}{\partial E} \simeq -\delta(E(\vec{k})-E_f)$

Take $\vec{\mathcal{E}}$ along the z-axis

$\int \cos^2\theta\,\sin\theta\,d\theta$

$$\Rightarrow \vec{j} = \hat{z}\,\frac{e^2}{4\pi^3}\left(\frac{\hbar}{m^*}\right)^2\mathcal{E}\;2\pi\,\frac{2}{3}\,\frac{m^*}{\hbar^2}\,k_f^3\,\tau(k_f)$$

$$= \vec{\mathcal{E}}\;e^2\,\tau(k_f)\,\frac{k_f^3}{3\pi^2}\,\frac{1}{m^*}$$

Thus, we get $\sigma = ne^2\tau(k_f)/m^*$, which is the usual formula for the conductivity in the scattering time approoximation. We must remember that the $\tau$ here is not the $\tau_0$, the av. time between scattering events. $\tau(k_f)$ can be quite different from $\tau_0(k_f)$. To see this, we use the form for $T(\vec{k},\vec{k}')$ in terms of phase shifts.

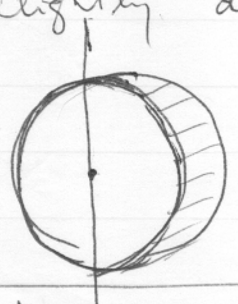
$$\frac{1}{\tau_0(k)} = \frac{4\pi n_i\,\hbar}{k\,m^*}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(k)$$

$$\frac{1}{\tau(k)} = \frac{4\pi n_i\hbar}{k\,m^*}\sum_{\ell=1}^{\infty}\ell\,\sin^2\left[\delta_\ell(k)-\delta_{\ell-1}(k)\right]$$

They are the same if $\delta_\ell(k) \neq 0$ only for $\ell = 0$. If other phase-shifts are present, then they will be different.

Also, note that $\tau(k_f)$ occurs in $\sigma$, although $\sigma$ is proportional to the total # density. This is not surprising, if we look at the physics

When the electric field is applied, all electrons begin to accelerate in the direction of the field. Scattering tends to bring it back to the original position. The elastic scatterings are possible only between the two annular regions which are close to the Fermi surface. Thus, only $\tau(k_f)$ enters. In the steady state, there is a drift velocity in the direction of $\vec{\mathcal{E}}$, so that the whole Fermi sphere is slightly displaced in this direction. The net current



comes from the electrons in the shaded region, whose volume is proportional to the volume of the sphere, i.e. to $n$.

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At finite temperatures, the temperature dependence comes through the term $\frac{\partial f(k)}{\partial E(k)}$, which is rather weakly dependent on T. Thus, the conductivity due to impurity scattering is not very much dependent on temperature. $\tau(k_f)$ is inversely $\propto n_i$. So the resistance $\propto$ concentration of impurities, as long as the concentration is small. This is observed experimentally.

## Phonon Scattering

This is the dominant mechanism for electrical resistance in metals or heavily doped semiconductors. This involves inelastic processes. We'll estimate the scattering term $\left.\frac{\partial f(\vec k)}{\partial t}\right|_{scatt}$ by treating the el-phonon interaction in first order perturbation theory.

$$H_{el-ph} = \frac{1}{\sqrt{N}} \sum_{\vec q, \vec k} D(\vec q)\; c^{\dagger}(\vec k+\vec q)\, c(\vec k)\left[a(\vec q) + a^{\dagger}(-\vec q)\right]$$

~~We have used~~

$$D(\vec q) = i\left[\frac{\hbar}{2\,\omega(q)\,M}\right]^{1/2} q\, C$$

Here, we have used the deformation potential form [$C \to$ constant] and considered only longitudinal acoustic phonons. We have to estimate now the rates of the following transition:

$$\vec k \to \vec k + \vec q \quad \begin{matrix}\text{emission of } (-\vec q)\\ \text{absorption of } (\vec q)\end{matrix} \Rightarrow \text{loss term.}$$

$$\vec k + \vec q \to \vec k \quad \left\{\begin{matrix}\text{emission of } (\vec q)\\ \text{absorption of } (-\vec q)\end{matrix}\right. \Rightarrow \text{gain term.}$$

We'll assume that the phonons are in thermal equilibrium. In principle, we should write down a Boltzmann equation for the phonons, involving a distribution for $n(\vec q, \vec r)$. Here, there is no $\vec r$ dependence. There will be departure from equilibrium due to the so called ~~el~~ "phonon drag", but this is a higher order effect so far as the electronic properties are concerned. [The phonon drag is caused by a strong electron-phonon interaction.

$\Rightarrow n(\vec q, \vec r) = n_0(\vec q)$

In the presence of a uniform electric field, the electrons acquire a net velocity in the direction opposite to that of the field. If the electron-phonon interaction is strong, then this causes an asymmetry in the phonon distribution i.e. $n(\vec{q}) \neq n(-\vec{q})$, whereas in equilibrium, $n(\vec{q}) = n(-\vec{q})$. This asymmetry, in turn, affects $f(\vec{k})$, but this is a higher order effect.] $\Rightarrow n_0(\vec{q}) = \dfrac{1}{e^{\hbar\omega(\vec{q})/k_BT} - 1}$

The first problem is to calculate the collision term $\left.\dfrac{\partial f}{\partial t}\right]_{\text{scat}}$. We need the transition rates $\vec{k} \to \vec{k}+\vec{q}$, and $\vec{k}+\vec{q} \to \vec{k}$. From the form of $H_{el\text{-}ph.}$, it is clear that, to first order in perturbation theory, Fermi's golden rule gives

$\vec{k} \to \vec{k}+\vec{q}$: ~~Em~~ ① Absorption of $\vec{q}$

$$\frac{2\pi}{\hbar}\frac{1}{N}\frac{\hbar}{2\omega(q)M}\, q^2 c^2\, n_0(\vec{q})\; \delta\left[E(\vec{k}+\vec{q}) - E(\vec{k}) - \hbar\omega(q)\right]$$

② Emission of $(-\vec{q})$

$$\frac{2\pi}{\hbar}\frac{1}{N}\frac{\hbar}{2\omega(q)M}\, q^2 c^2 \left[n_0(\vec{q}) + 1\right] \delta\left[E(\vec{k}+\vec{q}) + \hbar\omega(q) - E(\vec{k})\right]$$

$\vec{k}+\vec{q} \to \vec{k}$:

① Emission of $\vec{q}$:

$$\left[\qquad\qquad\right]\left[n_0(\vec{q}) + 1\right] \delta\left[E(\vec{k}+\vec{q}) - E(\vec{k}) - \hbar\omega(q)\right]$$

② Absorption of $-\vec{q}$:

$$\left[\qquad\qquad\right] n_0(\vec{q})\; \delta\left[E(\vec{k}+\vec{q}) + \hbar\omega(q) - E(\vec{k})\right]$$

Also, factor $f(\vec{k})\left[1 - f(\vec{k}+\vec{q})\right]$ with first two terms,
$f(\vec{k}+\vec{q})\left[1 - f(\vec{k})\right]$ second two terms.

$$\Rightarrow \frac{\partial f(\vec{k})}{\partial t}\Big]_{\text{scat.}} = \frac{\pi C^2}{NM}\sum_{q}\frac{q^2}{\omega(q)}\Big\{\Big[-f(\vec{k})\big(1-f(\vec{k}+\vec{q})\big)\,n_0(q)$$

$$+ f(\vec{k}+\vec{q})\big(1-f(\vec{k})\big)\big(n_0(q)+1\big)\Big]\,\delta\big(E(k+q)-\hbar\omega(q)-E(k)\big)$$

$$+\Big[-f(k)\big(1-f(\vec{k}+\vec{q})\big)\big(n_0(q)+1\big)+f(\vec{k}+\vec{q})\big(1-f(\vec{k})\big)$$

$$n_0(\vec{q})\Big]\,\delta\big(E(\vec{k}+\vec{q})+\hbar\,\omega(q)-E(\vec{k})\big)\Big\}$$

Check that detailed balance is satisfied:

$E_1 = E(\vec{k})$, $E_2 = E(\vec{k}+\vec{q}) = E_1 + \hbar\,\omega(q)$

$W(1,2) = \cancel{f(E_2)\,[1-f(E_1)]\,[n_0(q)+1]}$ ~~Constant~~ Constant × $[n_0(q)+1]$

$W(2,1) = \cancel{n_0(q)}$ Constant × $n_0(q)$

$W(1,2)/W(2,1) = e^{\hbar\omega(q)/k_BT} = e^{(E_2-E_1)/k_BT}$

$W(1,2)\,e^{-E_2/k_BT} = W(2,1)\,e^{-E_1/k_BT}$

$\Rightarrow P(1,2) = W(1,2)\,f_0(E_2)\,[1-f_0(E_1)] = W(2,1)\,f_0(E_1)\,[1-f_0(E_2)] = P(2,1)$

Similarly, for the second term. Thus, if we put $f = f_0$, then $\frac{\partial f}{\partial t}\Big]_{\text{scat}} = 0$. As before, we write

$f(\vec{k}) = f_0(k) + f_1(\vec{k})$ $\qquad f_1(k) = \phi(k)\,\frac{\partial f_0(\vec{k})}{\partial E(\vec{k})}$

$$= -\frac{1}{k_BT}\,\phi(\vec{k})\,f_0(\vec{k})\,[1-f_0(\vec{k})]$$

$\Rightarrow$ First term: $\displaystyle\sum_{\vec{q}} P(\vec{k},\vec{k}+\vec{q})\left(-\frac{1}{k_BT}\right)\left[\phi(\vec{k}+\vec{q})-\phi(\vec{k})\right]$

$$\delta\left[E(\vec{k}+\vec{q})-E(k)-\hbar\,\omega(q)\right]$$

$$P(\vec{k},\vec{k}+\vec{q}) = \frac{\pi C^2}{NM}\,\frac{q^2}{\omega(q)}\,[n_0(q)+1]\,f_0(\vec{k}+\vec{q})\big(1-f_0(\vec{k})\big)$$

$$= \frac{\pi C^2}{NM}\,\frac{q^2}{\omega(q)}\,n_0(q)\,f_0(k)\,[1-f_0(\vec{k}+\vec{q})]$$

Second term: $$\sum_{q} P'(\vec{k}, \vec{k}+\vec{q}) \left(-\frac{1}{k_B T}\right) \left[\phi(k+q) - \phi(k)\right] \delta\left(E(\vec{k}+\vec{q}) - E(\vec{k}) + \hbar\omega(q)\right)$$

$$P'(\vec{k}, \vec{k}+\vec{q}) = \frac{\pi C^2}{NM} \frac{q^2}{\omega(q)} f_0(k+q)\left(1 - f_0(k)\right) n_0(q)$$

$$\Rightarrow \quad \left.\frac{\partial f_1}{\partial t}\right|_{scat} = -\frac{\pi C^2}{NMk_BT} \sum_{q} \frac{q^2 n_0(q)}{\omega(q)} \left\{ f_0(\vec{k})\left(1 - f_0(\vec{k}+\vec{q})\right) \times \delta\left(E(\vec{k}+q) - E(\vec{k}) - \hbar\omega(q)\right) + f_0(k+q)\left(1 - f_0(\vec{k})\right) \times \delta\left(E(\vec{k}+\vec{q}) - E(\vec{k}) + \hbar\omega(q)\right) \right\} \left[\phi(\vec{k}+\vec{q}) - \phi(\vec{k})\right]$$

This is the right-hand side of the Boltzmann equation. The left-hand side is simple. We have only an electric field $\Rightarrow$

L.H.S $= -e\vec{v}(\vec{k})\cdot\mathcal{E} \dfrac{\partial f_0(\vec{k})}{\partial E(\vec{k})}$. This results in a rather complicated linear integral equation for $\phi$. [In the general case, no simple analytic solution is possible. We'll see that it reduces to simple forms in two limits. These two limits are

① High temperature. $T \gg \Theta_D$

② Low temperature $T \ll \Theta_D$.

1) $T \gg \Theta_D$!

The energies involved are much higher than typical phonon energies. $\Rightarrow$ Approximate $f_0(\vec{k}+\vec{q})$ by $f_0(k)$. Thus, we effectively have elastic scattering, and we'll see shortly that, in this case, it is possible to obtain a scattering time form for the solution $\phi(k)$.]

~~First, we have to get rid of the δ-functions.~~

~~$E(\vec{k}+\vec{q}) - E(\vec{k}) - \hbar\omega(q) = \dfrac{\hbar^2 q^2}{2m^*} + \dfrac{\hbar^2 \vec{k}\cdot\vec{q}}{m^*} - \hbar\omega(q) = 0$~~

We try a solution of the form

$$\phi(\vec{k}) = C(k)\,\vec{k}\cdot\vec{\mathcal{E}} \longrightarrow C(E)\,\vec{k}\cdot\vec{\mathcal{E}}$$

First term in $\left.\frac{\partial f_1}{\partial t}\right|_{scat}$ :

$$-\frac{\pi e^2}{NMk_BT}\frac{V}{(2\pi)^3}\int \frac{q^2 n_0(q)}{\omega(q)}\, f_0(E(\vec{k}))\left(1-f_0(E(\vec{k}+\vec{q}))\right)$$

$$\delta\left(\frac{\hbar^2 q^2}{2m^*} + \frac{\hbar^2\,\vec{k}\cdot\vec{q}}{m^*} - \hbar\omega(q)\right)\left[C(E(\vec{k}+\vec{q}))\,\vec{\mathcal{E}}\cdot(\vec{k}+\vec{q}) - C(E(\vec{k}))\,\vec{\mathcal{E}}\cdot\vec{k}\right] q^2\sin\theta\, d\theta\, d\phi$$

$\vec{k}\cdot\vec{q} = kq\cos\theta \rightarrow \phi$ $\qquad$ $\vec{k}$ along $z$ axis.

$\vec{k}\cdot\vec{\mathcal{E}} = k\mathcal{E}\cos\theta' \rightarrow \phi'$

$\vec{\mathcal{E}}\cdot\vec{q} = \mathcal{E}q\ \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi')$

↓ 0 when $\phi$ integral is done

$$\Rightarrow 2\pi\left\{C(E(\vec{k}+\vec{q}))\left[\mathcal{E}k\cos\theta' + \mathcal{E}q\cos\theta\cos\theta'\right] - C(E(\vec{k}))\,\mathcal{E}k\cos\theta'\right\}$$

$$= 2\pi\mathcal{E}\cos\theta'\left[C(E(\vec{k}+\vec{q}))\cdot(k+q\cos\theta) - C(E(k))\,k\right]$$

Now do the $\theta$ integration. The $\delta$-fn is satisfied for

$$\cos\theta = \frac{m^*\omega(q)}{\hbar kq} - \frac{q}{2k}.$$

First term : $\dfrac{qV_s}{V(k)\,q} = \dfrac{V_s}{V(k)}$

We are interested in $k \simeq k_f \Rightarrow \dfrac{V_s}{V_f} << 1.$

Second term: Consider monovalent metal

BZ radius $k_0$ given by $\frac{4\pi}{3}k_0^3 = (2\pi)^3\frac{1}{\Omega}.$

whereas $k_f$ is given by $\frac{4\pi}{3}k_f^3 = \frac{(2\pi)^3}{2}\frac{1}{\Omega}$

$\Rightarrow k_f \simeq \dfrac{k_0}{2^{1/3}}$ , $q_{max} \simeq k_0 \Rightarrow \dfrac{q_{max}}{2k_f} \simeq \dfrac{2^{1/3}}{2} < 1$

$$\boxed{\cancel{\Phi(E)}\quad \Phi(\vec{k}) = C(E(\vec{k}))\,\vec{k}\cdot\vec{\mathcal{E}} \qquad f_1(\vec{k}) = \Phi(\vec{k})\cdot\frac{\partial f_0}{\partial E}}$$

Thus, the value of $\cos\theta$ for which the $\delta$-fn is satisfied is between $-1, +1$ for all $\vec{q}, \vec{k}$, & there is no restriction on the magnitude of $q$. Same conclusion is obtd. for the second $\delta$ fn. [$\omega(q) \to -\omega(q)$, but this term is $\ll 1$ anyway]. ~~We~~ [This is not the case in doped semiconductors in which $k_f \ll k_0$, and the $q$ integration is not unrestricted]. Doing the $\theta$ integral gives

$$-\frac{\pi c^2}{NMk_BT}\frac{V}{(2\pi)^3}\cdot 2\pi\,\mathcal{E}\cos\theta' \int \frac{q^2 n_0(q)}{\omega(q)} f_0(E)\left[1-f_0(E+\hbar\omega(q))\right]$$

$$\times \frac{m^*}{\hbar^2 kq}\left[C(E+\hbar\omega(q))\left(k+\frac{m^*\omega(q)}{\hbar k}-\frac{q^2}{2k}\right)-C(E)k\right]$$

$$q^2\,dq$$

$\gamma = \frac{\hbar^2}{2m^*}$

$$\left.\frac{\partial f}{\partial t}\right|_{\text{scat.}} = -\frac{\pi c^2}{Mk_BT}\frac{\Omega}{(2\pi)^2}\mathcal{E}\cos\theta'\frac{m^*}{\hbar^2}\int\frac{q\,n_0(q)}{\omega(q)}\Big\{ f_0(E)\left[1-f_0(E+\hbar\omega(q))\right]$$

$$\times\left[C(E+\hbar\omega(q))\left(1+\frac{\hbar\omega(q)}{2E}-\frac{q^2}{2k^2}\right)-C(E)\right]$$

$$+ f_0(E-\hbar\omega)\left(1-f_0(E)\right)\left[C(E-\hbar\omega)\left(1-\frac{\hbar\omega}{2E}-\frac{q^2}{2k^2}\right) - C(E)\right]\Big\}\,q^2\,dq$$

This is a solution. $\mathcal{E}\cos\theta'$

## High Temperature limit

1) $\boxed{T \gg \Theta_D}$ $\qquad \hbar\omega \ll E$

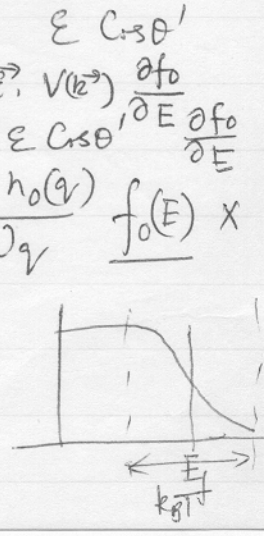
$$\text{L.H.S} = -e\vec{\mathcal{E}}\cdot V(\vec{k})\frac{\partial f_0}{\partial E} = -e\mathcal{E}\frac{\hbar k}{m^*}\mathcal{E}\cos\theta'\frac{\partial f_0}{\partial E}$$

$$\left.\frac{\partial f}{\partial t}\right|_{\text{scat.}} = -\frac{\pi c^2}{Mk_BT}\frac{\Omega}{(2\pi)^2}\mathcal{E}\cos\theta'\frac{m^*}{\hbar^2}\int\frac{q\,n_0(q)}{\omega_q}\underline{f_0(E)}\times$$

$$\underline{\left(1-f_0(E)\right)}\;\underline{C(E)}\left(-\frac{q^2}{2k^2}\right)2\;q^2\,dq$$

$\frac{f_1}{k}$

$$= -e\mathcal{E}\cos\theta'\frac{\hbar k}{m^*}\frac{\partial f_0}{\partial E}$$



But $\frac{\partial f_0}{\partial E} = -\frac{1}{k_BT} f_0(E)\left(1-f_0(E)\right)$

$$\Rightarrow \quad e\,\frac{\hbar k}{m^*} = \frac{\pi C^2}{M}\,\frac{\Omega}{(2\pi)^2}\,\frac{m^*}{\hbar^2}C(E)\int q\,\frac{n_0(q)}{\omega(q)}\,\frac{q^2}{k^2}\,q^2\,dq$$

This ~~q~~ determines $C(E)$. Also, it is obvious that

$$\left.\frac{\partial f_1}{\partial t}\right|_{\text{scat.}} = -\frac{f_1}{\tau(k)}$$

Thus, we can describe the conductivity in term of a scattering time.

$$\frac{1}{\tau(k)} = \frac{\pi C^2}{M}\,\frac{\Omega}{(2\pi)^2}\,\frac{m^*}{\hbar^2}\int \frac{q\,n_0(q)}{\omega(q)}\,\frac{q^2}{k^3}\,q^2\,dq.$$

High Tempr. $n_0(q) = \frac{k_BT}{\hbar v_s q}$ $\qquad \omega(q) = v_s q.$

$$\frac{1}{e^{\hbar\omega/k_BT}-1} \approx \frac{k_BT}{\hbar\omega}$$

$$\int_0^{q_m} \frac{q\,k_BT}{\hbar v_s^2 \cancel{q^2}}\,\frac{\cancel{q^2}}{k^3}\,q^2\,dq = \frac{k_BT}{\hbar v_s^2 k^3}\,\frac{q_m^4}{4}$$

$$\Rightarrow \quad \frac{\pi C^2}{M}\cdot\frac{\overset{3}{\cancel{6\pi^2}}}{q_m^3}\,\frac{1}{\cancel{(2\pi)^2}}\,\frac{m^*}{\hbar^2}\,\frac{k_BT}{\hbar v_s^2 k^3}\,\frac{q_m^4}{\cancel{4}\,8}$$

$$= \frac{m^*}{M}\,\frac{3\pi}{8}\,\frac{C^2 q_m^3}{\hbar k^3}\,k_BT\,\frac{1}{\hbar^2 v_s^2 q_m^2}$$

$$\Rightarrow \quad \frac{1}{\tau(k)} = \frac{m^*}{M}\,\frac{3\pi}{8}\,\frac{C^2 q_m^3}{\hbar k^3}\,\frac{k_BT}{(k_B\Theta_D)^2}$$

$$\hbar q_m v_s = k_B\Theta_D \qquad q_m = \left(\frac{6\pi^2}{\Omega}\right)^{1/3}$$

$$\tau(k_f) = \frac{M}{m^*}\,\frac{4}{3\pi}\,\frac{\hbar\,(k_B\Theta_D)^2}{C^2\,k_BT} \qquad k_f = \frac{q_m}{2^{1/3}}$$

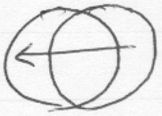
$\sigma = \frac{e^2 n\,\tau(k_f)}{m^*}$ gives $\sigma \propto \frac{1}{T}$

(Need to consider $\tau(k)$ for $k$ near $k_f$ because Fermi surface is smeared) $R \propto T$

at high temperatures. This is what is observed, although the constant of proportionality needs a better

Calculation. which include things like

1) Other phonons & a realistic phonon dispersion
2) Umklapp processes Also, realistic band structure.
3) Phonon drag effects ] etc.



Usually Umklapp.

## Low temperature limit

Here, we cannot neglect $\hbar\omega(\vec{q})$, and the calculation becomes complicated. One simplification is that the Fermi function is very much like a step function. We'll make use of this fact. First, let us write the equation for $\left.\frac{\partial f}{\partial t}\right]_{scat.}$ in a somewhat different form. We'll take out a factor

~~Divide both sides~~ $$-\frac{1}{k_BT} f_0(E)\left(1-f_0(E)\right) = \frac{\partial f_0(E)}{\partial E}$$

$$\Rightarrow \left.\frac{\partial f}{\partial t}\right]_{scat} = \frac{C^2\Omega}{4\pi M}\,\mathcal{E}\cos\theta'\,\frac{m^*}{\hbar^2}\,\frac{\partial f_0(E)}{\partial E}$$

$$\times \int \frac{q\, n_0(q)}{\omega(q)} \left\{ \frac{1-f_0(E+\hbar\omega)}{1-f_0(E)} \left[ C(E+\hbar\omega)\left(1+\frac{\hbar\omega}{2E}-\frac{q^2}{2k^2}\right) - C(E)\right] + \frac{f_0(E-\hbar\omega)}{f_0(E)}\left[ C(E-\hbar\omega)\left(1-\frac{\hbar\omega}{2E}-\frac{q^2}{2k^2}\right) - C(E)\right]\right\} q^2\,dq$$

$$1-f_0(E+\hbar\omega) = e^{(E+\hbar\omega-\mu)/k_BT} f_0(E+\hbar\omega)$$

$$= e^{\hbar\omega/k_BT}\,\frac{1-f_0(E)}{f_0(E)}\,f_0(E+\hbar\omega)$$

$$\Rightarrow \frac{1-f_0(E+\hbar\omega)}{1-f_0(E)} = e^{\hbar\omega/k_BT}\,\frac{f_0(E+\hbar\omega)}{f_0(E)}$$

Now, we'll combine these two terms by assuming that $\omega(q) = v_s q$ for all $q$. Then

$$\text{First term} = (\quad)\frac{\partial f_0}{\partial E}\int_0^{q_m} dq\, \frac{q^3}{v_s q}\, \frac{f_0(E+\hbar v_s q)}{f_0(E)}$$

$$\times \left[ C(E+\hbar v_s q)\left(1+\frac{\hbar v_s q}{2E}-\frac{q^2}{2k^2}\right) - C(E)\right] \frac{e^{\hbar v_s q/k_BT}}{e^{\hbar v_s q/k_BT}-1}$$

$$\downarrow$$

$$\frac{1}{1-e^{-\hbar v_s q/k_BT}}$$

Now, change variable from $q \to -q$ in the second term.

$$\Rightarrow \text{Second term} \quad (\quad) \int_{-q_m}^{0} dq\, \frac{q^3}{v_s q}\, \frac{f_0(E+\hbar v_s q)}{f_0(E)} \Big[ C(E+\hbar v_s q)$$

$$\times \left[1+\frac{\hbar v_s q}{2E}-\frac{q^2}{2k^2}\right] - C(E) \Big] \frac{1}{e^{-\hbar v_s q/k_BT}-1}$$

$$\downarrow$$

The integral is identical to that of the first term. Combine them to write

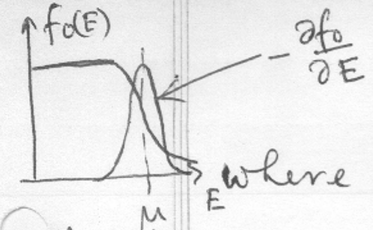
$$\left] \frac{1}{\left|1-e^{-\hbar v_s q/k_BT}\right|}\right.$$

$$\left.\frac{\partial f}{\partial t}\right]_{\text{scat.}} = \left(\frac{C^2\Omega}{4\pi M}\, \varepsilon \cos\theta'\, \frac{m^*}{\hbar^2}\right)\frac{\partial f_0(E)}{\partial E}$$

$$\times \int_{-q_m}^{q_m} dq\, \frac{q^2}{v_s} \left\{ \left(1+\frac{\hbar v_s q}{2E}-\frac{q^2}{2k^2}\right) C(\xi+x) - C(\xi) \right\}$$

$$\frac{f_0(\xi+x)}{f_0(\xi)} \quad \frac{1}{\left|1-e^{-x}\right|}$$

T28



width ~ $k_B T$

where $\xi = (E-\mu)/k_B T$, $x = \frac{\hbar v_s q}{k_B T}$

In $\xi$, width ~ $O(1)$

Also, note that $\frac{f_0(\xi+x)}{f_0(\xi)} = \frac{1+e^{\xi}}{1+e^{\xi+x}}$

This has to be equated to $-e\mathcal{E}\frac{\hbar k}{m^*}\cos\theta'\frac{\partial f_0}{\partial E}$

Now, we use the fact that the Fermi surface is sharp. Thus, we are interested in values of $C(\xi)$ near $\xi = 0$. We assume that near $\xi=0$, $C(\xi)$ does not vary rapidly with $\xi$ i.e. $C(\xi) = C(0)$. Note that the factor $\frac{\partial f_0(E)}{\partial E}$ restricts us close to the fermi surface, so that $\xi$ does not change very much from zero. Also, the $q$ integral involves values of $C$ over a range $\hbar v_s q$ near the Fermi surface. $\hbar v_s q_m = k_B \Theta_D \ll \mu$. Thus all we are assuming is that $C(E) = C(\mu)$ for $E$ close to $\mu$. It is possible to expand $C(E)$ about $E=\mu$ & determine the correction term.

$f_1$ varies rapidly with $E$ This comes from $f_1 \sim \frac{\partial f_0}{\partial E}$

$$\Rightarrow \left.\frac{\partial f}{\partial t}\right]_{scat} = \left(\frac{C^2\Omega}{4\pi M}\cancel{\mathcal{E}\cos\theta'}\frac{m^*}{\hbar^2}\right)\frac{\partial f_0(E)}{\partial E}C(0)$$

$$\times \int_{-q_m}^{q_m} dq\,\frac{q^2}{v_s}\left(\frac{\hbar v_s q}{2E} - \frac{q^2}{2k^2}\right)\frac{1+e^{\xi}}{1+e^{\xi+x}}\frac{1}{|1-e^{-x}|}$$

$$= -e\cancel{\mathcal{E}}\frac{\hbar k}{m^*}\cancel{\cos\theta'}\frac{\partial f_0}{\partial E}$$

Now, we integrate both sides w.r.t. $E$. On the R.H.S, we use $\frac{\partial f_0}{\partial E} = -\delta(E-\mu)$, which gives

$e\frac{\hbar k_f}{m^*}$

* Vary rapidly with $\xi$.

On the left hand side, we can not do this, because we are interested in the temperature dependence of $C(0)$, ~~Obviously, $C(0)$ is zero at exactly $T=0$.~~ which comes from the finite temperature smearing of the Fermi surface. Instead, we change the integration variable from $E$ to $\xi$.

$$\Rightarrow \left(\frac{c^2\Omega}{4\pi M}\,\frac{m^*}{\hbar^2}\right)C(0)\int \cancel{k_BT}\,d\xi\left(-\frac{1}{\cancel{k_BT}}\right)\frac{e^{\xi}}{(1+e^{\xi})^2}{}^{*}\int_{-q_m}^{q_m}dq\,\frac{q^2}{v_s}$$

$$\frac{\partial f_0(E)}{\partial E} = -\frac{1}{k_BT}\frac{e^{\xi}}{(1+e^{\xi})^2}$$

$$\times\left(\frac{\hbar v_s q}{2\mu}-\frac{q^2}{2k_f^2}\right)\frac{1+e^{\xi}}{1+e^{\xi+x}}{}^{*}\,\frac{1}{|1-e^{-x}|}$$

↑ We have replaced $E$ by $\mu$, $k$ by $k_f$ because the $\xi$ integrand is sharply peaked at $\xi=0$ i.e. at $E=\mu$.

So, finally, we have

$$e\frac{\hbar k_f}{m^*} = -\left(\frac{c^2\Omega}{4\pi M}\,\frac{m^*}{\hbar^2}\right)C(0)\int_{-q_m}^{q_m}dq\,\frac{q^2}{v_s}\left[\frac{\hbar v_s q}{2\mu}-\frac{q^2}{2k_f^2}\right)\frac{1}{|1-e^{-x}|}\underbrace{\int_{-\infty}^{\infty}d\xi\,\frac{1}{1+e^{\xi+x}}\,\frac{1}{1+e^{-\xi}}}_{\downarrow\; x/(e^x-1)}$$

Do $q$ integral $\Longrightarrow$ This determines $C(0)$

Then use
$$f_1(\vec{k}) = \frac{\partial f_0}{\partial E}\,\phi(\vec{k}) = C(0)\,\vec{\mathcal{E}}\cdot\vec{k}\,\frac{\partial f_0}{\partial E}$$

$$\vec{J} = -\frac{e}{4\pi^3}\int \vec{V}(\vec{k})\,f_1(\vec{k})\,d\vec{k}$$ to get $\sigma$

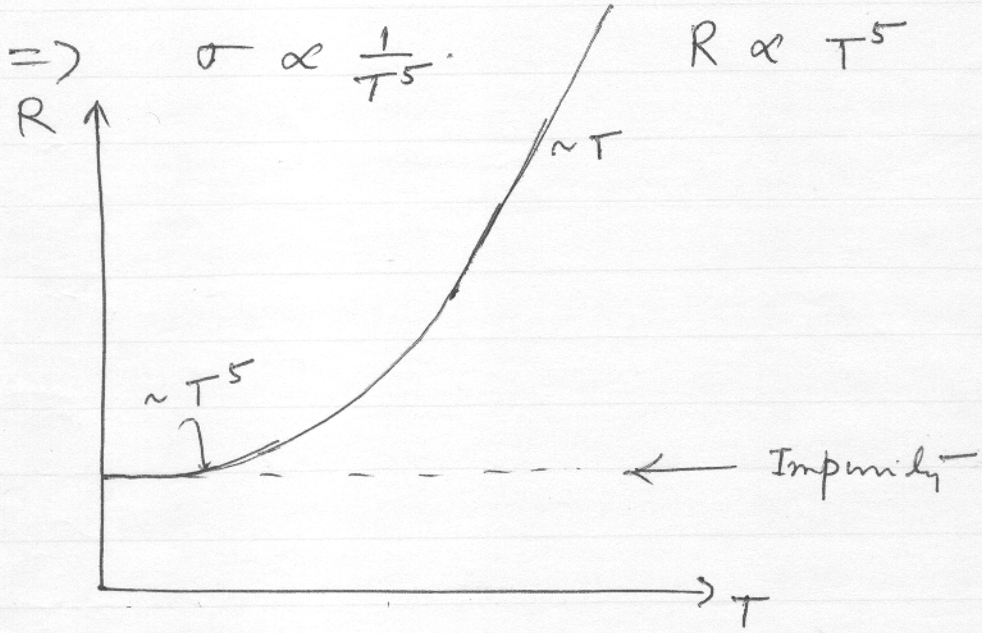
## Final result is

$$\sigma = \frac{2}{3\pi} \frac{M n e^2}{m^{*2}} \frac{\hbar k_f^3}{C^2 q_m^3} k_B \Theta_D \left(\Theta_D/T\right)^5 \frac{1}{J_5(\Theta_D/T)}$$

$$J_n(x) = \int_0^x y^n \Big/ \left[(e^y-1)(1-e^{-y})\right] dy$$

$\Theta_D >> T$ : $x \to \infty$ $J_5(\Theta_D/T) \longrightarrow 5!\,\zeta(5)$

$\Rightarrow$ $\sigma \propto \frac{1}{T^5}$. $R \propto T^5$



$$\int q^2 dq\, \delta\left(\frac{\hbar^2 |\vec{k}+\vec{q}|^2}{2m^*} - \frac{\hbar^2 k^2}{2m^*} - \hbar v_s q\right) \frac{q^2}{k^2} n_0(q)$$

$\sin\theta\, d\theta\, d\phi$