Boltzmann Equation

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I. Boltzmann Equantion

Boltzmann equation is used to describe the statistical behavior of the thermodynamic systems that are out of thermodynamic equilibrium.
The distribution function for electrons in an equilibrium system is Fermi-Dirac distribution $f_{n,\vec{k}}(\vec{r},t) = 1/(exp(\epsilon_{n,\vec{k}} - \mu)/k_B T) + 1)$. But when the system is out of equilibrium, the distribution function become time dependent,therefore we introduce the Boltzmann equation.

Boltzmann Equation:

$$\frac{\partial f}{\partial t} + \dot{\vec{r}}\frac{\partial f}{\partial \vec{r}} + \dot{\vec{k}}\frac{\partial f}{\partial \vec{k}} = (\frac{\partial f}{\partial t})_{coll}$$

The second term at the left of the equation corresponds to the flow of particles, the third term corresponds to the external field and the term at the right side stands for the collision effect,which depends on all sorts of disorders parameters of the metal.

II. Collision Term

As a simple but instructive case, we only consider the collisions between the electrons and the disorders.
The generalized collision term of the disorders goes as follow:

$$\frac{\partial f_k}{\partial t}|_{coll} = -\int \frac{d^3k'}{(2\pi)^3}[W_{kk'}f_k(1-f_{k'}) - W_{k'k}f_{k'}(1-f_k)]$$

Here $W_{kk'}$ is the transition rates and f_k is the distribution function for electrons with momentum $\vec{k}$.

II.1 Determination fo transition rates $W_{kk'}$

The form of $W_{kk'}$ depends largely on what problems we are dealing with. Now considering a system with weak perturbation: $H = H_0 + \Delta H$. We have:

$$W_{kk'} = \frac{2\pi}{\hbar}|< k'|\Delta H|k >|^2\delta(\epsilon_k - \epsilon_{k'})$$

Since while interchanging the k and k' $W_{kk'}$ would not change: $W_{kk'} = W_{k'k}$, with this result we can simplify the collision term:

$$\frac{\partial f_k}{\partial t}|_{coll} = -\int W_{kk'}(f_k - f_{k'})\frac{d^3k'}{(2\pi)^3}$$

II.2 Approximation of the distribution function

II.2.1 Linear Response

In a weak electric field $\vec{E}$, it is alright for us to linearize the distorted FD distribution as the following:

$$f_k \approx f_k^0 + \delta f_k \qquad f_k^0 >> \delta f_k$$

this is the so-call 'linear response', and f_k^0 is the FD distribution in equilibrium system. And now we can see the collision term becomes:

$$(\frac{\partial f}{\partial t})_{coll} = -\int W_{kk'}(\delta f_k - \delta f k')\frac{d^3k'}{(2\pi)^3}$$

II.2.2 Relaxation time approximation

However even after the above approximation, the equation is still a integral function and it is hard to get an analytic solution. Therefore we have to do another approximation:

$$-\int W_{kk'}(\delta f_k - \delta f_{k'})\frac{d^3k'}{(2\pi)^3} = -\frac{\delta f_k}{\tau_k}$$

This is called relaxation time approximation, and τ_k is called the relaxation time, which is a parameter used to describe the time scale for a non equilibrium system to recover its equilibrium.
With this approximation,we get the linearized B.E.:

$$\frac{\partial \delta f_k}{\partial t} - \frac{e\vec{E}}{\hbar}\vec{v}_k\frac{\partial f_k^0}{\partial \epsilon_{\vec{k}}} = -\frac{\delta f_k}{\tau_k}$$

III. Application

For the AC electric field case $\vec{E} = \vec{E}_0 cos\omega t$, we do a Fourier transformation $\delta f_k(\omega) = \int \delta f_k(t)e^{i\omega t}dt$, insert it into the linearized B.E. , then we get the deviation part of the distribution:

$$\delta f_k(\omega) = e(\vec{E}\vec{v}_k\frac{\partial f^0}{\epsilon_k})/(\frac{1}{\tau_k} - i\omega)$$

Since the current density is:

$$j^i = -2\int \frac{d^3k}{(2\pi)^3}ev_k^i f_k = -2\int \frac{d^3k}{(2\pi)^3}ev_k^i \delta f_k$$

(f_0 has no contribution), combine it with the definition of the conductivity:$j^i(\omega) = \sigma^{ij}(\omega)E^j(\omega)$, we have the formula for AC conductivity:

$$\sigma^{ij}(\omega) = -2\int \frac{d^3k}{(2\pi)^3}\frac{e\vec{v}_k^i\vec{v}_k^j\frac{\partial f^0}{\epsilon_k}\tau_k}{1 - i\omega\tau_k}$$

in order to get an analytic solution, we consider an isotropic system, in which the scattering only depends on the angle between $\vec{k}$ and $\vec{k'}$: the 'transport' relaxation rate is:

$$\frac{1}{\tau_k} = \int W_{kk'}(1 - cos\theta_{kk'})\frac{d^3k'}{(2\pi)^3}$$

This is the relaxation time for the case,which can tell us the conductivity of the metal under those conditions.

References

[1] Prof. Dr. A. Rosch 's scripts about Boltzmann equation

[2] Wikipedia, article of "Boltzmann Equation".