Karlsruher Institut für Technologie | Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie I WS 2018/19

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1. Dielektrische Funktion des nicht-wechselwirkenden Elektronengases:

Consider a total potential which includes both the external potential and the induced (screening) potential. Assume that the potential has a form of the plane wave

$$V_t e^{i(\boldsymbol{q}\boldsymbol{r}-\omega t)}.$$

Then the distribution function can be written down as the sum of the equilibrium distribution and a perturbation

$$f(\boldsymbol{p}) = f_0(\boldsymbol{p}) + f_1(\boldsymbol{p}) e^{i(\boldsymbol{q}\boldsymbol{r}-\omega t)}.$$

Substituting this expression into the Boltzmann equation in the τ-approximation we find an equation for $f_1(\mathbf{p})$:

$$-i\omega f_1 + \frac{\partial f_0}{\partial \epsilon}\boldsymbol{v}(-i\boldsymbol{q}V_t) + i\boldsymbol{q}\boldsymbol{v} f_1 = -\frac{f_1}{\tau} + \frac{\delta_n f_0}{\tau}.$$

Notice, that the right-hand side contains two terms. The first term is the usual deviation of the distribution function f_1. The second term is less standard - this is the variation of the equilibrium distribution due to the variation of particle density. Indeed, nonuniform electric fields cause fluctuations of the particle density. As a result, the chemical potential changes as well. Expanding the distribution function to the linear order in the variation of the chemical potential we find

$$\frac{\partial f_0}{\partial \mu}\delta\mu = -\frac{\partial f_0}{\partial \epsilon}\frac{\partial \mu}{\partial n}\delta n = -\frac{1}{\nu}\frac{\partial f_0}{\partial \epsilon}\delta n(\mathbf{r}) = \delta_n f_0,$$

where $\nu = \partial n/\partial \mu$ is the density of states at the Fermi level and $\delta n(\boldsymbol{r})$ is the variation of local particle density

$$\delta n(\boldsymbol{r}) = n_s e^{i(\boldsymbol{q}\boldsymbol{r}-\omega t)}.$$

Essentially, n_s is the density of the screening charge.

Now we use the Boltzmann equation to find the deviation of the distribution function f_1:

$$f_1 = \frac{i\boldsymbol{q}\boldsymbol{v}V_t\tau(\partial f_0/\partial \epsilon) + \delta_n f_0}{1 - i\omega\tau + i\boldsymbol{q}\boldsymbol{v}\tau}.$$

Now, the deviation of the distribution function results in the density variation

$$n_s = 2\int \frac{d^3p}{(2\pi)^3} f_1(\boldsymbol{p}).$$

Let us first average f_1 over the angle $\boldsymbol{qv} = qv\cos\theta$. As a result we find

$$\begin{aligned} \bar{f}_1(p) &= \frac{\delta_n f_0}{2iqv\tau} \ln \frac{1 - i\omega\tau + iqv\tau}{1 - i\omega\tau - iqv\tau} \\ &- V_t \frac{\partial f_0}{d\epsilon} \left[1 - \frac{1 - i\omega\tau}{2iqv\tau} \ln \frac{1 - i\omega\tau + iqv\tau}{1 - i\omega\tau - iqv\tau} \right]. \end{aligned}$$

Using the Fermi distribution as f_0 and recalling the density of states

$$\nu = \frac{p^2}{\pi^2 v},$$

we now find the equation for n_s, where we use the expression for $\delta_n f_0$ in the obtained solution $\bar{f}_1(p)$:

$$\begin{aligned} n_s &= \frac{n_s}{2iqv\tau} \ln \frac{1 - i\omega\tau + iqv\tau}{1 - i\omega\tau - iqv\tau} \\ &- \nu V_t \left[1 - \frac{1 - i\omega\tau}{2iqv\tau} \ln \frac{1 - i\omega\tau + iqv\tau}{1 - i\omega\tau - iqv\tau} \right]. \end{aligned}$$

This can be easily solved to obtain n_s

The screening charge n_s is proportional to the total potential V_t

$$n_s = X(q,\omega)V_t,$$

where the coefficient defines the dielectric response function

$$\epsilon(q,\omega) = 1 - \frac{4\pi e^2}{q^2} X(q,\omega).$$

Using the obtained solution for the screening charge we can now find the dielectric response function of the semi-classical non-interacting electron gas

$$\epsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2} \nu \frac{1 - \frac{1-i\omega\tau}{2iqv\tau} \ln \frac{1-i\omega\tau+iqv\tau}{1-i\omega\tau-iqv\tau}}{1 - \frac{1}{2iqv\tau} \ln \frac{1-i\omega\tau+iqv\tau}{1-i\omega\tau-iqv\tau}}.$$

2. Das thermoelektrische Effekt:

(a) Assuming a small temperature gradient

$$T = T_1 + (\boldsymbol{r}_1 - \boldsymbol{r}_2)\boldsymbol{\nabla} T,$$

one should note that the chemical potential also becomes position-dependent since μ depends on T. Thus the “initial” distribution function can be written as

$$f_0(\epsilon, \boldsymbol{r}) = \frac{1}{1 + \exp\left[\frac{\epsilon - \mu(\boldsymbol{r})}{T(\boldsymbol{r})}\right]}.$$

This is valid while the gradient is not too large, so that

$$\frac{T}{|\boldsymbol{\nabla} T|} \gg l \ldots,$$

where l represents the relaxation length in the system.
The left-hand side of the Boltzmann equation contains the following gradient

$$\boldsymbol{\nabla}_{\boldsymbol{r}} f_0(\epsilon, \boldsymbol{r}) = -\frac{\partial f_0}{\partial \epsilon}\left[\boldsymbol{\nabla}\mu(\mathbf{r}) + \frac{\epsilon-\mu}{T}\boldsymbol{\nabla} T\right].$$

To obtain the result one needs to notice the following

$$\boldsymbol{\nabla}_{\boldsymbol{r}} f_0(\epsilon, \boldsymbol{r}) = \frac{\partial f_0}{\partial \mu}\boldsymbol{\nabla}\mu(\boldsymbol{r}) + \frac{\partial f_0}{\partial T}\boldsymbol{\nabla} T,$$

and

$$\frac{\partial f_0}{\partial \mu} = -\frac{\partial f_0}{\partial \epsilon},$$

$$\frac{\partial f_0}{\partial T} = -\frac{\partial f_0}{\partial \epsilon}\frac{\epsilon-\mu}{T}.$$

Assuming that the gradient of the chemical potential is already taken into account by forming the electro-chemical potential, consider the responce of the system to the temperature gradient alone. The corresponding Boltzmann equation is

$$-\frac{\partial f_0}{\partial \epsilon}\frac{\epsilon-\mu}{T}\left(\boldsymbol{v}\boldsymbol{\nabla} T\right) = -\frac{f-f_0}{\tau_{tr}}.$$

The solution to this equation is then

$$\delta f = \tau_{tr}\frac{\epsilon-\mu}{T}\left(\boldsymbol{v}\boldsymbol{\nabla} T\right)\frac{\partial f_0}{\partial \epsilon}.$$

The electric current can be evaluated as always from the equation

$$\boldsymbol{j} = e\int (d\boldsymbol{p})\boldsymbol{v}\delta f.$$

Substituting the above solution δf one finds for the case of the isotropic spectrum

$$\boldsymbol{j} = \eta \boldsymbol{\nabla} T,$$

where

$$\eta = \frac{e}{T}\int d\epsilon \Big[\nu D\Big](\epsilon-\mu)\left(-\frac{\partial f_0}{\partial \epsilon}\right).$$

Here

$$D = \frac{1}{3}v_F^2\tau_{tr}.$$

is the diffusion coefficient.

Recall from the lecture that for the calculation of the Drude conductivity it was sufficient to use the approximation

$$-\frac{\partial f_0}{\partial \epsilon} \approx \delta(\epsilon-\mu).$$

Here however this is not sufficient since in this approximation the result would be strictly zero. Moreover, taking into account the derivative of the δ-function as it was done during the calculation of the thermal conductivity will not change this result.

What is the physics behind the effect? So far we have always neglected the energy dependence of the density of states (and/or the diffusion coefficient). In reality this is not so. The thermo-electric effect is an important example where one has to keep track of this dependence, i.e. one has to expand in the vicinity of the Fermi level

$$\nu D \approx \left[\nu D\right]\Big|_{E_F} + (\epsilon - \mu)\left[\nu D\right]'\Big|_{E_F}.$$

Substituting this expression into η and in addition taking into account that $\partial f_0/\partial\epsilon$ is not a δ-function

$$-\frac{\partial f_0}{\partial \epsilon} = \frac{1}{4T\cosh^2\frac{\epsilon-\mu}{2T}}$$

one finds

$$\eta = e\int d\epsilon \frac{(\epsilon-\mu)^2}{4T^2}\frac{1}{\cosh^2\frac{\epsilon-\mu}{2T}}\left[\nu D\right]'\Big|_{E_F} = \frac{\pi^2}{3}eT\left[\nu D\right]'\Big|_{E_F}.$$

The derivative appearing in the expression for η is the measure of the electron-hole asymmetry in the system. Indeed, particles react to the temperature gradient independently of their charge. Both electrons and holes move from hot to cold. But since their charges are opposite there has to be an asymmetry between them - i.e. different number of electrons and holes - for this flow to result in non-zero current.

(b) Consider now the contribution of the electric field to the Boltzmann equation. In the left-hand side we have the term

$$e\boldsymbol{E}\cdot\boldsymbol{\nabla}_{\boldsymbol{p}} f_0 = e\boldsymbol{E}\cdot\boldsymbol{\nabla}_{\boldsymbol{p}}\epsilon_{\boldsymbol{p}}\frac{\partial f_0}{\partial\epsilon} = e\boldsymbol{E}\cdot\boldsymbol{v}\frac{\partial f_0}{\partial\epsilon}.$$

Adding this term to the above kinetic equation we find

$$-\frac{\partial f_0}{\partial\epsilon}\frac{\epsilon-\mu}{T}(\mathbf{v}\nabla T) + e\boldsymbol{E}\cdot\boldsymbol{v}\frac{\partial f_0}{\partial\epsilon} = -\frac{f-f_0}{\tau_{tr}}.$$

The solution to this equation is

$$\delta f = \tau_{tr}\left[\frac{\epsilon-\mu}{T}(\mathbf{v}\nabla T) - e\boldsymbol{E}\cdot\boldsymbol{v}\right]\frac{\partial f_0}{\partial\epsilon}.$$

Now we will evaluate the current. The first term we have already integrated above, the second term yields

$$\int (d\boldsymbol{p})\boldsymbol{v}(\boldsymbol{E}\cdot\boldsymbol{v})\left(-\frac{\partial f_0}{\partial\epsilon}\right) = \frac{1}{2}v_F^2\boldsymbol{E}\nu(E_F),$$

which translates into the standard Drude formula

$$\boldsymbol{j} = \sigma_D\boldsymbol{E}.$$

In an open circuit, the current is zero which is achieved by the balance between the two above contributions. This means, that applying the thermal gradient we induce the electrical field

$$\boldsymbol{E} = \frac{\eta}{\sigma_D} \boldsymbol{\nabla} T,$$

where the above calculation yields the values of η and σ_D for the 3D electron gas with parabolic dispersion.