

EXERCISE / HOMEWORK SET 02
 ÚFV/TRANS/18 - Transport Properties of Solids
 lecture by Martin Gmitra
 Summer Semester 2022/2023

Exercise:

1. Derive stationary non-equilibrium distribution function in the presence of electrical field and temperature gradient [follow book by G. Grosso, G. P. Parravicini p. 509, Eq. (11.47)].
2. Use Sommerfeld expansion $\int \left(-\frac{\partial f^0}{\partial \varepsilon} \right) G(\varepsilon) d\varepsilon \simeq G(\mu) + \frac{\pi^2}{6} (k_B T)^2 \left(\frac{d^2 G}{d\varepsilon^2} \right)_{\varepsilon=\mu}$ written for any function $G(\varepsilon)$ to find expressions for the kinetic transport coefficients $K_n = e^{2-n} \int \left(-\frac{\partial f^0}{\partial \varepsilon} \right) (\varepsilon - \mu)^n \Sigma(\varepsilon) d\varepsilon$, $n = 0, 1, 2$, in leading terms of the generalized transport distribution function $\Sigma(\varepsilon)$ setting for $G(\varepsilon) = (\varepsilon - \mu)^n \Sigma(\varepsilon)$, where $\Sigma(\varepsilon)$ is defined as follows $\Sigma(\varepsilon) = \frac{1}{4\pi^3} \int \tau_{\mathbf{k}} (\mathbf{v}_{\mathbf{k}} \circ \mathbf{v}_{\mathbf{k}}) \delta[\varepsilon(\mathbf{k}) - \varepsilon] d\mathbf{k}$.

Homework:

1. [1 point] Show that the particle-current density for free-electrons is equal $\mathbf{j} = \frac{\hbar}{i} \frac{1}{2m_e} (\psi^* \nabla \psi - \psi \nabla \psi^*) = \frac{1}{V} \frac{\hbar \mathbf{k}}{m_e}$. Perform units analysis.
2. [1 point] Prove that in equilibrium the electric current vanishes $\mathbf{j}_e = -\frac{e}{4\pi^3} \sum_n \int_{1^{\text{st}} \text{BZ}} d^3 \mathbf{k} v_{n,\mathbf{k}} f^0(\varepsilon_{n,\mathbf{k}}) = 0$, using the periodicity of the energy spectrum in the reciprocal space, $\varepsilon_{n,\mathbf{k}+\mathbf{G}} = \varepsilon_{n,\mathbf{k}}$. From this also follows that a full band contributes no electric current (discuss how).
3. [1 point] Using expression for the conductivity tensor $\sigma_{\alpha,\beta} = \frac{e^2}{4\pi^3} \int d^3 \mathbf{k} v_{\mathbf{k},\alpha} v_{\mathbf{k},\beta} \tau(\varepsilon_{\mathbf{k}}) \left(-\frac{\partial f^0(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}} \right)$, derive Einstein's relation $\sigma_{\alpha,\beta} = e^2 g D_{\alpha,\beta}$, where g is the density of states and D is the diffusivity. Find expression for the $D_{\alpha,\beta}$.
4. [1 point] Find the vector \mathbf{a} satisfying the vector equation $e\mathbf{E} \cdot \mathbf{v} = -(1/\tau) \mathbf{v} \cdot \mathbf{a} + (e/m) \mathbf{v} \cdot (\mathbf{B} \times \mathbf{a})$. This vector is used to obtain conductivity tensor in the presence of magnetic field \mathbf{B} . (The result was used during lecture.)
5. [1 point] Find corresponding conductivity tensor for the case of the magnetic field along the z axis, $\mathbf{B} = (0, 0, B)$, knowing the resistivity tensor of an isotropic system $\rho(B) = \begin{pmatrix} \rho & -R_H B & 0 \\ R_H B & \rho & 0 \\ 0 & 0 & \rho \end{pmatrix}$.
6. [1 point] Find the expressions for the charge current $\mathbf{j}_e = K_0(\mathbf{E} + (1/e)\nabla\mu) + K_1(1/T)\nabla T$ and the heat current $\mathbf{j}_Q = -K_1(\mathbf{E} + (1/e)\nabla\mu) - K_2(1/T)\nabla T$ using definition of kinetic coefficients substituting the non-equilibrium distribution derived in exercise 1 to the general formulas for the currents.

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7. [4 points] Consider a conductor at a constant temperature in the presence of an electric field $E = -\nabla\phi$. Suppose that due to spin injection the chemical potentials of the spin up and spin down (with a predefined spin quantization axis) electrons are in general different and spatially dependent $\mu_{\uparrow} = \mu_{\uparrow}(\mathbf{r})$, $\mu_{\downarrow} = \mu_{\downarrow}(\mathbf{r})$. The local equilibrium distribution for spin up and spin down electrons is assumed in the form $f_{\ell,\lambda}^0(\varepsilon_k, \mathbf{r}) = [e^{(\varepsilon_k - e\phi(\mathbf{r}) - \mu_{\lambda}(\mathbf{r}))/k_B T} + 1]^{-1}$, where $\lambda = \uparrow, \downarrow$. Show that the steady-state distribution is

$$f_{k,\lambda} \approx f_{\ell,\lambda}^0(\varepsilon_k, \mathbf{r}) + \left(-\frac{\partial f_{\ell,\lambda}^0(\varepsilon_k)}{\partial \varepsilon_k} \right) \tau_k \mathbf{v}_k \cdot (-\nabla \mu_{\lambda})$$

Show also that the charge current $\mathbf{j}_e = \mathbf{j}_{e,\uparrow} + \mathbf{j}_{e,\downarrow}$, and the spin current $\mathbf{j}_s = \mathbf{j}_{e,\uparrow} - \mathbf{j}_{e,\downarrow}$ are given by $\mathbf{j}_e = \sigma(1/e)\nabla\mu$ and $\mathbf{j}_s = \sigma(1/e)\nabla\mu_s$, where the chemical potential $\mu = (\mu_{\uparrow} + \mu_{\downarrow})/2$ and the spin chemical potential (called *spin accumulation*) $\mu_s = (\mu_{\uparrow} - \mu_{\downarrow})/2$.