EXERCISE / HOMEWORK SET 02

ÚFV/TRANS/18 - Transport Properties of Solids
lecture by Martin Gmitra
Summer Semester 2020/2021

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 $\int\left(-\frac{\partial f^0}{\partial \varepsilon}\right) G(\varepsilon)\mathrm{d}\varepsilon \simeq G(\mu) + \frac{\pi^2}{6}(k_B T)^2\left(\frac{\mathrm{d}^2 G}{\mathrm{d}\varepsilon^2}\right)_{\varepsilon=\mu}$ written for any function $G(\varepsilon)$ to find expressions for the kinetic transport coefficients $K_n = e^{2-n}\int\left(-\frac{\partial f^0}{\partial \varepsilon}\right)(\varepsilon-\mu)^n \Sigma(\varepsilon)\mathrm{d}\varepsilon$, $n = 0, 1, 2$, 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 $\Sigma(\varepsilon) = \frac{1}{4\pi^3}\int \tau_{\mathbf{k}}(\mathbf{v}_{\mathbf{k}} \circ \mathbf{v}_{\mathbf{k}})\delta[\varepsilon(\mathbf{k}) - \varepsilon]\mathrm{d}\mathbf{k}$.

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 $\mathbf{j}_e = -\frac{e}{4\pi^3}\sum_n\int_{1^{\mathrm{st}}\mathrm{BZ}} \mathrm{d}^3\mathbf{k}\, v_{n,\mathbf{k}}\, f^0(\varepsilon_{n,\mathbf{k}}) = 0$, 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 $\sigma_{\alpha,\beta} = \frac{e^2}{4\pi^3}\int \mathrm{d}^3\mathbf{k}\, v_{\mathbf{k},\alpha}\, v_{\mathbf{k},\beta}\, \tau(\varepsilon_{\mathbf{k}})\left(-\frac{\partial f^0(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}}\right)$, 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 $\mathbf{B}$.
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 $f^0_{\ell,\lambda}(\varepsilon_k, \mathbf{r}) = [\mathrm{e}^{(\varepsilon_k - e\phi(\mathbf{r}) - \mu_\lambda(\mathbf{r}))/k_B T} + 1]^{-1}$, where $\lambda = \uparrow, \downarrow$. Show that the steady-state distribution is
$f_{k,\lambda} \approx f^0_{\ell,\lambda}(\varepsilon_k, \mathbf{r}) + \left(-\dfrac{\partial f^0(\varepsilon_k)}{\partial \varepsilon_k}\right) \tau_k \mathbf{v}_k \cdot (-\nabla \mu_\lambda)$
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*) $\mu_s = (\mu_\uparrow - \mu_\downarrow)/2$.