Problem set 2

Phy-801

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1. **Drude dynamics and the single relaxation time approximation:** In class we used a simple model in which each collision resets an electron's momentum to $\boldsymbol{p} = 0$. In this problem you will analyse this model and several generalisations, and determine when they yield the same Drude dynamics.

   (a) Consider electrons in an electric field, with collisions occurring as a Poisson process with mean interval length τ, and each collision resetting the momentum to zero, $\boldsymbol{p} \to 0$.

   i. Derive
   $$\frac{d\langle \boldsymbol{p} \rangle}{dt} = -e\boldsymbol{E} - \frac{\langle \boldsymbol{p} \rangle}{\tau} \tag{1}$$
   where $\langle \boldsymbol{p} \rangle$ is the average electron momentum, and τ is the mean time between collisions.

   ii. Hence find the drift momentum $\boldsymbol{p}_{\mathrm{d}}$ (the steady-state value of $\boldsymbol{p}$) and the Drude conductivity σ_0.

   iii. Show that the connected two-time correlator
   $$C_{ij}(t,s) = \langle p_i(t+s)p_j(t) \rangle - \langle p_i(t+s) \rangle \langle p_j(t) \rangle \tag{2}$$
   obeys
   $$C_{ij}(t,s) = C_{ij}(0,0)\mathrm{e}^{-|s|/\tau} \tag{3}$$

   (b) More generally, suppose scattering is characterised by a transition rate kernel $W_{\boldsymbol{p}\to\boldsymbol{p}'}$: in an infinitesimal interval dt, an electron with momentum $\boldsymbol{p}$ scatters to $\boldsymbol{p}'$ with probability $W_{\boldsymbol{p}\to\boldsymbol{p}'}dt$. Let $f(\boldsymbol{r},\boldsymbol{p},t)$ be the phase-space density of electrons at position $\boldsymbol{r}$ and momentum $\boldsymbol{p}$. The *Boltzmann equation* is
   $$\frac{\partial f}{\partial t} - e\boldsymbol{E}\cdot\nabla_{\boldsymbol{p}} f = \int d^3\boldsymbol{q}\,\Big(W_{\boldsymbol{q}\to\boldsymbol{p}} f(\boldsymbol{r},\boldsymbol{q},t) - W_{\boldsymbol{p}\to\boldsymbol{q}} f(\boldsymbol{r},\boldsymbol{p},t)\Big). \tag{4}$$
   Here the left-hand side is the *free transport term*, while the right-hand side is the *collision integral*. The quantity
   $$\int d^3\boldsymbol{q}\,(\boldsymbol{q}-\boldsymbol{p})\,W_{\boldsymbol{p}\to\boldsymbol{q}} \tag{5}$$
   gives the rate of change of momentum for electrons with momentum $\boldsymbol{p}$. Using (4), show that the Drude dynamics (1) for
   $$\langle \boldsymbol{p} \rangle \equiv \frac{1}{N}\int d^3\boldsymbol{r}d^3\boldsymbol{p}\, f(\boldsymbol{r},\boldsymbol{p})\boldsymbol{p}$$
   is obtained if
   $$\int d^3\boldsymbol{q}\,(\boldsymbol{q}-\boldsymbol{p})\,W_{\boldsymbol{p}\to\boldsymbol{q}} = -\frac{\boldsymbol{p}}{\tau}. \tag{6}$$
   This condition is in fact necessary and sufficient for Drude relaxation (1) for arbitrary $f(\boldsymbol{r},\boldsymbol{p})$.

   (c) A widely used simplification is the *single relaxation time approximation*, in which
   $$W_{\boldsymbol{p}\to\boldsymbol{p}'} = \frac{f_0(\boldsymbol{p}')}{n\tau}, \tag{7}$$

where $n = \int d^3\boldsymbol{p}\, f_0(\boldsymbol{p}) = \int d^3\boldsymbol{p}\, f(\boldsymbol{p})$ is the electron density, and f_0 is an equilibrium distribution satisfying

$$\int d^3\boldsymbol{p}\, f_0(\boldsymbol{p})\, \boldsymbol{p} = 0. \tag{8}$$

Show that (7) satisfies (6), and that it reduces the Boltzmann equation to

$$\frac{\partial f}{\partial t} - e\boldsymbol{E} \cdot \nabla_{\boldsymbol{p}} f = \frac{f_0 - f}{\tau}. \tag{9}$$

2. **A failure of Drude's theory: the thermoelectric correction**: in this question you will derive the transport coefficients of Drude theory using linear response.

(a) One method of finding transport coefficients is studying the linear response of the solutions to the Boltzmann equation. Here we have now included the effect of spatial variation ($\boldsymbol{r}$ dependence)

$$\frac{\partial f}{\partial t} + \dot{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{r}} f + \dot{\boldsymbol{p}} \cdot \nabla_{\boldsymbol{p}} f = \frac{f_0 - f}{\tau}, \tag{10}$$

with $\dot{\boldsymbol{r}} = \boldsymbol{p}/m$ and $\dot{\boldsymbol{p}} = -e\boldsymbol{\mathcal{E}}$ given by the electrochemical force $\boldsymbol{\mathcal{E}} = \boldsymbol{E} + \frac{1}{e}\nabla\mu$. For constant T and $\boldsymbol{\mathcal{E}} = 0$, the equilibrium state is the Maxwell–Boltzmann distribution

$$f_0(\boldsymbol{r}, \boldsymbol{p}) = \frac{n}{(2\pi m k_{\mathrm{B}} T)^{3/2}} \exp\left(-\frac{p^2}{2mk_{\mathrm{B}}T}\right). \tag{11}$$

In the presence of a weak electrochemical force $\boldsymbol{\mathcal{E}}$ and a weak spatial temperature variation ∇T. Let $\boldsymbol{X}_1 = \boldsymbol{\mathcal{E}}$ and $\boldsymbol{X}_2 = -\nabla T$. we Taylor expand f to linear order

$$f = f_0 + \delta f_1 + \delta f_2, \qquad \delta f_j = \boldsymbol{X}_j \cdot \nabla_{\boldsymbol{X}_j} f\big|_{\boldsymbol{X}_j = 0} \tag{12}$$

and neglect higher order terms. By using that f is a static solution to (10), show that

$$\delta f_i = \frac{\boldsymbol{F}_i \cdot \boldsymbol{v}\,\tau}{k_{\mathrm{B}}T} f_0, \tag{13}$$

where $\boldsymbol{F}_1$ and $\boldsymbol{F}_2$ are the electrochemical force, and the force due to the temperature gradient respectively

$$\boldsymbol{F}_1 = -e\boldsymbol{\mathcal{E}}, \quad \boldsymbol{F}_2 = -\left(\frac{p^2}{2m} - \frac{3}{2}k_{\mathrm{B}}T\right)\frac{\nabla T}{T}. \tag{14}$$

(b) The corresponding linear-response electrical and heat current densities are

$$\begin{aligned} \langle \boldsymbol{j} \rangle &= \frac{1}{V}\int d^3\boldsymbol{r}\, d^3\boldsymbol{p}\, f(\boldsymbol{r}, \boldsymbol{p}) \boldsymbol{j}_{\mathrm{el.}}(\boldsymbol{p}), \\ \langle \boldsymbol{j}_{\mathrm{q}} \rangle &= \frac{1}{V}\int d^3\boldsymbol{r}\, d^3\boldsymbol{p}\, f(\boldsymbol{r}, \boldsymbol{p}) \boldsymbol{j}_{\mathrm{q,el.}}(\boldsymbol{p}) \end{aligned} \tag{15}$$

where $\boldsymbol{j}_{\mathrm{el.}}(\boldsymbol{p}) = -e(\boldsymbol{p}/m)$ and $\boldsymbol{j}_{\mathrm{q,el.}}(\boldsymbol{p}) = (p^2/(2m) - \mu)(\boldsymbol{p}/m)$ are the electrical and heat current per electron.

These are related to thermal and electrical gradients by the relation

$$\begin{pmatrix} \langle \boldsymbol{j} \rangle \\ \langle \boldsymbol{j}_q \rangle \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} \boldsymbol{\mathcal{E}} \\ -\boldsymbol{\nabla} T \end{pmatrix}, \tag{16}$$

Using your result for f, compute the Drude values for L_{12}.

You may use: standard Maxwell-Boltzmann expectation values

$$\langle v_i v_j \rangle = \tfrac{1}{3}\delta_{ij}\langle v^2 \rangle, \quad \langle \tfrac{1}{2}mv^2 \rangle = \langle \varepsilon \rangle = \tfrac{3}{2}k_{\mathrm{B}}T, \quad \sigma_\varepsilon^2 = \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2 = \tfrac{3}{2}(k_{\mathrm{B}}T)^2 \tag{17}$$

(c) Using the following definitions, express the matrix L_{ab} in terms of σ, κ, S and T

- The electrical conductivity σ is defined by $\langle \boldsymbol{j} \rangle = \sigma \boldsymbol{\mathcal{E}}$ for $\nabla T = 0$.
- The thermal conductivity κ is defined by $\langle \boldsymbol{j}_q \rangle = -\kappa \nabla T$ for $\langle \boldsymbol{j} \rangle = 0$
- The Seebeck coefficient S is defined by $\boldsymbol{\mathcal{E}} = S\, \nabla T$ under open-circuit conditions $\langle \boldsymbol{j} \rangle = 0$
- The Peltier coefficient Π is defined by $\langle \boldsymbol{j}_q \rangle = \Pi \langle \boldsymbol{j} \rangle$ for $\nabla T = 0$.
- The relation $\Pi = TS$ due to Kelvin.

(d) Hence compute the Drude linear response value of the Seebeck coefficient S.

(e) The thermal conductivity receives a correction if a current is allowed to flow by closing the circuit. In terms of σ, κ, S and T, determine

i. The thermal conductivity κ_{closed}, defined by $\langle \boldsymbol{j}_q \rangle = -\kappa_{\text{closed}} \nabla T$ for $\boldsymbol{\mathcal{E}} = 0$

ii. The dimensionless thermoelectric correction to the thermal conductivity

$$\delta\tilde{\kappa} = \frac{\kappa_{\text{closed}} - \kappa}{\kappa} \tag{18}$$

(f) Finally, evaluate the Drude prediction for $\delta\tilde{\kappa}$. Compare your answer for (2(e)ii) to the empirical value of $\delta\tilde{\kappa}$ for copper at room temperature. Comment on the success of Drude theory.

You may use: your calculation for S, the relations

$$\sigma_0 = \frac{ne^2\tau}{m}, \quad \kappa = \frac{5}{2}\frac{n\tau k_{\text{B}}^2 T}{m}, \quad \Pi = ST \tag{19}$$

and the following properties of copper at room temperature: Seebeck coefficient $S = 2 \times 10^{-6}\,\text{V}\,\text{K}^{-1}$, conductivity $\sigma_0 = 5.9 \times 10^7\,\Omega^{-1}\text{m}^{-1}$ and thermal conductivity $400\,\text{W}\,\text{m}^{-1}\text{K}^{-1}$.

3. **The plasma frequency and the transparency of metals:** Consider a Drude metal in an incident electromagnetic wave with electric field

$$\boldsymbol{E}(\boldsymbol{r}, t) = \boldsymbol{E}_0 \cos(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t). \tag{20}$$

Typically the mean free path of an electron $\lambda \ll k^{-1} = c/\omega$, so we may neglect the spatial dependence and write

$$\boldsymbol{E}(t) = \boldsymbol{E}_0 \cos(\omega t). \tag{21}$$

(a) Consider a general superposition of frequencies,

$$\boldsymbol{E}(t) = \int d\omega\, \mathrm{e}^{-i\omega t} \boldsymbol{E}(\omega), \tag{22}$$

and look for solutions to (1) of the form

$$\langle \boldsymbol{p}(t) \rangle = \int d\omega\, \mathrm{e}^{-i\omega t} \langle \boldsymbol{p}(\omega) \rangle. \tag{23}$$

Find the AC conductivity $\sigma(\omega)$, defined by $\boldsymbol{j}(\omega) = \sigma(\omega)\boldsymbol{E}(\omega)$, in terms of the DC conductivity σ_0, ω and τ.

(b) Using Maxwell's equations with no net charge density,

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = 0, \quad \boldsymbol{\nabla} \cdot \boldsymbol{B} = 0, \quad \boldsymbol{\nabla} \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}, \qquad \boldsymbol{\nabla} \times \boldsymbol{B} = \mu_0 \boldsymbol{J} + \epsilon_0\mu_0 \frac{\partial \boldsymbol{E}}{\partial t}, \tag{24}$$

together with standard vector identities, show that

$$\nabla^2 \boldsymbol{E} = -\frac{\omega^2}{c^2}\epsilon(\omega)\boldsymbol{E}(\omega) \tag{25}$$

and find the complex dielectric function $\epsilon(\omega)$ in terms of σ_0.

(c) Show that for $\omega\tau \gg 1$,

$$\epsilon(\omega) = 1 - \frac{\omega_{\mathrm{p}}^2}{\omega^2}, \tag{26}$$

where ω_{p} is the plasma frequency. Find the classical Drude value of ω_{p}.

(d) For sufficiently low frequency, the metal is opaque, and solutions of (25) decay exponentially with a characteristic length ξ (the penetration depth). Assuming a low frequency (but still with $\omega\tau \gg 1$) calculate ξ in terms of ω_{p} and show that it diverges as ω is increased through ω_{p}.

(e) For sufficiently high frequency, the metal is transparent and solutions of (25) are propagating waves with wavelength λ. Express λ in terms of ω_{p} and show that it also diverges, this time as ω is decreased through ω_{p}.

(f) The plasma wavelength is $\lambda_{\mathrm{p}} = 2\pi c/\omega_{\mathrm{p}}$. Calculate λ_{p} for lithium (in Ångström units). Compare your result with the wavelength at which lithium becomes transparent ($\lambda_{\mathrm{p}} = 1850\text{Å}$).

You may use: lithium is monovalent, with molar mass $m_{\mathrm{mol}} = 6.94\,\mathrm{g\,mol^{-1}}$ and density $\rho = 0.534\,\mathrm{g\,cm^{-3}}$.