ICFP Master Program
Condensed Matter Theory (B. Douçot, B. Estienne, L. Messio)
Homework for the fall vacation, 2019

This homework will count for 25% of the total note.

1 Electromagnetic response functions

Let us impose an external electromagnetic field to a physical system composed of charged fermions, each carrying a charge $-e$. This field is described by the combination of a scalar potential V and a vector potential $\mathbf{A}$. Although we will consider non-relativistic systems, it will be convenient to introduce the four-component vector $A^\mu \equiv (V, \mathbf{A})$. Here the scalar part corresponds to $\mu = 0$ and the vector part to $\mu = 1, 2, 3$. In the sequel, we shall label these three-dimensional spatial components by Latin superscripts such as i or j, whereas Greek letters such as μ, ν, will be used to label four-vectors components. In this problem, we shall adopt the following conventions for Fourier transforms:

$$\begin{aligned} f(\mathbf{r}, t) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i(\mathbf{q}.\mathbf{r}-\omega t)} \tilde{f}(\mathbf{q}, \omega) \\ \tilde{f}(\mathbf{q}, \omega) &= \int d^3\mathbf{r} \int dt e^{-i(\mathbf{q}.\mathbf{r}-\omega t)} f(\mathbf{r}, t) \end{aligned}$$

The system response to this electromagnetic field will be described by the local charge density $\delta\rho(\mathbf{r}, t)$ and the charge current $\mathbf{J}(\mathbf{r}, t)$, which will also be cast into a four-component vector $J^\mu \equiv (\delta\rho, \mathbf{J})$. In the linear response regime, we may write:

$$J^\mu(\mathbf{r}, t) = -\int d^3\mathbf{r}' \int dt' \sum_{\nu=0}^{3} K^{\mu\nu}(\mathbf{r}, t; \mathbf{r}', t') A^\mu(\mathbf{r}', t').$$

1) Under which conditions can we write $K^{\mu\nu}(\mathbf{r}, t; \mathbf{r}', t') = K^{\mu\nu}(\mathbf{r} - \mathbf{r}'; t - t')$?

2) Explain briefly why this allows us to write, in Fourier space:

$$\tilde{J}^\mu(\mathbf{q}, \omega) = -\sum_{\nu=0}^{3} \tilde{K}^{\mu\nu}(\mathbf{q}, \omega) \tilde{A}^\nu(\mathbf{q}, \omega).$$

3) Using the local condition of charge conservation, show that that, for each $\nu \in \{0, 1, 2, 3\}$, the component $\tilde{K}^{0\nu}$ can be expressed in terms of the three components $\tilde{K}^{i\nu}$ with $i \in \{1, 2, 3\}$.

4) Consider a gauge transformation:

$$A^\mu = (-\frac{\partial\lambda}{\partial t}, \boldsymbol{\nabla}\lambda),$$

where $\lambda(\mathbf{r}, t)$ is an arbitrary scalar function. Express then the four-vector $\tilde{K}^{\mu\nu}(\mathbf{q}, \omega)$ as a function of the scalar function $\tilde{\lambda}(\mathbf{q}, \omega)$.

5) Show that gauge invariance implies that the components $\tilde{K}^{\mu 0}$ can be expressed in terms of the three components $\tilde{K}^{\mu j}$ with $j \in \{1, 2, 3\}$.

6) Combining the results of questions 3 and 5, show that $\tilde{K}^{00}$ can be expressed as a function of the spatial components $\tilde{K}^{ij}$ with $i, j \in \{1, 2, 3\}$. Show that $\tilde{K}^{00} = -e^2\chi_c$, where χ_c is the charge susceptibility defined in the lectures.

7) To simplify further the spatial response tensor $\tilde{K}^{ij}$, we are going to assume that both the system Hamiltonian and its unperturbed state are invariant under arbitrary rotations. The vector $\mathbf{q}$ at which the response is evaluated sets a particular direction in space if $\mathbf{q} \neq 0$. For an arbitrary spatial vector $\mathbf{v}$, we decompose it as $\mathbf{v} = \mathbf{v}_{\parallel} + \mathbf{v}_{\perp}$, where

$$\mathbf{v}_{\parallel} = \frac{\mathbf{v}.\mathbf{q}}{\mathbf{q}.\mathbf{q}}\,\mathbf{q},$$

so that $\mathbf{v}_{\perp}.\mathbf{q} = 0$. Let us perform an arbitrary rotation along an axis parallel to $\mathbf{q}$. What happens to $\mathbf{J}(\mathbf{q}, \omega)$?

8) Deduce from this that there are three functions $\tilde{K}_{\parallel}(q, \omega)$, $\tilde{K}_{\perp}(q, \omega)$, and $\tilde{K}_{\mathrm{odd}}(q, \omega)$ (we have set $q = |\mathbf{q}|$), such that:

$$\begin{aligned}
\delta\tilde{\mathbf{J}}_{\parallel}(\mathbf{q}, \omega) &= -\tilde{K}_{\parallel}(q, \omega)\tilde{\mathbf{A}}_{\parallel}(\mathbf{q}, \omega) \\
\delta\tilde{\mathbf{J}}_{\perp}(\mathbf{q}, \omega) &= -\tilde{K}_{\perp}(q, \omega)\tilde{\mathbf{A}}_{\perp}(\mathbf{q}, \omega) - \tilde{K}_{\mathrm{odd}}(q, \omega)\frac{\mathbf{q} \wedge \tilde{\mathbf{A}}_{\perp}(\mathbf{q}, \omega)}{|\mathbf{q}|}
\end{aligned}$$

9) Show that if both the system Hamiltonian and its unperturbed state are invariant under reflections with respect to arbitrary mirror planes, then $\tilde{K}_{\mathrm{odd}}(q, \omega) = 0$. Can you think of a physical situation where this would not apply? In the remainding part of this problem, we shall assume that $\tilde{K}_{\mathrm{odd}}(q, \omega) = 0$.

10) Show that we get then:

$$\tilde{K}^{ij}(\mathbf{q}, \omega) = \tilde{K}_{\parallel}(q, \omega)\frac{q^i q^j}{q^2} + \tilde{K}_{\perp}(q, \omega)(\delta^{ij} - \frac{q^i q^j}{q^2})$$

11) Deduce from this that:

$$\begin{aligned}
\tilde{K}^{00}(\mathbf{q}, \omega) &= -\frac{q^2}{\omega^2}\tilde{K}_{\parallel}(q, \omega) \\
\tilde{K}^{0j}(\mathbf{q}, \omega) &= \tilde{K}_{\parallel}(q, \omega)\frac{q^j}{\omega} \\
\tilde{K}^{i0}(\mathbf{q}, \omega) &= -\frac{q^i}{\omega}\tilde{K}_{\parallel}(q, \omega)
\end{aligned}$$

12) We define the longitudinal conductivity $\tilde{\sigma}_{\parallel}(\mathbf{q}, \omega)$ by the relation $\tilde{\mathbf{J}}_{\parallel}(\mathbf{q}, \omega) = \tilde{\sigma}_{\parallel}(\mathbf{q}, \omega)\tilde{\mathbf{E}}_{\parallel}(\mathbf{q}, \omega)$, where $\mathbf{E}$ is the external electric field defined by $\mathbf{E} = -\boldsymbol{\nabla} V - \partial\mathbf{A}/\partial t$. Show that $\tilde{\sigma}_{\parallel}(\mathbf{q}, \omega)$ can be expressed uniquely as a function of $\tilde{K}_{\parallel}(q, \omega)$.

13) Consider a free electron system, and a wave-vector $q \ll 2k_{\mathrm{F}}$, where k_{F} is the Fermi wave-vector. Using the results of the lectures, give the expressions of $\tilde{\sigma}_{\parallel}(q, \omega)$ when $\omega \gg v_{\mathrm{F}}q$ (v_{F} being the Fermi velocity) and of the real part of $\tilde{\sigma}_{\parallel}(q, \omega)$ when $\omega < v_{\mathrm{F}}q$. What do you think of these results? What is the origin of dissipation when $\omega < v_{\mathrm{F}}q$?

2 Comparison between longitudinal and transverse responses

14) Give a physical argument to show that $\tilde{K}_{\parallel}(q \to 0, \omega) = \tilde{K}_{\perp}(q \to 0, \omega)$, when $\omega \neq 0$.

15) Show that $\tilde{K}_{\parallel}(q, \omega = 0) = 0$.

16) For a free electron system, the static transverse response, when $q \ll k_{\mathrm{F}}$, is given by:

$$\tilde{K}_{\perp}(q, \omega = 0) = \frac{ne^2}{m} \frac{q^2}{4k_{\mathrm{F}}^2}$$

Are you surprised by the fact that $\tilde{K}_{\parallel}(q, \omega = 0) \neq \tilde{K}_{\perp}(q, \omega = 0)$?

17) Do you know some physical systems in which the difference between these two static response functions is even stronger at small q?

3 Response of a free fermion systems to a static magnetic field

18) We suppose that our system is exposed to a static external magnetic field $\mathbf{B}_{\mathrm{ext}}$. This magnetic field induces a current $\mathbf{J}_{\mathrm{ind}}$ in the system, which in turn generates an induced magnetic field $\mathbf{B}_{\mathrm{ind}}$. Ampère's equation gives $\boldsymbol{\nabla} \times \mathbf{B}_{\mathrm{ind}} = \mu_0 \mathbf{J}_{\mathrm{ind}}$. We introduce a vector potential $\mathbf{A}_{\mathrm{ind}}$ such that $\boldsymbol{\nabla} \times \mathbf{A}_{\mathrm{ind}} = \mathbf{B}_{\mathrm{ind}}$. Working in the Coulomb gauge $\boldsymbol{\nabla}.\mathbf{A}_{\mathrm{ind}} = 0$, express the Fourier transform $\tilde{\mathbf{A}}_{\mathrm{ind}}(\mathbf{q})$ as a function of $\tilde{\mathbf{J}}_{\mathrm{ind}}(\mathbf{q})$.

19) In a mean-field approximation, we assume that the system reacts as a non-interacting one to the local vector potential $\mathbf{A}_{\mathrm{loc}} = \mathbf{A}_{\mathrm{ext}} + \mathbf{A}_{\mathrm{ind}}$. Express then the Fourier amplitude $\tilde{\mathbf{A}}_{\mathrm{loc}}(\mathbf{q})$ as a function of $\tilde{\mathbf{A}}_{\mathrm{ext}}(\mathbf{q})$.

20) Using the expression given in question 16, specialize this result to the small q limit. How would you characterize this type of screening for an external magnetic field? Give an order of magnitude estimate for the correction to $\mathbf{A}_{\mathrm{ext}}$ due to induced currents.

4 Charge susceptibility in a semi-conductor

In the lectures, we have computed the charge susceptibility for a non-interacting Fermi sea, in the absence of any periodic potential. Let us now assume that electrons are subjected to such periodic potential. The eigenstates of the corresponding single particle Hamiltonian are normalized Bloch waves $|\alpha, \mathbf{k}\rangle$, whose spatial form reads $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}.\mathbf{r}} u_{\alpha,\mathbf{k}}(\mathbf{r})$, where $u_{\alpha,\mathbf{k}}(\mathbf{r})$ is a periodic function. We assume that the system is a semi-conductor, so that the Fermi energy lies in an energy gap of the single particle Hamiltonian.

21) Explain why the charge susceptibility can be expressed as:

$$\tilde{\chi}_c(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{\alpha \notin F; \beta \in F} \sum_{\mathbf{k},\, \mathbf{k}'} \Big\{ e^{i(\mathbf{k}-\mathbf{k}')(\mathbf{r}-\mathbf{r}')} \frac{u^*_{\beta\mathbf{k}'}(\mathbf{r}) u_{\alpha\mathbf{k}}(\mathbf{r}) u^*_{\alpha\mathbf{k}}(\mathbf{r}') u_{\beta\mathbf{k}'}(\mathbf{r}')}{\hbar\omega - \varepsilon_\alpha(\mathbf{k}) + \varepsilon_\beta(\mathbf{k}') + i\eta} - e^{-i(\mathbf{k}-\mathbf{k}')(\mathbf{r}-\mathbf{r}')} \frac{u^*_{\beta\mathbf{k}'}(\mathbf{r}') u_{\alpha\mathbf{k}}(\mathbf{r}') u^*_{\alpha\mathbf{k}}(\mathbf{r}) u_{\beta\mathbf{k}'}(\mathbf{r})}{\hbar\omega + \varepsilon_\alpha(\mathbf{k}) - \varepsilon_\beta(\mathbf{k}') + i\eta} \Big\}$$

In this sum, $\alpha \notin F$ means that band α is empty, and $\beta \in F$ means that band β is filled.

22) On a lattice, translational symmetry is limited to the underlying Bravais lattice vectors $\mathbf{R}$. This means that $\tilde{\chi}_c(\mathbf{r}+\mathbf{R},\mathbf{r}'+\mathbf{R};\omega) = \tilde{\chi}_c(\mathbf{r},\mathbf{r}';\omega)$. So in general, $\tilde{\chi}_c(\mathbf{r},\mathbf{r}';\omega)$ is not a function of just $\mathbf{r}-\mathbf{r}'$ as in the absence of a periodic potential. To circumvent this, we consider the double spatial Fourier transform:

$$\tilde{\chi}_c(\mathbf{q};\omega) = \frac{1}{V}\int d^3\mathbf{r}\int d^3\mathbf{r}' e^{-i\mathbf{q}.(\mathbf{r}-\mathbf{r}')}\tilde{\chi}_c(\mathbf{r},\mathbf{r}';\omega),$$

where V denotes the total volume of the system. Show that this quantity can be simplified into:

$$\tilde{\chi}_c(\mathbf{q};\omega) = \frac{1}{V}\sum_{\alpha\notin F;\beta\in F}\sum_{\mathbf{k}}\left\{\frac{|\langle u_{\beta,\mathbf{k}-\frac{\mathbf{q}}{2}}|u_{\alpha,\mathbf{k}+\frac{\mathbf{q}}{2}}\rangle|^2}{\hbar\omega-\varepsilon_\alpha(\mathbf{k}+\frac{\mathbf{q}}{2})+\varepsilon_\beta(\mathbf{k}-\frac{\mathbf{q}}{2})+i\eta} - \frac{|\langle u_{\beta,\mathbf{k}+\frac{\mathbf{q}}{2}}|u_{\alpha,\mathbf{k}-\frac{\mathbf{q}}{2}}\rangle|^2}{\hbar\omega+\varepsilon_\alpha(\mathbf{k}-\frac{\mathbf{q}}{2})-\varepsilon_\beta(\mathbf{k}+\frac{\mathbf{q}}{2})+i\eta}\right\}$$

To obtain this expression, one has to modify the normalization of the Bloch functions, and to impose that the integral of $|u_{\alpha,\mathbf{k}}(\mathbf{r})|^2$ over a unit cell should be equal to 1. The scalar products which appear in the numerators of the above formula are also defined as integrals over a single unit cell.

23) Deduce from this that the static charge susceptibility $\tilde{\chi}_c(\mathbf{q};\omega=0)$ vanishes as $\mathbf{q}\to 0$.

24) Assuming that $\tilde{\chi}_c(\mathbf{q};\omega=0)\simeq -c\,\mathbf{q}^2$ at small q, with $c>0$, analyze the screening of an external electric charge along the lines presented in the lectures. Do you see a qualitative difference with the case of metallic screening? How would you characterize such behavior?