Quantum Theory of Condensed Matter II

Mesoscopic Physics

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Sheet 4

1. Kubo formula for a uniform external perturbation $(q = 0)$

In this exercise you will derive the Kubo formula for non-interacting electrons in a uniform electric field $\mathbf{E}$. The interaction between the electrons and the electric field is well described in this case by the dipole coupling.

$$\hat{V}(t) = e\hat{\mathbf{X}} \cdot \mathbf{E}(t)$$

where e is the (absolute value of the) electronic charge and $\hat{\mathbf{X}} = \sum_i \hat{\mathbf{r}}_i$ with $\hat{\mathbf{r}}_i$ the position operator of the i-th electron.

1. Prove that the dipole moment operator for a collection of electrons reads $\hat{\mathcal{P}} = -e\hat{\mathbf{X}}$, thus justifying the coupling Hamiltonian. Moreover, prove that the current operator reads instead $\hat{\mathcal{J}} = -e\hat{\mathbf{P}}/m = -e/m \sum_i \hat{\mathbf{p}}_i$ where $\hat{\mathbf{p}}_i$ is the momentum operator of the i-th electron.

   Hint: Start from the definition of the density and current density operators in first quantization.

2. Describe the perturbation on the current $J(t) \equiv \langle \hat{\mathcal{J}} \rangle$ within the linear response theory. Calculate explicitly the response function in the frequency domain, thus obtaining the classical result

$$\sigma_{\alpha\beta}(\omega) = i\frac{e^2 n}{m\omega}\,\delta_{\alpha\beta}$$

   Hint: The following representation of the step function could be of interest:

$$\theta(t) = \lim_{\eta \to 0^+} \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \frac{i}{\omega + i\eta}$$

3. Use than the relation $\dot{\mathbf{X}} = \mathbf{P}/m$ and a partial integration to obtain, starting from the linear response expression of 1.2, the more familiar Kubo formula

$$\sigma(\omega) = \frac{i}{\omega}\left(\mathbf{\Pi}(\omega) + \frac{e^2 n}{m}\right)$$

   where the polarization $\mathbf{\Pi}(\omega)$ reads, in components:

$$\Pi_{\alpha\beta}(\omega) = \frac{i}{\hbar V}\int_0^{+\infty} \mathrm{d}t\, \langle [\hat{\mathcal{J}}_\beta, \hat{\mathcal{J}}_\alpha(t)] \rangle_0\, e^{i\omega t},$$

   with V the volume of the system and $\langle \bullet \rangle_0$ the thermal average with respect to the unperturbed, free electron Hamiltonian.

4. Prove that:

$$\Pi_{\alpha\beta}(\omega = 0) = -\frac{e^2 n}{m}\delta_{\alpha\beta}.$$

   Do you see any contradiction with the results obtained at points 1.2 and 1.3 ?

(8 Points)

2. Classical limit of the Kubo formula

In the lecture the following expression for the conductivity of charged Fermions has been derived

$$\sigma_{\mathrm{xx}}(\omega) = i\frac{e^2}{\omega V}\sum_{\mathrm{n,m}} |v_{\mathrm{nm}}|^2 \frac{f(\epsilon_{\mathrm{n}}) - f(\epsilon_{\mathrm{m}})}{\epsilon_{\mathrm{n}} - \epsilon_{\mathrm{m}} + \hbar\omega + i\eta} + i\frac{e^2 n}{m\omega}, \tag{1}$$

where V is the volume of the system and v_{nm} is the matrix element of the velocity operator in the single particle basis.
Derive the Kubo formula in the classical (*i.e.* non-degenerate) limit in which the Fermi-Dirac distribution is approximated by $f(\epsilon) \approx e^{-\beta(\epsilon-\mu)}$.

1. First simplify equation (1) by means of the given approximation for $f(\epsilon)$ and expand the numerator in powers of the difference $\beta(\epsilon_{\mathrm{n}} - \epsilon_{\mathrm{m}})$.
2. Divide the resulting sum in two terms. One term is proportional to ω^{-1} and cancels exactly the diamagnetic term in equation (1). Bear in mind that, in the classical limit the following substitution holds

   $$1/V\ \mathbf{Tr}[v_{\mathrm{x}} e^{-\beta H/2} v_{\mathrm{x}} e^{-\beta H/2}] = n\langle v_{\mathrm{x}}^2\rangle = nkT/m,$$

   where the square parentheses represent the thermal single particle average.
3. Analogously, derive from the second term the classical result already derived in Sheet 2.

(6 Points)

Frohes Schaffen!