Karlsruher Institut für Technologie | Institut für Theorie der Kondensierten Materie

Übungen zur Theorie der Kondensierten Materie II SS 18

Prof. Dr. J. Schmalian
Dr. J. M. Link, Egor Kiselev

Blatt 10
Besprechung 6.07.2018

---

1. Kubo formula for conductivity (10 + 10 + 10 + 70 Points)

(a) Consider the Lagrangian of a particle in an electromagnetic field (with the scalar potential Φ and the vector potential $\boldsymbol{A}$)

$$L = \frac{1}{2} m v^2 + q \boldsymbol{v} \cdot \boldsymbol{A} - q\Phi.$$

Show that the correct equations of motion follow from this Lagrangian. Perform a Legendre transform and show that the Hamiltonian is given by

$$H = \frac{1}{2m} \left(\boldsymbol{p} - q\boldsymbol{A}\right)^2 + q\Phi,$$

where $\boldsymbol{p}$ is the canonical momentum. How is this Hamiltonian generalized to many non-interacting particles? Show that the electric current $\boldsymbol{J} = q\sum_i \boldsymbol{v}_i$ is obtained by varying H with respect to the vectro potential $\boldsymbol{A}$ ($\boldsymbol{A}$ and $\boldsymbol{p}$ are independent variables in the Hamiltonian picture).

$$q\frac{\partial H}{\partial \boldsymbol{A}} = -q\sum_i \boldsymbol{v}_i = -\boldsymbol{J}.$$

(b) In second quantization the Hamiltonian reads

$$H = \frac{1}{2m} \sum_\alpha \int d^d x \psi_\alpha^\dagger(x) \left(\frac{\hbar}{i}\nabla - q\boldsymbol{A}\right)^2 \psi_\alpha(x).$$

$\boldsymbol{A}$ is not quantized. Calculate the first variation of H with respect to $\boldsymbol{A}$: $H(\boldsymbol{A} + \delta\boldsymbol{A}) - H(\boldsymbol{A})$. Be carefull with the non-commuting $\boldsymbol{A}$ and ∇! Show that

$$\begin{aligned} \boldsymbol{j} &= \frac{\hbar q}{2mi} \sum_\alpha \int d^d x \left[\psi_\alpha^\dagger(x)\left(\nabla\psi_\alpha(x)\right) - \left(\nabla\psi_\alpha^\dagger(x)\right)\psi_\alpha(x)\right] \\ &- \sum_\alpha \int d^d x \frac{q^2}{m} \boldsymbol{A} \psi_\alpha^\dagger(x)\psi_\alpha(x). \end{aligned}$$

The first term of $\boldsymbol{j}$ is called the paramagnetic contribution $\boldsymbol{j}_p$, the second is called the diamagnetic contribution $\boldsymbol{j}_{dia}$.

(c) Remembering that the current operator was obtained as a first variation of H with respect to $\boldsymbol{A}$, it is easy to write down the coupling Hamiltonian H_{EM} in terms of the current $\boldsymbol{j}(x)$ and the vector potentian $\boldsymbol{A}(x)$. Show that

$$\langle \boldsymbol{j}(t)\rangle = \langle \boldsymbol{j}_p(t)\rangle - \frac{q^2}{m}\boldsymbol{A}(t)\langle \rho\rangle_0 .$$

Using the Kubo formula demonstrate that

$$\begin{aligned}
&\left\langle j^i(t,x)\right\rangle = \int_{-\infty}^{\infty} d^d x' \\
&\times \left[-i\int_{-\infty}^{\infty} dt'\theta(t-t')\left\langle\left[j_p^i(t,x), j_p^k(t',x')\right]\right\rangle_0 - \int_{-\infty}^{\infty} dt'\delta(x-x')\delta(t-t')\delta_{ki}\frac{q^2}{m}\langle\rho\rangle_0\right] \\
&A^k(x',t') .
\end{aligned}$$

Disregard all non-linearities in $\boldsymbol{A}$. By Fourier transforming this result, show that for the conductivity $\sigma_{ik}(\omega, q)$ holds

$$\sigma_{ik}(\omega,q) = \frac{1}{i\omega}C_{ik}^R(\omega,q) - \frac{1}{i\omega}\delta_{ki}\frac{q^2}{m}\langle\rho\rangle_0 ,$$

where $C_{ik}^R(\omega,q)$ is the Fourier transform of the correlator

$$-i\int_{-\infty}^{\infty} dt'\theta(t-t')\left\langle\left[j_p^i(t,x), j_p^k(t',x')\right]\right\rangle_0 . \tag{1}$$

Use the gauge $\Phi = 0$.

(d) Calculate the real part of the conductivity

$$\mathrm{Re}\left[\sigma_{jk}(\omega\to 0, q=0)\right] = \lim_{\omega\to 0}\mathrm{Re}\left[\frac{1}{i\omega}C_{ik}^R(\omega, q=0)\right].$$

Use the Matsubara formalism. The corresponding Matsubara Green's function is

$$C_{ik}(\tau,\tau') = C_{ik}(\tau-\tau') = -\left\langle T_\tau\left\{j_p^i(\tau,q)\, j_p^k(\tau',-q)\right\}\right\rangle ,$$

where τ is the imaginary time $t\to -i\tau$. In the frequency and momentum representation the Green's function reads

$$C_{ik}(\omega_n,q) = -\left\langle\left\langle j_p^i(\omega_n,q)\, j_p^k(-\omega_n,-q)\right\rangle\right\rangle . \tag{2}$$

Use the single particle Green's function

$$G_{\boldsymbol{q},i\omega_n} = \frac{1}{i\omega_n - \epsilon_{\boldsymbol{q}} + \frac{i}{2\tau}\mathrm{sgn}\omega_n},$$

Where the term $\frac{i}{2\tau}\mathrm{sgn}\omega_n$ is a self-energy contribution due to impurity scattering. To calculate the correlator (2) you need to consider the diagram shown in Abbildung 1. Continue analytically to real frequencies **before** performing the integration over momenta. For the Matsubara summation you will need a threefold contour with two brunch-cuts. Show, finally, that the old Drude-result is obtained

$$\sigma_{xx} = \frac{e^2\tau n}{m}.$$

For more hints take a look at standard literature such as the books by Altland & Simons and Bruus & Flensberg.

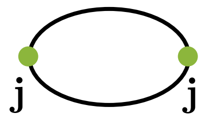

Abbildung 1: Diagrammatic representation of the current-current correlation function