Sheet 3:

Hand-out: Tuesday, Nov. 7, 2023; Solutions: Tuesday, Nov. 14, 2023

Problem 1 Drude conductivity

We consider electrons in a disorder-averaged scattering potential described by the Green's function with momentum k and Matsubara frequencies $i\omega_n$,

$$G(k, i\omega_n) = \frac{1}{i\omega_n - \xi_k + \frac{i}{2\tau}\mathrm{sgn}(\omega_n)}. \tag{1}$$

Here, ξ_k is the dispersion relation and τ is the scattering time scale. The goal is to compute the Drude conductivity, constituted by the diamagnetic and paramagnetic current response, using Kubo's formula. The latter relates the conductivity $\sigma(\nu)$ to the current-current fluctuations

$$\sigma(\nu) = \frac{1}{-i\nu}\left\{\frac{ne^2}{m} - i\nu\Big\langle[j(q\to 0,\nu), j(q\to 0,-\nu)]\Big\rangle\right\} \tag{2}$$

with current $j(q\to 0,\nu) \equiv j(\nu)$. For the optical conductivity in metals, the wavevector $q \ll k_F$ is much smaller than the Fermi momentum k_F, which justifies to consider the $q = 0$ component. To obtain the real frequency response of the system, we first need to derive the auto-correlation function on the imaginary frequency axis and then do the analytic continuation. We use the boundary condition (DC current in metals) to re-write the conductivity in imaginary time as

$$\sigma(i\nu_n) = \frac{1}{\nu_n}\Big[\big\langle j(\nu')j(-\nu')\big\rangle\Big]_{\nu'=0}^{\nu'=i\nu_n} \tag{3}$$

with $\langle j(i\nu_n)j(-i\nu_n)\rangle = \int_0^\beta d\tau e^{i\nu_n\tau}\langle Tj(\tau)j(0)\rangle$.

(1.a) For a parabolic dispersion, $\xi_k = k^2/2m$, the current operator at $q = 0$ is given by

$$j(q=0) = \frac{e}{2m}\sum_k 2k\hat{c}_k^\dagger\hat{c}_k. \tag{4}$$

Use Feynman rules to show that the current fluctuations can be expressed as

$$\langle j(i\nu_n)j(-i\nu_n)\rangle = -2e^2T\sum_{k,i\omega_n}\frac{k^2}{m^2}G(k, i\omega_n + i\nu_n)G(k, i\omega_n). \tag{5}$$

(1.b) Show that the contribution for $i\nu_n \to 0$ exactly cancels the diamagnetic term in Eq. (2). *Hint: Use the Ward identity* $\frac{k}{m}G^2(k) = \nabla_k G(k)$.

(1.c) Now, we want to evaluate (5) using the Matsubara summation technique by writing the Matsubara sum as an integral over the complex variable z using the Fermi-Dirac distribution $n_F(\omega)$. Show that it can be be expressed as an integral over products of retarded and advanced Green's functions along the real axis.
Hint: The integrand has branch cuts and you need to consider three contours.

(1.d) Evaluate the frequency integration.
Hint: Use that for $T \ll E_F$, we can express $n_F(\epsilon+\omega) - n_F(\epsilon) = -\omega\delta(\epsilon)$.

(1.e) Take the continuum limit and change variables

$$\int \frac{d^3k}{(2\pi)^3} \to \int \frac{d\Omega}{4\pi}\frac{N(\xi)d\xi}{2\pi}, \tag{6}$$

where $N(\xi)$ is the density of states. Assume that at low-energy contributions at the Fermi surface are dominant and evaluate the integral.

(1.f) Analytically continue Eq. (5) and insert into Eq. (2). Show that we have obtained the known result for Drude conductivity.

Problem 2 Analytic properties of Green's functions

In many-body theory, we often encounter various kinds of Green's functions. In this problem, we figure out the intimate connection between different types of Green's functions. Especially, we see that all of them can be obtained from the imaginary time-ordered Green's function using analytic continuation in the complex frequency plane. Some important Green's functions are the following,

- Imaginary time-ordered Greens function

$$(-1)\mathcal{G}_{AB}(\tau-\tau') = \langle \mathcal{T}_\tau\{\hat{A}(\tau)\hat{B}(\tau')\}\rangle = \theta(\tau-\tau')\langle\hat{A}(\tau)\hat{B}(\tau')\rangle + \zeta\theta(\tau'-\tau)\langle\hat{B}(\tau')\hat{A}(\tau)\rangle\,. \tag{7}$$

- Real time-ordered Green's function

$$iG_{AB}(t-t') = \langle \mathcal{T}_t\{\hat{A}(t)\hat{B}(t')\}\rangle = \theta(t-t')\langle\hat{A}(t)\hat{B}(t')\rangle + \zeta\theta(t'-t)\langle\hat{B}(t')\hat{A}(t)\rangle\,. \tag{8}$$

- Retarded Green's function

$$G^R_{AB}(t-t') = i\theta(t-t')\langle[\hat{A}(t),\hat{B}(t')]_\zeta\rangle\,. \tag{9}$$

- Advanced Green's function

$$G^A_{AB}(t-t') = -i\theta(t'-t)\langle[\hat{A}(t),\hat{B}(t')]_\zeta\rangle\,. \tag{10}$$

- Spectral function

$$A_{AB}(\omega) = \mathrm{Im}\{G^R_{AB}(\omega)\}\,,\quad G^R_{AB}(\omega) = \int dt e^{i(\omega+i0^+)t}G^R_{AB}(t) \tag{11}$$

Here, $\langle\cdots\rangle = \mathrm{Tr}\big(e^{-\beta(\hat{K}-\Omega)}\cdots\big)$, $\hat{K} = \hat{H}-\mu\hat{N}$, $e^{-\beta\Omega} = \mathrm{Tr}\big(e^{-\beta\hat{K}}\big)$, $\hat{A}(\tau) = e^{\tau\hat{K}}\hat{A}e^{-\tau\hat{K}}$, and $[\cdot,\cdot]_\zeta$ is the commutator (anti-commutator) for bosons (fermions).

(2.a) Show that $\mathcal{G}_{AB}(\tau+\beta) = \zeta\, \mathcal{G}_{AB}(\tau)$ for $-\beta \le \tau < 0$. Thus, $\mathcal{G}_{AB}(\tau)$ is (anti-)periodic for bosons (fermions), and can be Fourier expanded in terms of bosonic (fermionc) Matsubara frequencies $\omega_n = 2\pi n/\beta$ ($\omega_n = \pi/\beta(2n+1)$) as $\mathcal{G}_{AB}(\tau) = 1/\beta \sum_n e^{-i\omega_n \tau} \mathcal{G}_{AB}(i\omega_n)$.

(2.b) Derive the Lehman representation of $A_{AB}(\omega)$ by expanding Eq. 11 in terms of the complete set of eigenstates of $\hat{H}$.

(2.c) Derive the *Kramers-Krönig relations*, which states that for every analytic function $\chi(z) = \chi_R(z) + i\chi_I(z)$ in the closed upper-half plane (upper half plane including the real axis),

$$\begin{aligned} \chi_R(\omega) &= \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\chi_I(\omega')}{\omega'-\omega}\,, \\ \chi_I(\omega) &= -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\chi_R(\omega')}{\omega'-\omega}\,. \end{aligned} \tag{12}$$

Hint: use the Cauchy's theorem, which for $\chi(z)$, states that $0 = \int d\omega' \chi(\omega')/(\omega' - \omega + i0^+)$. Then use the relation $1/(\omega' - \omega + i0^+) = \mathcal{P}\{1/(\omega' - \omega)\} - i\pi\delta(\omega - \omega')$. Kramers-Krönig relations are crucial identities relating the real and imaginary parts of the Fourier transform of any causal function. Since response functions in physics are always causal, the Kramers-Krönig relations hold for every response function in the universe.

(2.d) From Kramers-Krönig relations, show that

$$\begin{aligned} G^R_{AB}(\omega) &= \int \frac{d\omega'}{\pi} \frac{1}{\omega' - \big(\omega + i0^+\big)} A_{AB}(\omega')\,, \\ G^A_{AB}(\omega) &= \int \frac{d\omega'}{\pi} \frac{1}{\omega' - \big(\omega - i0^+\big)} A_{AB}(\omega')\,. \end{aligned} \tag{13}$$

Verify Eqs. 13 explicitly using Lehman representation of $G^R_{AB}(\omega)$, $G^A_{AB}(\omega)$, and $A_{AB}(\omega)$.

(2.e) Using the Lehman representation of $\mathcal{G}_{AB}(i\omega_n)$, $G^R_{AB}(\omega)$ and $G^A_{AB}(\omega)$, show that all are related to $\mathcal{G}_{AB}(z)$ defined by

$$\mathcal{G}_{AB}(z) = \int d\omega' \frac{1}{\omega' - z} A_{AB}(\omega')\,, \tag{14}$$

such that $G^R_{AB}(\omega) = \mathcal{G}_{AB}(z = \omega + i0^+)$, $G^A_{AB}(\omega) = \mathcal{G}_{AB}(z = \omega - i0^+)$, and $\mathcal{G}_{AB}(i\omega_n) = \mathcal{G}_{AB}(z = i\omega_n)$.

(2.f) Show that the imaginary part of $\mathcal{G}_{AB}(z)$ has a branch cut along the real axis, with a discontinuity of its imaginary part equal to $2A_{AB}(\omega)$.