Prof. Dr. J. von Delft, Dr. O. Yevtushenko, F. Kugler Jan. 14, 2020

Problem Set 11: Conductivity of disordered metals

The goal of this problem set is to show how methods of many-body theory can be used to study non-interacting electrons in a random potential. In particular, we will compute the disorder-averaged single-particle Green's function as well as the conductivity using the Kubo formula. We start by showing how we can make use of all the many-body theory tools, because averaging over disorder generates an effective interaction between electrons.
Consider free electrons in a random potential $V(x)$ described by the action

$$S[\bar{c},c] = \int_0^\beta d\tau \int d^d x\, c^\dagger(x,\tau)\Big[\partial_\tau - \frac{\nabla^2}{2m} + V(x)\Big]c(x,\tau) \tag{1}$$

with a Gaussian disorder distribution

$$p[V(x)] \;\propto\; \exp\left[-\int d^d x \int d^d y\, V(x)\Delta(x-y)V(y)\right], \tag{2}$$

i.e., $\langle V(x)\rangle_{\rm dis} = 0$ and $\langle V(x)V(y)\rangle_{\rm dis} = D(x-y)$, with $\int d^d z\, \Delta(x-z)D(z-y) = \delta(x-y)$.
Let's consider the disorder-averaged partition function

$$\langle Z\rangle_{\rm dis} = \int \mathcal{D}V\, \mathcal{D}(\bar{c},c)\, e^{-S[\bar{c},c]}\, p[V(x)]. \tag{3}$$

1) Perform the Gaussian integral over the disorder realizations $V(x)$. Show that this disorder average generates an effective two-body interaction between the electrons, with an interaction potential given by the disorder correlation function $D(x)$.

For this reason, it seems that we can straight-forwardly employ our many-body theory methods to compute disorder-averaged quantities. There is one caveat, though: when computing disorder-averaged propagators, the partition function Z appears in the denominator, which causes problems and requires to introduce a few more tricks. However, these go beyond the scope of this problem set.
Let's simplify further and take a Gaussian white noise model where the disorder potential is uncorrelated at different positions, i.e., the disorder correlation function takes the form $D(x) = \frac{1}{2\pi\nu_0\tau_{\rm ei}}\,\delta(x)$. Here, ν_0 is the density of states at the Fermi energy and $\tau_{\rm ei}$ is the characteristic electron–impurity scattering time.
The disorder-averaged Green's function (GF) is given by

$$G^{-1} = G_0^{-1} - \Sigma, \tag{4}$$

where $G_0^{-1} = i\omega_n - \xi_k$ is the bare (free) GF and Σ is the self-energy generated by the disorder. We assume that the disorder is weak and we will calculate Σ in the leading approximation. We start from the perturbative expansion of the GF, Fig. 1(a), and perform disorder averaging by pairing V-vertices in a given order of the expansion in all possible ways. An example of the leading diagram is shown in Fig. 1(b).

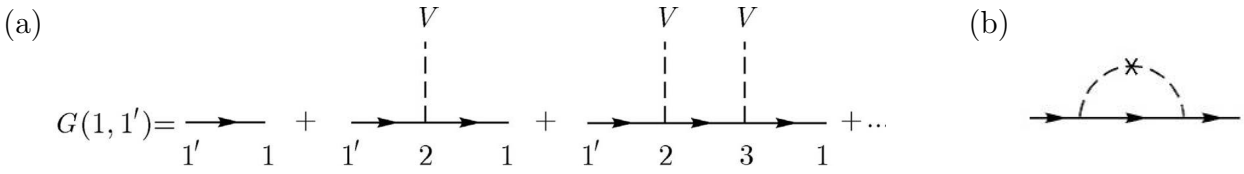

Figure 1: (a) Perturbative expansion of the GF in the potential V before averaging over disorder. (b) Leading contribution to the disorder-averaged GF. The dashed line with a cross denotes the disorder correlation function $\langle V(x)V(x')\rangle_{\rm dis}$.

Let us analyze the disorder-averaged GF.

2) Explain why there are no diagrams of order $O(V^{2k+1})$ in the disorder-averaged Green's function.

3) Draw all possible diagrams of order $O(V^4)$; compare their structure with the diagrammatic expansion of the GF in the electron interactions.
Hint: You have to look at the 2nd order in the interaction.

4) Single out the self-energy from the leading diagram, Fig. 1(b), write down the corresponding analytical expression, calculate the integrals, do the analytic continuation, and show that

$$\bar{G}^{R/A}(\omega,k) \equiv \langle G^{R/A}(\omega,k)\rangle_{\rm dis} \simeq \frac{1}{\omega - \xi_k \pm i/2\tau_{\rm ei}}. \tag{5}$$

5) Explain the physical meaning of $\mathrm{Im}(\Sigma)$ in Eq. (5).

6) Which series of diagrams is taken into account in Fig. 1(a).

Now we will use the disorder-averaged GFs to calculate the longitudinal conductivity using the Kubo formula

$$\sigma_{xx}(\omega) = \frac{1}{-i\omega}\left(\lim_{\mathbf{q}\to 0}\chi^R_{j_x,j_x}(\mathbf{q},\omega) + e^2 n/m\right), \tag{6}$$

where $\chi^R_{j_x,j_x}(\mathbf{q},\omega)$ is the retarded current-current correlation function, and e, n, m appearing in the diamagnetic term are the electron charge, density, and mass, respectively. To obtain χ^R, we have to derive the current auto-correlation function on the imaginary frequency axis,

$$\chi_{j_x,j_x}(\mathbf{q},i\Omega_n) = -\frac{1}{V}\int_0^\beta d\tau e^{i\Omega_n\tau}\langle \hat{T}_\tau j_x(\mathbf{q},\tau) j_x(-\mathbf{q},0)\rangle, \tag{7}$$

and do the analytic continuation $i\Omega_n \to \omega + i0^+$. For electrons with dispersion $\varepsilon_k = k^2/(2m)$ the current operator in second quantization takes the form

$$\mathbf{j}(\mathbf{q}) = \frac{e}{2m}\sum_{\mathbf{k}}(2\mathbf{k}+\mathbf{q})\, c^\dagger_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}}. \tag{8}$$

Let us at first find more convenient expressions before disorder averaging.

7) Insert Eq. (8) into Eq. (7) and use Wick's theorem to express the current auto-correlation function in terms of the GFs.

8) Show that in the limit $\mathbf{q} \to 0$ the disconnected part vanishes and χ_{j_x,j_x}, after summation over the spin indices, can be written as

$$\chi_{j_x,j_x}(\mathbf{q}=0, i\Omega_n) = 2e^2 \int_0^\beta d\tau e^{i\Omega_n \tau} \int \frac{d^3k}{(2\pi)^3}\, v_x^2(\mathbf{k})\, G(\tau,\mathbf{k}) G(-\tau,\mathbf{k}). \tag{9}$$

Here, $v_x(\mathbf{k}) = k_x/m$ is the x-component of the electron velocity calculated at momentum $\mathbf{k}$.

9) Do the Fourier transform and rewrite Eq. (9) via a sum over the Matsubara frequency, and draw the corresponding diagram.

10) Single out the part $\chi^R_{j_x,j_x}(\omega = 0)$, calculate it, and prove that it exactly cancels the diamagnetic term in Eq. (6).
Hints: (a) Regularize the expression by introducing $e^{i\omega_n 0^+}$ (cf. the derivation of the density by using the Green's functions);
(b) prove the (Ward) identity $v_x G^2(\mathbf{k}) = \nabla_{\mathbf{k}} G(\mathbf{k})$;
(c) use it, integrate once by parts, and single out the electron density.

11) *Advanced*: Which physical symmetry prohibits the existence of the diamagnetic term in the equation for the conductivity of normal metals?

Now we can average $\chi_{j_x,j_x}(\mathbf{q}, i\Omega_n)$ over the disorder. The classical part of this response function is given by the so-called Drude–Boltzmann approximation.

12) Consider the difference $\chi_{j_x,j_x}(i\Omega_n) - \chi_{j_x,j_x}(0)$ and substitute the disorder averaged GFs for the GFs of the free electrons. Analyze this expression and check the convergence of all integrals. Convince yourself that it is determined by pole contributions.

13) Calculate the Matsubara sum by converting it to a contour integral and keeping only those terms which yield finite pole contributions.
Hint: We consider a good metal where p_F and E_F are very large and $T, \omega \ll E_F$; this allows one to simplify the integrals in a small vicinity of the Fermi surface.

14) Change variables

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

and simplify the expression for the Drude conductivity, using the fact that the dominant contribution comes from the vicinity of the Fermi surface.

15) Calculate the angular integral and the integral over the energy ξ and show that this yields the classical Drude conductivity

$$\sigma_{xx}(\omega) \simeq \frac{e^2 n \tau_{\rm ei}}{m} \frac{1}{1 - i\omega\tau_{\rm ei}}. \tag{10}$$

16) *Advanced*: Which important diagrams are not included in the Drude–Boltzmann approximation? These diagrams describe quantum corrections to the classical conductivity (e.g. the weak-localization correction).

Discussion of the problem set on Jan. 21, 2020.