Statistical Physics & Condensed Matter Theory I: Exercise

Conductance through an Anderson impurity

The influence of interactions on electronic transport properties can be observed in many nanostructures, in particular in a so-called quantum dot, namely a spatially isolated island in and out of which electrons can tunnel. Due to its small size, the quantum dot supports discretely-spaced energy levels; considering only one of these levels for simplicity, we model the dot with the Hamiltonian

$$H_d = \sum_{\sigma=\uparrow,\downarrow} \xi_{d\sigma} d_\sigma^\dagger d_\sigma + U n_{d\uparrow} n_{d\downarrow}$$

in which $d_\sigma, d_\sigma^\dagger$ are the annihilation/creation operators for a spin-σ electron in the considered level on the dot (they obey the canonical equal-time anticommutation relations $\{d_\sigma, d_{\sigma'}^\dagger\} = \delta_{\sigma\sigma'}$), $\xi_{d\sigma} = \varepsilon_{d\sigma} - \mu$ is the on-site energy (including chemical potential shift set by a gate voltage), $n_{d\sigma} \equiv d_\sigma^\dagger d_\sigma$ and U is a Hubbard-like repulsive interaction which is counted if the dot is doubly occupied.

To investigate transport properties through the dot, we put two conducting leads to the left and right. These leads are described by the Hamiltonians (in which the index k can be thought of as a momentum-like label)

$$H_l = \sum_{k\sigma} \xi_k l_{k\sigma}^\dagger l_{k\sigma}, \qquad H_r = \sum_{k\sigma} \xi_k r_{k\sigma}^\dagger r_{k\sigma},$$

in which $l_{k\sigma}, l_{k\sigma}^\dagger$ are the annihilation/creation operators for fermions in the left lead, which obey the canonical equal-time anticommutation relations $\{l_{k\sigma}, l_{k'\sigma'}^\dagger\} = \delta_{kk'}\delta_{\sigma\sigma'}$, and $r_{k\sigma}, r_{k\sigma}^\dagger$ are the corresponding ones for the right lead. For simplicity, we have taken the set of one-body energies ξ_{lk}, ξ_{rk} to be the same in the left and right leads $\xi_{lk} = \xi_{rk} \equiv \xi_k$, and are neglecting any interaction effects in the leads.

Since they are in close proximity, the leads and the dot hybridize, meaning that electrons can effectively hop from/to leads to/from dot. This is modelled using the tunneling Hamiltonian

$$H_t = H_{ld} + H_{rd} = \sum_{k\sigma} \left[t_l l_{k\sigma}^\dagger d_\sigma + t_l^* d_\sigma^\dagger l_{k\sigma} \right] + \sum_{k\sigma} \left[t_r r_{k\sigma}^\dagger d_\sigma + t_r^* d_\sigma^\dagger r_{k\sigma} \right]$$

in which t_l and t_r are complex amplitudes quantifying the intensity of the hopping. The whole setup, whose full Hamiltonian is thus $H = H_d + H_l + H_r + H_t$, is illustrated in Fig. AndersonDot 1.

The leads will act as reservoirs for electrons: putting the leads at different chemical potentials (voltage), electrons will tend to hop from one lead to the dot and then to the other lead, leading to an observable current. Since the dot can only accommodate up to two electrons at a time, and since the electrons are strongly interacting when they sit on the dot, this current will be a complicated function of the applied voltages, interaction U and tunneling coefficients. This exercise aims at calculating the so-called conductance through the dot.

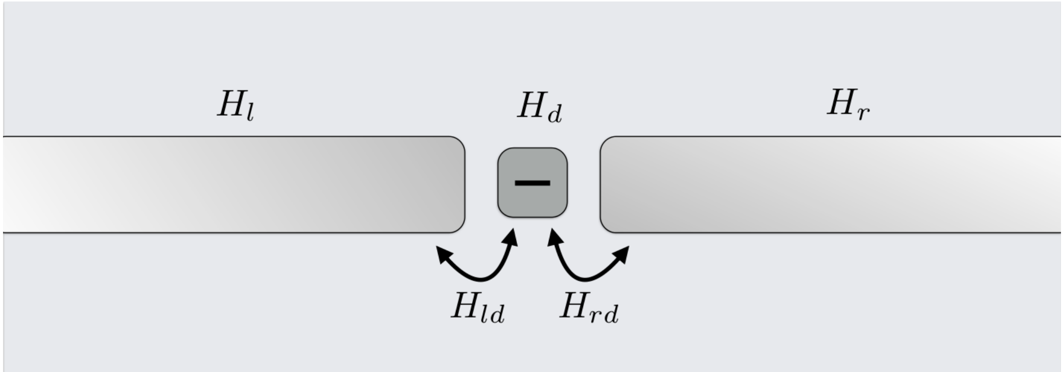

Figure 1: Cartoon of the experimental setup for measuring the conductance through an Anderson-type impurity. The left and right leads, on which a finite (static) voltage difference is applied to drive the current, couple to the dot via the tunneling Hamiltonians $H_{ld} + H_{rd}$. On the dot itself, a single level is available, with a Hubbard-type interaction energy cost U for double occupancy. The dot has a chemical potential set by a gate voltage. `AndersonDot`

a) The (particle number) current going into the left lead can be written as the time derivative of the total number of electrons in the left lead,

$$I_l = \frac{d}{dt}N_l = i\,[H, N_l]\,, \qquad N_l \equiv \sum_{k\sigma} l^\dagger_{k\sigma} l_{k\sigma}.$$

Show explicitly that

$$I_l = J_l + J_l^\dagger, \quad \text{where} \quad J_l \equiv -it_l \sum_{k\sigma} l^\dagger_{k\sigma} d_\sigma.$$

Note (you don't need to rederive this, it's obvious) that this implies the similar-looking formula

$$I_r = \frac{d}{dt}N_r = J_r + J_r^\dagger, \quad \text{where} \quad J_r \equiv -it_r \sum_{k\sigma} r^\dagger_{k\sigma} d_\sigma$$

which will be of use later on.

b) It is possible to choose a smart basis for our fermions. Namely, in each fixed k, σ subsector, let us define the unitary transformation $\boldsymbol{U}$ into even and odd combinations (u, v are parameters to be determined later; they do not depend on k, σ)

$$\begin{pmatrix} e_{k\sigma} \\ o_{k\sigma} \end{pmatrix} \equiv \boldsymbol{U} \begin{pmatrix} l_{k\sigma} \\ r_{k\sigma} \end{pmatrix} = \begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix} \begin{pmatrix} l_{k\sigma} \\ r_{k\sigma} \end{pmatrix}, \qquad |u|^2 + |v|^2 = 1.$$

Since this tranformation is by definition unitary, the $e_{k\sigma}$ and $o_{k\sigma}$ obey canonical equal-time anticommutation relations $\{e_{k\sigma}, e^\dagger_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}$ and similarly for $o_{k\sigma}$, with e and o operators having trivial (vanishing) anticommutation relations with each other. The lead Hamiltonians thus naturally preserve their form under this transformation,

$$H_l + H_r = H_e + H_o, \qquad H_e = \sum_{k\sigma} \xi_k e^\dagger_{k\sigma} e_{k\sigma}, \quad H_o = \sum_{k\sigma} \xi_k o^\dagger_{k\sigma} o_{k\sigma}.$$

Show that a smart choice of the parameters u, v (which you are asked to give explicitly) turns the tunneling Hamiltonian into the particularly simple form

$$H_t = H_{ld} + H_{rd} = \sum_{k\sigma} \bar{t} \left[e^\dagger_{k\sigma} d_\sigma + d^\dagger_\sigma e_{k\sigma} \right], \qquad \bar{t} \equiv \sqrt{|t_l|^2 + |t_r|^2},$$

in other words that the tunneling Hamiltonian only involves the even and impurity fermion modes, but not the odd ones.

c) Let us now apply a perturbation in the form of a static voltage difference between the leads. A time-independent current will develop, which we define as $I = I_l$. Note however that in this time-independent situation, we must have $I_l = -I_r$ by charge conservation (the dot cannot accumulate charge). Therefore, we are entitled to equivalently consider any linear combination of the form

$$I = \alpha I_l - (1-\alpha) I_r.$$

Show that under a judicious choice of the free parameter α (which you are asked to give explicitly), we can write the current operator in terms of the impurity modes d and the odd fermion modes o only,

$$I = J + J^\dagger, \qquad J \equiv i\tilde{t} \sum_{k\sigma} o^\dagger_{k\sigma} d_\sigma, \qquad \tilde{t} \equiv \frac{t_l t_r}{\bar{t}}.$$

d) Let us now treat the voltage difference between the leads perturbatively using linear response theory. Our starting point is the retarded current-current correlation function,

$$\mathcal{C}^{II}_{ret}(t) \equiv -i\theta(t)\langle [I(t), I(0)] \rangle$$

where the average is taken using the full unperturbed Hamiltonian $H = H_d + H_e + H_o + H_t$ for $\xi_{lk} = \xi_{rk} \equiv \xi_k$ (in the unperturbed system, the leads are at same voltage).

Using the following definitions of the 'greater' and 'lesser' Green's functions of the odd electrons and of the impurity (*careful with the time arguments!*),

$$\mathcal{G}^{o,>}_{k\sigma}(t_1 - t_2) \equiv -i\langle o_{k\sigma}(t_1) o^\dagger_{k\sigma}(t_2)\rangle, \qquad \mathcal{G}^{o,<}_{k\sigma}(t_1 - t_2) \equiv i\langle o^\dagger_{k\sigma}(t_2) o_{k\sigma}(t_1)\rangle,$$
$$\mathcal{G}^{d,>}_{\sigma}(t_1 - t_2) \equiv -i\langle d_{\sigma}(t_1) d^\dagger_{\sigma}(t_2)\rangle, \qquad \mathcal{G}^{d,<}_{\sigma}(t_1 - t_2) \equiv i\langle d^\dagger_{\sigma}(t_2) d_{\sigma}(t_1)\rangle,$$

show that the retarded current-current function can be written as

$$\mathcal{C}^{II}_{ret}(t) = -i\theta(t) \sum_{k\sigma} |\tilde{t}|^2 \left[\mathcal{G}^{o,<}_{k\sigma}(-t)\mathcal{G}^{d,>}_{\sigma}(t) - \mathcal{G}^{o,>}_{k\sigma}(-t)\mathcal{G}^{d,<}_{\sigma}(t) - (t \to -t) \right].$$

For future reference, the conductance G which we will want to calculate is defined by the zero-frequency limit of the (time) Fourier transform of $\mathcal{C}^{II}_{ret}$,

$$G \equiv \lim_{\omega \to 0} \frac{-e^2}{\omega} \mathrm{Im}\, \mathcal{C}^{II}_{ret}(\omega), \qquad \mathcal{C}^{II}_{ret}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \mathcal{C}^{II}_{ret}(t).$$

N.B.: INFO BLOCK !!!
You can use the equations in this greyed-out part without rederivation.

The retarded current-current function can be Fourier transformed to frequency space as follows. Using the facts that

$$[\mathcal{G}^{o,>}(t)]^* = [-i\langle o(t) o^\dagger(0)\rangle]^* = i\langle o(0) o^\dagger(t)\rangle = -\mathcal{G}^{o,>}(-t), \qquad [\mathcal{G}^{o,<}(t)]^* = -\mathcal{G}^{o,<}(-t)$$

and similar-looking equations for $\mathcal{G}^d$, it can easily be shown that

$$\mathrm{Im}(\mathcal{C}^{II}_{ret}(\omega)) = \frac{-1}{2} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{k\sigma} |\tilde{t}|^2 \left[\mathcal{G}^{o,<}_{k\sigma}(-t)\mathcal{G}^{d,>}_{\sigma}(t) - \mathcal{G}^{o,>}_{k\sigma}\mathcal{G}^{d,<}_{\sigma}(t) - (t \to -t) \right].$$

Using the conventions

$$\mathcal{G}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \mathcal{G}(\omega), \qquad \mathcal{G}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \mathcal{G}(t),$$

leads after simple manipulations to

$$\text{Im}\ \mathcal{C}^{II}_{ret}(\omega) = -\frac{|\tilde{t}|^2}{2}\sum_{k\sigma}\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\left\{\mathcal{G}^{o,<}_{k\sigma}(\omega_1)\left[\mathcal{G}^{d,>}_{\sigma}(\omega_1+\omega) - \mathcal{G}^{d,>}_{\sigma}(\omega_1-\omega)\right]\right.$$
$$\left. -\mathcal{G}^{o,>}_{k\sigma}(\omega_1)\left[\mathcal{G}^{d,<}_{\sigma}(\omega_1+\omega) - \mathcal{G}^{d,<}_{\sigma}(\omega_1-\omega)\right]\right\}.$$

Making use of the following identities relating the greater/lesser Green's functions to the spectral function

$$\mathcal{G}^{>}(\omega) = -i(1-n_F(\omega))A(\omega), \qquad \mathcal{G}^{<}(\omega) = in_F(\omega)A(\omega),$$

in which $n_F(\omega) = \frac{1}{e^{\beta\omega}+1}$ is the usual Fermi-Dirac distribution, the imaginary part of the retarded current-current function can then be rewritten as

$$\text{Im}\ \mathcal{C}^{II}_{ret}(\omega) = \frac{|\tilde{t}|^2}{2}\sum_{k\sigma}\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}A^{o}_{k\sigma}(\omega_1)\left\{A^{d}_{\sigma}(\omega_1+\omega)[n_F(\omega_1+\omega)-n_F(\omega_1)] - (\omega\to-\omega)\right\}.$$

e) At this point, you should notice the truly remarkable fact that Im $\mathcal{C}^{II}_{ret}(\omega)$ is given by correlations of the *odd* fermions and impurity ones. Remember that we had shown earlier that only the *even* fermions couple to the dot! Therefore, the odd fermions still are described by the free Hamiltonian $H_o = \sum_{k\sigma}\xi_k o^{\dagger}_{k\sigma}o_{k\sigma}$, and they do not couple to the rest of the system.

Show that the retarded Green's function of the odd fermions is

$$\mathcal{G}^{o,ret}_{k\sigma}(\omega) = \frac{1}{\omega - \xi_k + i\eta}.$$

You can do this either by using the Matsubara formulation of the functional field integral to calculate the imaginary-time function $\mathcal{G}^{o}_{k\sigma}(i\omega_n) \equiv \langle\bar{\psi}_{k\sigma n}\psi_{k\sigma n}\rangle$ (performing the substitution $i\omega_n \to \omega + i\eta$ at the end of the calculation) or by calculating this function 'canonically' from its definition

$$\mathcal{G}^{o,ret}_{k\sigma}(t) = -i\theta(t)\langle\left\{o_{k\sigma}(t), o^{\dagger}_{k\sigma}(0)\right\}\rangle$$

and Fourier transforming the result using the conventions $\mathcal{G}^{ret}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t - \eta|t|}\mathcal{G}^{ret}(t)$ (including a convergence factor $\eta\to 0^+$).

f) Using the relationship between the retarded function and the spectral function

$$A(\omega) = -2\text{Im}\ \mathcal{G}^{ret}(\omega)$$

and the relation Im $\frac{1}{\omega-\xi+i\eta} = -\pi\delta(\omega-\xi)$ coming from the Dirac identity, simplify the imaginary part of the current-current function to

$$\text{Im}\ \mathcal{C}^{II}_{ret}(\omega) = \frac{|\tilde{t}|^2}{2}\sum_{k\sigma}\left\{A^{d}_{\sigma}(\xi_k+\omega)\left[n_F(\xi_k+\omega)-n_F(\xi_k)\right] - A^{d}_{\sigma}(\xi_k-\omega)\left[n_F(\xi_k-\omega)-n_F(\xi_k)\right]\right\}.$$

Show that the conductance itself (see again the definition given earlier in d) is given by

$$G = e^2\sum_{k\sigma}|\tilde{t}|^2 A^{d}_{\sigma}(\xi_k)\left[-\frac{\partial n_F(\xi)}{\partial\xi}\right]\Bigg|_{\xi_k}.$$

The conductance is thus a direct measurement of the spectral function of electrons on the dot.

g) Let us now turn to the problem of calculating $A^d_\sigma(\omega)$. The leftover part of our Hamiltonian (H_o has been dealt with and is thus ignored from now on) is

$$H = H_d + H_e + H_t = \sum_\sigma \xi_{d\sigma} d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} \xi_k e^\dagger_{k\sigma} e_{k\sigma} + \sum_{k\sigma} \left[\bar{t}\, e^\dagger_{k\sigma} d_\sigma + \bar{t}^* d^\dagger_\sigma e_{k\sigma} \right].$$

Let us now consider the functional field integral representation for this Hamiltonian (directly in the Matsubara representation). Introducing Grassmann coherent states $\psi_{k\sigma n}, \bar{\psi}_{k\sigma n}$ for the even fermion modes (n is thus the Matsubara frequency index), and $\phi_{\sigma n}, \bar{\phi}_{\sigma n}$ for the impurity modes, we can write the partition function as

$$\mathcal{Z} = \int \mathcal{D}(\bar{\phi}, \phi) \int \mathcal{D}(\bar{\psi}, \psi) e^{-S_d - S_e - S_t}$$

in which

$$S_d[\bar{\phi}, \phi] \equiv \sum_{\sigma n} \bar{\phi}_{\sigma n} \left[-i\omega_n + \xi_{d\sigma} \right] \phi_{\sigma n} + \frac{U}{\beta} \sum_{n,n',m} \bar{\phi}_{\uparrow n+m} \bar{\phi}_{\downarrow n'-m} \phi_{\downarrow n'} \phi_{\uparrow n},$$

$$S_e[\bar{\psi}, \psi] \equiv \sum_{k\sigma n} \bar{\psi}_{k\sigma n} \left[-i\omega_n + \xi_k \right] \psi_{k\sigma n}, \qquad S_t[\bar{\psi}, \psi; \bar{\phi}, \phi] \equiv \sum_{k\sigma n} \left[\bar{t}\, \bar{\psi}_{k\sigma n} \phi_{\sigma n} + \bar{t}^* \bar{\phi}_{\sigma n} \psi_{k\sigma n} \right].$$

The even modes appear as bilinears; show that they can be 'integrated out', yielding the effective theory for the impurity modes

$$e^{-S_d[\bar{\phi},\phi]} \int \mathcal{D}(\bar{\psi}, \psi) e^{-S_e[\bar{\psi},\psi] - S_t[\bar{\psi},\psi;\bar{\phi},\phi]} = C \times e^{-S_{eff}[\bar{\phi},\phi]}$$

where C is some $\phi, \bar{\phi}$-independent quantity (so we can forget about it and set it to 1 here) and

$$S_{eff}[\bar{\phi}, \phi] \equiv \sum_{\sigma n} \bar{\phi}_{\sigma n} \left[-i\omega_n + \xi_{d\sigma} + \Sigma(i\omega_n) \right] \phi_{\sigma n} + \frac{U}{\beta} \sum_{n,n',m} \bar{\phi}_{\uparrow n+m} \bar{\phi}_{\downarrow n'-m} \phi_{\downarrow n'} \phi_{\uparrow n},$$

in terms of the even electron 'self-energy' function which is defined as

$$\Sigma(i\omega_n) \equiv \sum_k \frac{|\bar{t}|^2}{i\omega_n - \xi_k}.$$

h)* The effective theory we have obtained is actually quite simple, since it only involves the impurity fermions. Let us now make the further simplifying assumption that the even electron self-energy is equal to some constant, $\Sigma(i\omega_n) \equiv \Sigma - \frac{i}{2}\Gamma$ (with $\Sigma, \Gamma \in \mathbb{R}$). Show[1] that the retarded Green's function of the impurity fermions then takes the form (here, for spin $\uparrow$, the expression for $\mathcal{C}^{d,ret}_\downarrow$ being similar)

$$\mathcal{C}^{d,ret}_\uparrow(\omega) = \frac{1 - \langle n_{d\downarrow} \rangle}{\omega - \xi_{d\uparrow} - \Sigma + \frac{i}{2}\Gamma} + \frac{\langle n_{d\downarrow} \rangle}{\omega - \xi_{d\uparrow} - U - \Sigma + \frac{i}{2}\Gamma}.$$

Show that the spectral function then is given by the sum of two Lorentzians,

$$A^d_\uparrow(\omega) = -2\text{Im}\, \mathcal{C}^{d,ret}_\uparrow(\omega) = \frac{(1 - \langle n_{d\downarrow} \rangle)\Gamma}{(\omega - \xi_{d\uparrow} - \Sigma)^2 + (\Gamma/2)^2} + \frac{\langle n_{d\downarrow} \rangle \Gamma}{(\omega - \xi_{d\uparrow} - U - \Sigma)^2 + (\Gamma/2)^2}.$$

Make a sketch of the expected conductance G as a function of $\xi_{d\uparrow}$ (thus as a function of the gate voltage applied on the dot), assuming that the interaction U and inverse lifetime $\simeq \Gamma$ take some nonzero values (you can put Σ to zero), and that the temperature is zero. Give a physical interpretation of whichever peaks you find in the conductance $G(\xi_{d\uparrow})$.

[1]Hint: consider inserting the identity $1 = (1 - n_{d\downarrow}) + n_{d\downarrow}$ in the correlation function for the spin-up impurity modes, and using the fact that $1 - n_{d\downarrow}$ projects onto the subspace with $n_{d\downarrow} = 0$, and that $n_{d\downarrow}$ projects onto the subspace with $n_{d\downarrow} = 1$.