Übungen zur Theorie der Kondensierten Materie II SS 18

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1. The Green's functions $G_l^<(t-t')$ and $G_l^>(t-t')$ (30 Points)

In the lecture you encountered the retarded, advanced and causal Green's functions G^r, G^a, G^c. Here we will introduce two further Green's functions that will be useful in the second problem below.
We restrict ourselves to fermions and assume that the Hamiltonian of the problem respects homogeneity in time. The two new Green's functions are defined as

$$\begin{aligned} G^>_{\alpha,\beta}(t-t') &\equiv -i\langle c_\alpha(t)c^\dagger_\beta(t')\rangle = -iZ^{-1}\mathrm{tr}\left[e^{-\beta H}c_\alpha(t)c^\dagger_\beta(t')\right] \\ G^<_{\alpha,\beta}(t-t') &\equiv i\langle c^\dagger_\beta(t')c_\alpha(t)\rangle = iZ^{-1}\mathrm{tr}\left[e^{-\beta H}c^\dagger_\beta(t')c_\alpha(t)\right], \end{aligned}$$

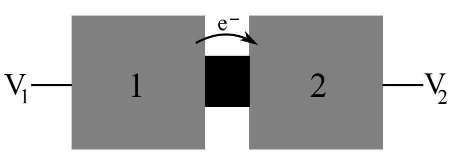
where $c_\alpha(t)$ and $c^\dagger_\beta(t)$ are respectively fermionic annihilation and creation operators in the Heisenberg picture.This defines the so-called *greater* and *lesser* Green's functions.
By carrying out the trace in the exact eigenbasis of the Hamiltonian, prove that in frequency space $G^<$ and $G^>$ are related to the retarded Green's function G^r via the relations

$$\begin{aligned} G^>_l(\omega) &= 2i(1-n_F(\omega))\mathrm{Im}\left[G^r_l(\omega)\right] \\ G^<_l(\omega) &= -2in_F(\omega)\mathrm{Im}\left[G^r_l(\omega)\right], \end{aligned}$$

where l labels a complete set of quantum states, $G^>_l(t-t') = -i\langle c_l(t)c^\dagger_l(t')\rangle$ and $n_F(\omega) = (1+e^{\beta\omega})^{-1}$ is the Fermi function. Recalling that $J_l(\omega) = -2n_F(\omega)\mathrm{Im}G^r_l(\omega)$, it is clear that these relations connect the spectral function $J_l(\omega)$ to $G^<_l(\omega)$ and $G^>_l(\omega)$.

2. Differential conductance (5 + 15 + 30 + 20 Points)

In this problem we study how the spectral function $J(\omega)$, that was introduced in the lectures, can be related to differential conductance measurements. Consider the setup shown in the figure. We have two metallic conductors 1 and 2 that are in close proximity



to each other, seperated by an insulating material (black). Upon bringing the systems to different electrostatic potentials, V_1 and V_2, an electric current will flow between the two conductors. This happens by a process where electrons tunnel between systems 1 and 2. The Hamiltonian of the combined system is given by three parts $H = H_1 + H_2 + H_T$. The first two terms characterize the two metals, whereas the third term describes the tunneling process. The quantum states in the two metallic systems are well-described by a non-interacting theory, thus we write $H_i = \sum_l (\epsilon_{i,l} + eV_i) c_{i,l}^\dagger c_{i,l}$, where l are the labels of the conductors' single-particle states, V_i is the electrostatic potential on conductor i, $i = 1, 2$. Also $c_{i,l}^\dagger$ and $c_{i,l}$ are fermionic creation/annihilation operators for system i and state l. The coupling between the two systems is described by the *tunneling Hamiltonian*

$$H_T = \sum_{l,m} \left[T_{l,m} c_{1,l}^\dagger c_{2,m} + T_{m,l}^* c_{2,m}^\dagger c_{1,l} \right].$$

In the following we want to calculate the tunneling current I that flows between the two conductors as a result of the potential difference $V = V_2 - V_1$. Then we will relate the so-called *differential conductance* $\frac{dI}{dV}$ to the spectral function $J(\omega)$.

(a) Check that the total Hamiltonian H is Hermitian. Why is this important? (1 pt.)

(b) The current between the conductors can be calculated as the rate of change of the number of occupied states of either conductor. The total number of occupied states of system 1 is $N_1(t) = \sum_l c_{1,l}^\dagger(t) c_{1,l}(t)$, where we work in the Heisenberg picture. Using the Heisenberg equation of motion, show that

$$I \equiv \frac{d}{dt} N_1(t) = -i \sum_{l,m} \left[T_{l,m} c_{1,l}^\dagger c_{2,m} - T_{m,l}^* c_{2,m}^\dagger c_{1,l} \right]$$

and interpret the two terms. (3 pts.)

(c) We are interested in the thermal average of this operator, i.e. $\langle I(t) \rangle$. We will assume that the tunneling barrier between the metals is so high that the $T_{l,m}$ can all be considered small. In this case the Kubo formula, that was derived in the lectures, can be applied with H_T being the perturbation. The Kubo formula in this case reads

$$\langle I(t) \rangle = -i \int_{-\infty}^{\infty} dt' \theta(t - t') \langle [I(t), H_T(t')] \rangle_0,$$

where all operators are expressed in the Heisenberg picture with $H_1 + H_2$ as Hamiltonian.
Insert the expressions for I and H_T into this formula and obtain

$$\langle I(t) \rangle = 2\mathrm{Re} \int_{-\infty}^{\infty} dt'' \theta(-t'') \sum_{lm} |T_{lm}|^2 e^{ieVt''} \left[G_{1,l}^>(-t'') G_{2,m}^<(t'') - G_{1,l}^<(-t'') G_{2,m}^>(t'') \right],$$

where $G_{i,m}^>(t) = -i \langle c_{i,m}(t) c_{i,m}^\dagger(0) \rangle$ etc. You will need to use the so called Wick theorem, which says that mean values of four, or more creators and annihilators can be written in terms products of mean values of two operators. For our purposes you will need to use the identities (special case!)

$$\begin{aligned}
\left\langle c_{2,m}^\dagger(t)\, c_{1,l}(t)\, c_{1,j}^\dagger(t')\, c_{2,k}(t') \right\rangle_0 &= \left\langle c_{2,m}^\dagger(t)\, c_{2,k}(t') \right\rangle_0 \left\langle c_{1,l}(t)\, c_{1,j}^\dagger(t') \right\rangle_0 \\
\left\langle c_{1,j}^\dagger(t')\, c_{2,k}(t')\, c_{2,m}^\dagger(t)\, c_{1,l}(t) \right\rangle_0 &= \left\langle c_{1,j}^\dagger(t')\, c_{1,l}(t) \right\rangle_0 \left\langle c_{2,k}(t')\, c_{2,m}^\dagger(t) \right\rangle_0 .
\end{aligned}$$

Transform $\langle I(t)\rangle$ to frequency space and use the relation derived in problem 1 to replace the Green's functions by $J_l^{(i)}(\omega)$, where i refers to system 1 or 2. Obtain the formula

$$\langle I(t)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_{l,m} |T_{l,m}|^2 \frac{J_l^{(1)}(\omega)}{n_F(\omega)} \frac{J_m^{(2)}(\omega+eV)}{n_F(\omega+eV)} \left[n_F(\omega+eV) - n_F(\omega)\right]$$

as the final result. (5 pts.)

(d) Finally we come to the conductance $\frac{dI}{dV}$. Let us assume that system 2 has a constant density of states. In this case $\frac{J_m^{(2)}(\omega+eV)}{n_F(\omega+eV)}$ does not vary much with V. In carrying out the derivative with respect to V we can treat this factor as a constant. Also ignore the l dependence of $\sum_m |T_{l,m}|^2$. Argue that at low temperatures the relation

$$\frac{dI}{dV} \propto \sum_l J_l^{(1)}(-eV)$$

holds. (3 pts.)

Thus by measuring dI/dV for varying V the spectral function of system 1 can be determined.