University of Regensburg Summer Semester 2008

Quantum Theory of Condensed Matter

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Sheet 11

1. Tunnelling spectroscopy

The spectral function is a measure of the single particle property of a many body system. A direct measure of the spectral function can be achieved via a tunnelling experiment in which a metal (for example a Scanning Tunnelling Microscope tip) is brought in tunnelling contact with a sample and, by applying a bias voltage (V) current is driven from the metal through the sample (see Fig.1). The derivative of the current with respect of the voltage is proportional to the spectral function of the sample as you will derive in this exercise.

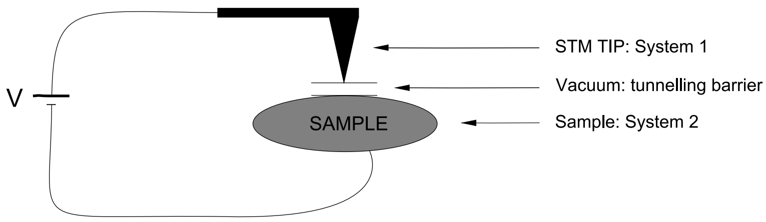

Fig.1

In order to model the experimental set up sketched in Figure 1 consider the following Hamiltonian:

$$H = \sum_k (\varepsilon_k - eV) c^\dagger_{1k} c_{1k} + \sum_i \varepsilon_i c^\dagger_{2i} c_{2i} + \sum_{ki} \left(T_{ki} c^\dagger_{1k} c_{2i} + T^*_{ki} c^\dagger_{2i} c_{1k} \right)$$

where for simplicity we have omitted the spin degree of freedom which is not playing any particular role in the calculation. The subscripts 1 and 2 indicate the system 1 and 2 respectively.

- Calculate the current operator as the derivative of the number of electrons present in the STM tip. *Hint:* Use the Heisenberg pictures in which the time evolution is associated to the operators.
- Prove that the average current to lowest non-vanishing order in the tunnelling T_{ik} in the tunnelling can be written as:

$$\langle I \rangle (t) = \int_{t_0}^{+\infty} dt' C^r_{I\,H_T}(t,t'), \tag{1}$$

where

$$C^r_{I\,H_T}(t,t') = -i\theta(t-t')\langle [I(t), H_T(t')] \rangle_0,$$
$$H_T = \sum_{ki} \left(T_{ki} c^\dagger_{1k} c_{2i} + T^*_{ki} c^\dagger_{2i} c_{1k} \right),$$

the time development and the average $\langle \bullet \rangle_0$ are calculated with respect of $H - H_T$ and t_0 is the initial time at which all the representations coincide. Prove also that, since the Hamiltonian does not explicitly depends on time, if $t_0 \to -\infty$, then also the average current does not depend on time. Assume from now on this limit. *Hint:* Use the general expression of the Kubo formula derived in the lecture.

- Simplify the expression for the current given in (1) by evaluating the average inside the integral. You should obtain:

$$\langle I \rangle = 2\mathrm{Re} \int_{-\infty}^{0} dt' \sum_{ik} |T_{ik}|^2 \left[G_{1k}^{>}(-t') G_{2i}^{<}(t') - G_{1k}^{<}(-t') G_{2i}^{>}(t') \right] \tag{2}$$

  Hint: Remember that $H - H_T$ conserves the number of particles in system 1 and 2 separately. Wick's theorem is also valid, namely:

$$\langle c_{2i}^{\dagger}(t) c_{1k}(t) c_{1k}^{\dagger}(t') c_{2i}(t') \rangle_0 = \langle c_{2i}^{\dagger}(t) c_{2i}(t') \rangle_0 \, \langle c_{1k}(t) c_{1k}^{\dagger}(t') \rangle_0$$

- Prove that (2) can be rewritten in the Fourier space as:

$$\langle I \rangle = \lim_{\omega' \to 0} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \sum_{ik} |T_{ik}|^2 \left[G_{1k}^{>}(\omega) G_{2i}^{<}(\omega + \omega') - G_{1k}^{<}(\omega) G_{2i}^{>}(\omega + \omega') \right]$$

  Hint: remember that $[G_{\alpha}^{<}(t)]^* = -G_{\alpha}^{<}(-t)$ and $[G_{\alpha}^{>}(t)]^* = -G_{\alpha}^{>}(-t)$.

- Eventually insert the relations between the Green's functions and the spectral functions:

$$\begin{aligned}
G_{2i}^{<}(\omega) &= \imath A_2(\varepsilon_i, \omega) n_F(\omega) \\
G_{2i}^{>}(\omega) &= -\imath A_2(\varepsilon_i, \omega)[1 - n_F(\omega)] \\
G_{1k}^{<}(\omega) &= \imath A_1(\varepsilon_k - eV, \omega) n_F(\omega - eV) \\
G_{1k}^{>}(\omega) &= -\imath A_1(\varepsilon_k - eV, \omega)[1 - n_F(\omega - eV)]
\end{aligned}$$

  which you can check using the Lehmann representation for the Green's functions. With the observation that the spectral function for the system 1 (the metal) is a delta function and we assume a weak dependence of the tunnelling amplitude on the sample quantum number i, prove that you will obtain:

$$\langle I \rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} K A_2(\varepsilon_i, \omega)[n_F(\omega) - n_F(\omega - eV)]$$

  where $K = \sum_k |T_{ik}|^2 \delta(\varepsilon_k - eV - \omega)$ is a constant. Which is the sign of the current that you just calculated for a positive bias? Can you explain why?

- Calculate the limit $T \to 0$ of the differential conductance $G(V) \equiv \frac{d\langle I \rangle}{dV}$ thus proving that it is a direct mesure of the spectral function for the sample (system 2).

Frohes Schaffen!