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Advanced Condensed Matter Theory — SS10

Exercise 7

7.1 Tunnel current (25 points)

In the lecture, it was mentioned that one can measure the local density of states (DOS) of a substrate by performing a scanning tunneling microscope experiment. In this exercise, we will derive an elementary relation between the DOS and the measured dI/dV signal. For that purpose, consider the model Hamiltonian (see Fig. 1)

$$\begin{aligned}
\mathcal{H} &= \sum_{\mathbf{k}} (\epsilon_{\mathrm{T}}(\mathbf{k}) - \mu_{\mathrm{T}})\, c^{\dagger}_{\mathbf{k},\mathrm{T}}\, c_{\mathbf{k},\mathrm{T}} + \sum_{\mathbf{k}} (\epsilon_{\mathrm{S}}(\mathbf{k}) - \mu_{\mathrm{S}})\, c^{\dagger}_{\mathbf{k},\mathrm{S}}\, c_{\mathbf{k},\mathrm{S}} \\
&\quad + \sum_{\mathbf{k},\mathbf{k}'} \left(t_{\mathbf{k}\mathbf{k}'}\, c^{\dagger}_{\mathbf{k},\mathrm{T}}\, c_{\mathbf{k}',\mathrm{S}} + t^{*}_{\mathbf{k}\mathbf{k}'}\, c^{\dagger}_{\mathbf{k}',\mathrm{S}}\, c_{\mathbf{k},\mathrm{T}} \right) \\
&\equiv \mathcal{H}_T + \mathcal{H}_S + \mathcal{H}_{hyb} \\
&\equiv \mathcal{H}_0 + \mathcal{H}_{hyb}
\end{aligned} \tag{1}$$

The indices S and T denote the substrate and the tip, respectively.

a) The current flowing between tip and substrate is given by

$$I(t) = e_0 \frac{dN_{\mathrm{S}}}{dt}(t) = -e_0 \frac{dN_{\mathrm{T}}}{dt}(t), \qquad N_{\mathrm{S(T)}}(t) = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\mathrm{S(T)}}(t)\, c_{\mathbf{k},\mathrm{S(T)}}(t)$$

where here the operators are represented in the Heisenberg representation. In the Heisenberg representation the equation of motion is given by the *time-independent* Hamiltonian as

$$\frac{dN_{\mathrm{S}}}{dt}(t) = -i \left[N_{\mathrm{S(T)}}(t), \mathcal{H} \right]$$

Use the Heisenberg equation of motion to derive

$$\langle I(t) \rangle = e_0 \mathrm{i} \sum_{\mathbf{k},\mathbf{k}'} \left(t_{\mathbf{k}'\mathbf{k}}\, \langle c^{\dagger}_{\mathbf{k}',\mathrm{T}}(t)\, c_{\mathbf{k},\mathrm{S}}(t) \rangle - t^{*}_{\mathbf{k}'\mathbf{k}}\, \langle c^{\dagger}_{\mathbf{k},\mathrm{S}}(t)\, c_{\mathbf{k}',\mathrm{T}}(t) \rangle \right).$$

b) Show that in leading order of the tunneling amplitude the current expectation value finally reads

$$\begin{aligned}
\langle I(t) \rangle &= e_0 \sum_{\mathbf{k},\mathbf{k}'} \left| t_{\mathbf{k}'\mathbf{k}} \right|^2 \int_{-\infty}^{\infty} dt' \Big(\langle c^{\dagger}_{\mathbf{k}',\mathrm{T}}(t)\, c_{\mathbf{k},\mathrm{S}}(t) c^{\dagger}_{\mathbf{k},\mathrm{S}}(t')\, c_{\mathbf{k}',\mathrm{T}}(t') \rangle_0 \\
&\qquad - \langle c^{\dagger}_{\mathbf{k},\mathrm{S}}(t)\, c_{\mathbf{k}',\mathrm{T}}(t) c^{\dagger}_{\mathbf{k}',\mathrm{T}}(t')\, c_{\mathbf{k},\mathrm{S}}(t') \rangle_0 \Big) \\
&\equiv I_{\mathrm{S}\to\mathrm{T}} - I_{\mathrm{T}\to\mathrm{S}}.
\end{aligned}$$

Hint: Remind yourselves of the section on linear response theory in Theoretical Condensed Matter Theory last semester. There you learned that, we can derive the response function of a system to an external perturbation $\mathcal{H}_{hyb}$ via the formula (using our problem Hamiltonian as an example)

$$\langle I(t) \rangle \quad = \quad -ie_0 \int_{-\infty}^{\infty} dt' \ \langle \left[\dot{N}_S(t), \mathcal{H}_{hyb}(t') \right] \rangle_0 \tag{2}$$

Here we stress that the operators $\dot{N}_S(t)$ and $\mathcal{H}_{hyb}(t')$ are now in the *interaction* representation, i.e., $\dot{N}_S(t) \equiv e^{i\mathcal{H}_0 t} N_S e^{-i\mathcal{H}_0 t}$, and the same for $\mathcal{H}_{hyb}(t')$. Also, the notation $\langle \cdots \rangle_0$ denotes taking the average value over the ground state. Now the reason for the fact that we have now our operators in the *interaction* representaion is due to the derivation of the linear response formula itself, in the following way: lets assume we want to derive the *current response* operator $J(\mathbf{r}, t)$ from the *current* operator $j(\mathbf{r}, t)$ (the explicit form of the respective operators does not concern us here; this is only an illustrative example)

$$\begin{aligned} J(\mathbf{r}, t) &= \langle \psi' \mid e^{i\mathcal{H}t} j(\mathbf{r}) e^{-i\mathcal{H}t} \mid \psi' \rangle \\ &= \langle \psi' \mid e^{i(\mathcal{H}_0 + \mathcal{H}_{hyb})t} j(\mathbf{r}) e^{-i(\mathcal{H}_0 + \mathcal{H}_{hyb})t} \mid \psi' \rangle \end{aligned}$$

where $\mid \psi' \rangle$ is the wave function at $t = 0$ for an *interacting* system (with the full $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{hyb}$ involved, where $\mathcal{H}_{hyb}$ is again a perturbation part). Now we also know that

$$\begin{aligned} e^{-i(\mathcal{H}_0 + \mathcal{H}_{hyb})t} &= e^{-it\mathcal{H}_0} U(t) \\ \Rightarrow U(t) &= e^{-it\mathcal{H}_0} e^{-i(\mathcal{H}_0 + \mathcal{H}_{hyb})t} \\ \Rightarrow J(\mathbf{r}, t) &= \langle \psi' \mid U^\dagger(t) e^{i\mathcal{H}_0 t} j(\mathbf{r}) e^{-i\mathcal{H}_0 t} U(t) \mid \psi' \rangle \end{aligned}$$

where $U(t) = T \exp \left[-i \int_0^t dt' \mathcal{H}_{hyb}(t') \right]$ is the well-known time development operator, T the time-ordering operator. Now since $\mid \psi' \rangle = T \exp \left[-i \int_{-\infty}^{0} dt' \mathcal{H}_{hyb}(t') \right] \mid \psi \rangle$, with $\mid \psi \rangle$ denoting the ground state we see also that $U(t) \mid \psi' \rangle = T \exp \left[-i \int_{-\infty}^{t} dt' \mathcal{H}_{hyb}(t') \right] \mid \psi \rangle \equiv S(t, -\infty) \mid \psi \rangle$. Now we can rewrite

$$\begin{aligned} J(\mathbf{r}, t) &= \langle \psi' \mid U^\dagger(t) e^{i\mathcal{H}_0 t} j(\mathbf{r}) e^{-i\mathcal{H}_0 t} U(t) \mid \psi' \rangle \\ &= \langle \psi \mid S^\dagger(t, -\infty) j(\mathbf{r}, t) S(t, -\infty) \mid \psi' \rangle \end{aligned}$$

where $j(\mathbf{r}, t)$ is now in the *interaction* picture. Expanding $S(t, -\infty)$ up to 1st order in $\mathcal{H}_{hyb}$ and resubstituting it we see that

$$\begin{aligned} J(\mathbf{r}, t) &= \langle \psi \mid S^\dagger(t, -\infty) j(\mathbf{r}, t) S(t, -\infty) \mid \psi \rangle \\ &= \langle \psi \mid \left[1 + i \int_{-\infty}^{t} dt' \mathcal{H}_{hyb}(t') \right] j(\mathbf{r}, t) \left[1 - i \int_{-\infty}^{t} dt' \mathcal{H}_{hyb}(t') \right] \mid \psi \rangle \\ &= \langle \psi \mid \left[j(\mathbf{r}, t) - i \int_{-\infty}^{t} dt' \left[j(\mathbf{r}, t) \mathcal{H}_{hyb}(t') - \mathcal{H}_{hyb}(t') j(\mathbf{r}, t) \right] \right] \mid \psi \rangle \end{aligned}$$

and assuming $\langle\ \psi | j(\mathbf{r},t)\ |\ \psi\ \rangle\ = 0$ you have the expression

$$J(\mathbf{r},t) = -i \int_{-\infty}^{t} dt'\ \langle\ \psi\ |\ [j(\mathbf{r},t), \mathcal{H}_{hyb}(t')]\ |\ \psi\ \rangle$$

Therefore one starts with all the operators in the Heisenberg picture, but since we want to do the calculation with $\mathcal{H}_{hyb}$ as a perturbation, the perturbation part goes into the time evolution operator and the rest of the operators in the commutator is defined in the *interaction* picture. This final expression looks very much like (2), of course.

c) Denote the joint many body states of sample and tip by $|n, n'\rangle \equiv |n\rangle_{\mathrm{T}} |n'\rangle_{\mathrm{S}}$ to derive the spectral representation

$$\begin{aligned} I_{\mathrm{S}\to\mathrm{T}} &= \frac{2\pi e_0}{Z_{\mathrm{G}}} \sum_{\mathbf{k},\mathbf{k}'} \sum_{n,n'} \sum_{m,m'} \left| t_{\mathbf{k}'\mathbf{k}} \right|^2 \left| \langle n, n' | c^\dagger_{\mathbf{k}',\mathrm{T}} c_{\mathbf{k},\mathrm{S}} | m, m' \rangle \right|^2 \mathrm{e}^{-\beta(E_n - \mu_{\mathrm{T}})}\, \mathrm{e}^{-\beta(E_{n'} - \mu_{\mathrm{S}})} \\ &\quad \times \delta(E_n + E_{n'} - E_m - E_{m'}) \end{aligned}$$

and the corresponding one for $I_{\mathrm{T}\to\mathrm{S}}$.

Show that $I_{\mathrm{S}\to\mathrm{T}}$ can be expressed as

$$I_{\mathrm{S}\to\mathrm{T}} = 2\pi e_0 \sum_{\mathbf{k},\mathbf{k}'} \left| t_{\mathbf{k}'\mathbf{k}} \right|^2 \int d\omega\, A_{\mathbf{k}',\mathrm{T}}(\omega)\, A_{\mathbf{k},\mathrm{S}}(\omega)\, f_{\mathrm{T}}(\omega)\, (1 - f_{\mathrm{S}}(\omega)),$$

where

$$f_{\mathrm{S(T)}}(\omega) = \frac{1}{\mathrm{e}^{\beta(\omega - \mu_{\mathrm{S(T)}})}}.$$

Derive also the corresponding expression for $I_{\mathrm{T}\to\mathrm{S}}$.

Hint:

- Use the definition of the spectral function from the lecture, i.e.,

$$A_{\mathbf{k},S}(\omega) = \frac{1}{Z_G^S} \sum_{n',m'} \left| \langle n' | c^\dagger_{\mathbf{k},\mathrm{S}} | m' \rangle \right|^2 (e^{-\beta \tilde{E}_{n'}} + e^{-\beta \tilde{E}_{m'}}) \delta(\omega + E_{n'} - E_{m'})$$

  and similarly for $A_{\mathbf{k}',T}(\omega)$, where $\tilde{E}_n \equiv E_n - \mu_T$, $\tilde{E}_{n'} \equiv E_{n'} - \mu_S$ inserting this into the expression for $I_{S\to T}$ given on the sheet, try to recover expression for $I_{\mathrm{S}\to\mathrm{T}}$ given above.
- $Z_G = Z_G^S \cdot Z_G^T$
- $\left| \langle n, n' | c^\dagger_{\mathbf{k}',\mathrm{T}} c_{\mathbf{k},\mathrm{S}} | m, m' \rangle \right|^2 \equiv \left| \langle n | c^\dagger_{\mathbf{k}',\mathrm{T}} | m \rangle \right|^2 \left| \langle n' | c_{\mathbf{k},\mathrm{S}} | m' \rangle \right|^2$
- The average value $\langle \cdots \rangle_0 \equiv \frac{1}{Z_G} \sum_{n,n'} \langle n, n' | e^{-\beta \mathcal{H}_0} \cdots | n, n' \rangle$

d) For simplicity, we assume $\left|t_{\mathbf{k}'\mathbf{k}}\right|^2 \approx |t|^2 = const$. Furthermore, the local density of states of the tip is typically a smooth and slowly varying function and we can approximate

$$N_{\mathrm{T}}(\omega) \;=\; \sum_{\mathbf{k}} A_{\mathbf{k},\mathrm{T}}(\omega) \;\approx\; N_0 .$$

The difference of the chemical potentials arises from the applied voltage V: $\mu_{\mathrm{T}} - \mu_{\mathrm{S}} = e_0 V$. Show that then the dI/dV-measurement is related to the local DOS of the substrate via

$$\frac{d\langle I\rangle}{dV} \;=\; e_0^2 \Gamma N_{\mathrm{S}}(\mu_{\mathrm{S}} + e_0 V), \qquad \Gamma \;=\; 2\pi N_0 |t|^2 .$$

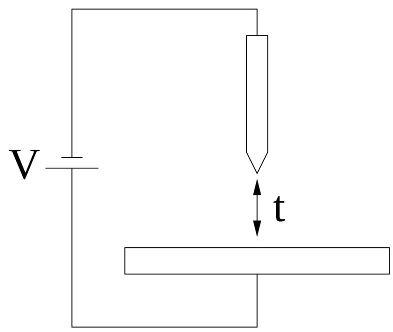

Figure 1: STM setup