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Physikalisches Institut
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Advanced Theoretical Condensed Matter Physics — SS09

Exercise 5

(Please return your solutions before Fr. 19.6.2009, 12h)

5.1. Screening in an electron gas II: Thomas-Fermi approximation and Friedel oscillations (15 points)

We will continue with our calculation of the response of an electron gas to a static impurity with charge $q_0 = e_0$ in three dimensions. On the last sheet we derived the expression for the induced change of the charge density

$$\Delta n(\mathbf{r},t) \;=\; -e_0 \int \frac{d^3q}{(2\pi)^3}\, \mathrm{e}^{-\mathrm{i}\mathbf{qr}}\, \hat{\phi}_{el}(\mathbf{q})\, \Pi(\mathbf{q}). \tag{1}$$

a) Show that according to Eq. (1), with the bare Coulomb interaction $\hat{\phi}_{\rm el}(\mathbf{q})$, the induced charge

$$\Delta Q \;=\; -e_0 \int d^3r\, \Delta n(\mathbf{r},t)$$

is infinite!

b) To obtain a physically meaningful result we must take into account the screening of the Coulomb interaction by the electron gas. For that purpose, we will re-sum the leading contributions (*random phase approximation*) to get an effective interaction

corresponding to

$$\hat{\phi}_{\rm eff}(\mathbf{q}) \;=\; \hat{\phi}_{el}(\mathbf{q}) + \hat{\phi}_{el}(\mathbf{q})e_0\Pi(\mathbf{q})\hat{\phi}_{el}(\mathbf{q}) + \hat{\phi}_{el}(\mathbf{q})e_0\Pi(\mathbf{q})\hat{\phi}_{el}(\mathbf{q})e_0\Pi(\mathbf{q})\hat{\phi}_{el}(\mathbf{q}) + \ldots$$

Replace in Eq. (1) the bare Coulomb interaction by the effective one and show that it yields

$$\Delta n(\mathbf{r},t) \;=\; -\int \frac{d^3q}{(2\pi)^3}\, \mathrm{e}^{-\mathrm{i}\mathbf{qr}} \left(\frac{1}{\kappa(\mathbf{q})} - 1\right), \tag{2}$$

with

$$\kappa(\mathbf{q}) \;=\; 1 + \frac{q_{\rm TF}^2}{q^2}\, g(q/k_{\rm F}) \quad , \qquad q_{\rm TF} \;=\; \sqrt{\frac{4e_0^2 m}{\pi} k_{\rm F}}, \qquad g(x) \;=\; \left(\frac{1}{2} + \frac{1-(x/2)^2}{2x} \ln\left|\frac{1+\frac{x}{2}}{1-\frac{x}{2}}\right|\right).$$

c) Show that the induced charge now becomes

$$\Delta Q \;=\; -e_0,$$

which shows that the additional charge at the origin becomes completely screened at large distances.

d) To get a rough estimate on the asymptotic behaviour of $\Delta n(\mathbf{r},t)$ for $r \to \infty$, we set $g(q/k_{\rm F}) \approx g(0)$ (*Thomas-Fermi approximation*). Show that this yields

$$\Delta n(\mathbf{r},t) \;\overset{r\to\infty}{\approx}\; -\frac{q_{\rm TF}^2}{4\pi}\, \frac{\mathrm{e}^{-q_{\rm TF} r}}{r}.$$

e) A careful evaluation of Eq. (2) shows that the correct result is

$$\Delta n(\mathbf{r},t) \;\overset{r\to\infty}{\approx}\; -\frac{4e_0}{\pi}\, \frac{q_{\rm TF}^2/k_{\rm F}^2}{(8 + q_{\rm TF}^2/k_{\rm F}^2)^2}\, \frac{\cos(2k_{\rm F} r)}{r^3}.$$

The long-range oscillations with wavelength $\pi/k_{\rm F}$ are called *Friedel oscillations* and arise from the presence of a sharp Fermi surface. To obtain them one has to take into account the singularity of $g(x)$, $g'(x) \approx -\delta(x-2)$. Using the asymptotics of $g(x)$ we approximate

$$\Delta n(\mathbf{r},t) \;=\; -\int \frac{d^3q}{(2\pi)^3}\, \mathrm{e}^{-\mathrm{i}\mathbf{qr}} \left(\frac{1}{\kappa(\mathbf{q})} - 1\right) \;\simeq\; q_{\rm TF}^2 \int \frac{d^3q}{(2\pi)^3}\, \mathrm{e}^{-\mathrm{i}\mathbf{qr}}\, \frac{g(q/k_{\rm F})}{q^2 + q_{\rm TF}^2}.$$

Use integration by parts and approximate

$$F(x) \;=\; \int_0^x dy\, \frac{y}{y^2 + r^2 q_{\rm TF}^2} \sin(y) \quad \Rightarrow \quad F(2k_{\rm F} r) \;\simeq\; -\frac{\cos(2k_{\rm F} r)}{r}$$

to obtain the Friedel oscillations of the density modulation.

5.2. Tunnel current (15 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)

$$\begin{aligned}\mathcal{H} \;=\; & \sum_{\mathbf{k}} (\epsilon_{\rm T}(\mathbf{k}) - \mu_{\rm T})\, c_{\mathbf{k},\rm T}^\dagger c_{\mathbf{k},\rm T} + \sum_{\mathbf{k}} (\epsilon_{\rm S}(\mathbf{k}) - \mu_{\rm S})\, c_{\mathbf{k},\rm S}^\dagger c_{\mathbf{k},\rm S} \\ & + \sum_{\mathbf{k},\mathbf{k}'} \left(t_{\mathbf{k}\mathbf{k}'}\, c_{\mathbf{k},\rm T}^\dagger c_{\mathbf{k}',\rm S} + t_{\mathbf{k}\mathbf{k}'}^*\, c_{\mathbf{k}',\rm S}^\dagger c_{\mathbf{k},\rm T} \right).\end{aligned} \tag{3}$$

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

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

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

Use the Heisenberg equation of motion to derive

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

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

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

b) 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

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

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

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

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

where

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

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

c) 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

$$\frac{d\langle I\rangle}{dV} \overset{T\to 0}{=} e_0^2 \Gamma N_{\mathrm{S}}(\mu_{\mathrm{S}} + e_0 V), \qquad \Gamma = 2\pi N_0 |t|^2.$$

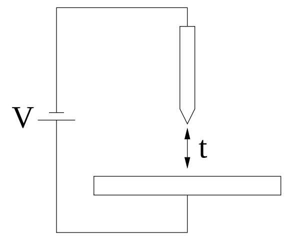

Figure 1: STM setup