LMU München
WS 2016/2017
Lehrstuhl für Theoretische Nanophysik
PD Dr. F. Heidrich-Meisner
Jan Stolpp, *Questions: jan.stolpp@physik.uni-muenchen.de*

12. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, January 27, 2017.

Exercise 1: Charge density waves

This exercise treats a very simple model of electrons in a solid which includes the possibility of an instability of the electron gas induced by Coulomb interactions. We study a one-dimensional system of spinless electrons with the Hamiltonian

$$H = -t\sum_{l=1}^{2L}(c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1}) + V\sum_{l=1}^{2L} c_{l+1}^\dagger c_{l+1} c_l^\dagger c_l. \tag{1}$$

The kinetic energy is described by the hopping matrix element $t > 0$. Of the full Coulomb interaction only the largest matrix element $V > 0$ is considered.

a. Argue why the consideration of only the largest matrix element of the Coulomb interaction leads to the Hamiltonian (1).

b. The particle number operator is defined as $N = \sum_{l=1}^{2L} c_l^\dagger c_l$. Show that the Hamilton operator Eq. (1) commutes with the particle number operator. What does that mean?

c. Calculate the groundstate energy E_0 of the non-interacting system ($V = 0$) in the thermodynamic limit. You should obtain: $\frac{E_0}{2L} = -\frac{2t}{\pi}\sin(\pi\rho)$, where $\rho = \frac{n}{2L}$ is the filling.

From here on we consider the interacting system ($V > 0$).

d. We treat the interaction in the following Hartree-Fock decomposition:

$$\hat{V} = V\sum_{l=1}^{2L}(n_{l+1}\rho_l + \rho_{l+1}n_l - \rho_l\rho_{l+1}),$$

where $\rho_l = \langle n_l\rangle$. Is this decomposition complete? Visualize the groundstate for $\rho = \frac{1}{2}$ and $\frac{V}{t} \to \infty$. From this, motivate the ansatz $\rho_{2l-1} = \rho + \delta,\ \rho_{2l} = \rho - \delta$.

e. Show that the potential term then becomes

$$\hat{V} = -2V\delta\sum_{l=1}^{L}(n_{2l-1} - n_{2l}) + 2LV(\delta^2 + \rho^2).$$

f. Next, we define operators $b_q = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} \mathrm{e}^{-iq2l} c_{2l}$ and $d_q = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} \mathrm{e}^{-iq(2l-1)} c_{2l-1}$ where $q = \frac{\pi}{L}\left[-\frac{L}{2}+1, \dots, 0, \dots, \frac{L}{2}\right]$. Putting them into the Hamiltonian you should arrive at

$$H = \sum_q \begin{pmatrix} b_q^\dagger & d_q^\dagger \end{pmatrix} \begin{pmatrix} -\Delta & \epsilon_q \\ \epsilon_q & \Delta \end{pmatrix} \begin{pmatrix} b_q \\ d_q \end{pmatrix} + 2LV(\delta^2 + \rho^2),$$

where $\Delta = -2V\delta$. Diagonalize this operator to arrive at

$$H = \sum_{q,\mu=\pm 1} E_{\mu q} g_{\mu q}^\dagger g_{\mu q} + 2LV(\delta^2 + \rho^2),$$

with $E_{\mu q} = \mu\sqrt{\epsilon_q^2 + \Delta^2}$ and $\mu = \pm 1$. Sketch $E_{\mu q}$ and interpret the parameter Δ.

g. Show that the groundstate energy of the interacting system is given by

$$\frac{E}{2L} = -\frac{1}{\pi} \int_0^{\pi\rho} \sqrt{\epsilon_q^2 + \Delta^2} dq + V(\delta^2 + \rho^2).$$

Plot the groundstate energy as a function of Δ for $\rho = \frac{1}{2}$. Which value of Δ is physically realized?

h. From the groundstate energy, calculate the defining equation for Δ: the so-called self-consistency equation

$$\Delta = \frac{1}{\pi} \int_0^{\pi\rho} \frac{2V\Delta}{\sqrt{\epsilon_q^2 + \Delta^2}} dq. \tag{2}$$

This equation always has $\Delta = 0$ as a solution. How can one interpret this case?

i. The question whether there are additional solutions as well can be answered as follows: First, one divides Eq. (2) by Δ to split off the trivial solution ($\Delta = 0$). The remaining equation can be used to derive the parameters ρ and V: One assumes that a critical curve (i.e. a critical $V_c(\rho)$) exists in the parameter space where Δ is exactly zero. This $V_c(\rho)$ can be derived from the self-consistency equation. Qualitatively, explain the two distinct regimes in parameter space. How do you interpret $V_c(\frac{1}{2})$?

j. Calculate Δ as a function of V and ρ and assure yourself that (for $V > V_c$) the solution with finite Δ really gives the lower groundstate energy.
Hint: You can check that numerically.

Exercise 2: Friedel oscillations

The static dielectric function for a three-dimensional system of free electrons is given by

$$\epsilon(\boldsymbol{q}, \omega = 0) = 1 + \frac{4e^2 m k_F}{\pi q^2} \left\{ \frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right\}. \tag{3}$$

We want to calculate the effect of a point charge at the origin ($n_a(\boldsymbol{r}) = n_{a0}\delta(\boldsymbol{r})$) on the density distribution $n(\boldsymbol{r})$. The change in the electron density distribution can be deduced from the Poisson equation:

$$\delta n(\boldsymbol{r}) = \int \frac{d^3q}{(2\pi)^3} \left\{ \frac{1}{\epsilon(\boldsymbol{q}, 0)} - 1 \right\} n_a(\boldsymbol{q}) \mathrm{e}^{i\boldsymbol{q}\boldsymbol{r}}. \tag{4}$$

a. Using partial integration show that this gives

$$\delta n(\boldsymbol{r}) = \frac{n_{a0}}{r^3} \int_0^\infty g''(q) \sin(qr) dq, \tag{5}$$

where $g(q) = \frac{q}{2\pi^2} \frac{\epsilon(q)-1}{\epsilon(q)}$.

b. Show that around $q \sim 2k_F$, the approximation

$$g''(q) \approx \frac{A}{q - 2k_F},$$

can be made.

c. Use this as well as the assumption that $k_F r \gg 1$ to arrive at the following form of the integral:

$$\delta n(r) \approx \frac{A n_{a0}}{r^3} \int_{2k_F-\Lambda}^{2k_F+\Lambda} \frac{\sin((q-2k_F)r)\cos(2k_F r) + \cos((q-2k_F)r)\sin(2k_F r)}{q - 2k_F} dq$$

with a cut-off $\Lambda \to \infty$. Why can you make the change of the integration bounds compared to Eq. (5)?

d. Solve the integral to get

$$\delta n(r) \approx \pi A n_{a0} \frac{\cos(2k_F r)}{r^3}.$$

Interpret this result.