University of Regensburg Summer Term 2018

Quantum Theory of Condensed Matter I

Prof. John Schliemann
Dr. Paul Wenk **Mo.** 08:00-10:00 c.t., PHY 5.0.21

Sheet 1

1. Non-Interacting Jellium Model .... [8P]

Consider a metal (in $3D$) of volume V at zero temperature and approximate the periodic ion distribution with the jellium model. By neglecting the electron-electron interaction:

a)(3P) Calculate the relation between the density of electrons $n = N/V$ and the Fermi wavelength k_F. *Hint:* Look at the expectation value of the particle number operator in the Fermi sea/ Fermi sphere.

b)(2P) Estimate the value of the Fermi wavelength, and Fermi energy ϵ_F for copper knowing that it is monovalent and with a typical interatomic distance of 2Å.

c)(3P) Calculate the energy of the ground state $E^{(0)}$ of the metal in the jellium model. Which is the energy per particle?

2. Perturbation Theory for Interacting Jellium .... [12P]

Now, let us consider the previous model including electron-electron interaction.

a)(3P) Due to the infinite range of the Coulomb potential the integrals appearing in this problem are divergent. However, one can solve them by adding a convergence generating factor $\exp(-\mu|\mathbf{r}-\mathbf{r}'|)$ with $\mu > 0$ and taking the limit $\mu \to 0$ in the end. With this and the general V_{int} derived in the lecture, show that the Hamiltonian which represents the electron-electron interaction is written in the *Bloch-representation* as

$$V_{\text{el}-\text{el}} = \frac{1}{2V} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}} \sum_{\sigma_1\sigma_2} \frac{e^2}{\epsilon_0 q^2} c^\dagger_{(\mathbf{k}_1+\mathbf{q})\sigma_1} c^\dagger_{(\mathbf{k}_2-\mathbf{q})\sigma_2} c_{\mathbf{k}_2\sigma_2} c_{\mathbf{k}_1\sigma_1}. \tag{1}$$

b)(3P) Show that the contributions steming from H_{++} and H_{+-}, which describe the ion-ion and the ion-electron interaction, respectively, cancel the divergent term for of $q = 0$ in Eq. (1). For simplicity you can assume that the charge density of the ions is homogeneously distributed, i.e., $n_{\text{ion}} = \textit{const}$.

c)(4P) Calculate the energy per particle of the ground state for the jellium model to first order perturbation in the interaction $V_{\text{el-el}}$ and express the result in terms of the dimensionless measure r_s.
Hint: Distinguish between a “direct” and “exchange” term and use the fact that we can neglect the term where $q = 0$. Recall that r_s can be defined by the relation

$$\frac{4\pi}{3}(r_s a_0)^3 = \frac{V}{N} \tag{2}$$

where a_0 is the Bohr radius, V is the volume of the metal and N the total number of electrons. Moreover, the expectation value of the particle number operators in respect of the ground state will yield an integral of the form

$$\int \mathrm{d}^3k \int \mathrm{d}^3q \frac{1}{q^2} \theta(k_F - |\mathbf{k}+\mathbf{q}|)\theta(k_F - k). \tag{3}$$

To solve this integral, perform a substitution $\mathbf{k} \to \mathbf{x} = \mathbf{k} + 1/(2\mathbf{q})$ and relate the result to segments of spheres ...

d)(2P) Show that the first order perturbation of the jellium model predicts the stability of the metals.
Hint: How does - aside from higher order corrections - the ground state energy depend on r_s*?*