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# Quantum Field Theory of Many-Particle Systems - Problem Set 8

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**Abgabe:** The problem set will be discussed in the tutorial on **Tuesday, 08.12.2015, 11:00**

**Internet:** The problem sets can be downloaded from
http://home.uni-leipzig.de/stp/QFT_of_MPS_WS1516.html

## 14. Screening in the Thomas Fermi approximation *3+3+3 Punkte*

Imagine placing a test charge into a jellium electron system. At first the potential due to the added test charge extends its influence to the far reaches of the system, falling off slowly as $1/r$. However, mobile electrons nearby rapidly react to the test charge, and the motions they make in response have the effect of almost completely canceling out its electric field, except within a characteristic distance called the screening length. This phenomenon can be studied in the context of Thomas-Fermi theory. The Thomas-Fermi theory allows to determine the local electron density from the following equation

$$\frac{\hbar^2}{2m}(3\pi^2)^{2/3}n^{2/3}(\mathbf{r}) + U(\mathbf{r}) + \int d^3r' \frac{e^2 n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \mu.$$

This equation can be understood by realising that for a homogeneous electron system, the first term is the kinetic energy for particles at the Fermi level, and that at zero temperature the sum of kinetic energy, potential energy, and interaction energy for particles at the Fermi level has to be equal to the chemical potential.

**a)** Show that the first term is indeed the kinetic energy of a particle at the Fermi level, i.e. calculate the kinetic energy $\epsilon(k_F)$ and express $k_F$ in terms of the density.

**b)** Suppose that $n_0$ is the solution of this equation when the potential $U(\mathbf{r})$ of the positive background neutralises the Coulomb potential due to the average electron density $n_0$ as discussed in Problem 13 of the previous sheet. If now a small potential $\delta U(\mathbf{r})$ is added, find the equation governing deviations $\delta n(\mathbf{r})$ of the density from perfect uniformity to first order in $\delta U$.

**c)** Consider adding one extra electron to the uniform electron gas and therefore specialise to the case $U(\mathbf{r}) = e^2/|\mathbf{r}|$. Solve the linearised equation for $\delta n(\mathbf{r})$ by Fourier transform. The answer should be of the form $\delta n(\mathbf{r}) \sim e^{-|\mathbf{r}|/\xi}$. Identify the screening length $\xi$, and calculate the effective potential

$$V_{\text{eff}}(\mathbf{r}) = U(\mathbf{r}) + \int d^3r' \frac{e^2 \delta n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}.$$

## 15. Hartree-Fock theory

*4+2+4 Punkte*

Consider a system of interacting electrons with Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \xi(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} V(\mathbf{q}) c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma}.$$

In this problem we will treat the system within a mean-field theory.

**a)** Writing pairs of operators in terms of their deviation from their average value $c^\dagger c - \langle c^\dagger c \rangle$ and keeping only the leading terms in the deviation, show that the interaction part of the Hamiltonian can be written as $H_{\text{int}} = H^H + H^F$, where the so-called Hartree and Fock terms are given by

$$H^{\text{H}} = \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} V(\mathbf{q}) \left[ \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} \rangle c^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'} c_{\mathbf{k}'\sigma'} + \langle c^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'} c_{\mathbf{k}'\sigma'} \rangle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} \right],$$

and

$$H^{\text{F}} = -\frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} V(\mathbf{q}) \left[ \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} \rangle c^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma} + \langle c^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma} \rangle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} \right].$$

Hint: In this problem you may assume number conservation and neglect terms like $\langle c^\dagger c^\dagger \rangle$ and $\langle cc \rangle$.

**b)** Using that $\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} \rangle = \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} = n_{\mathbf{k}\sigma} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$ show that the Hamiltonian can be written as

$$H^{\text{HF}} = \sum_{\mathbf{k}\sigma} \xi^{\text{HF}}_\sigma(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma},$$

where $\xi^{\text{HF}}_\sigma(\mathbf{k}) = \xi(\mathbf{k}) - \Sigma^{\text{HF}}(\mathbf{k})$ with

$$\Sigma^{\text{HF}}(\mathbf{k}) = \sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q},\sigma} V(\mathbf{q}) - nV(0),$$

denoting the Hartree-Fock self-energy. In this expression we have defined the total density $n = \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}$.

**c)** Consider now electrons interacting via a local interaction $V(\mathbf{q}) = U$ and define $\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma}\rangle = \delta_{\mathbf{k}\mathbf{k}'}\bar{n}_{\mathbf{k}\sigma}$. Show that

$$\xi^{\mathrm{HF}}_\sigma(\mathbf{k}) = \xi(\mathbf{k}) + U(\bar{n}_\uparrow + \bar{n}_\downarrow - \bar{n}_\sigma) = \xi(\mathbf{k}) + U\bar{n}_{\bar{\sigma}}.$$

This gives rise to the self-consistency equations

$$\bar{n}_\sigma = \sum_{\mathbf{k}} n_F(\xi^{\mathrm{HF}}_\sigma(\mathbf{k})).$$

By converting the sum into an integral show that, at zero temperature, these self-consistency equations are equivalent to

$$\frac{\hbar^2}{2m}(6\pi)^{2/3}\bar{n}_\uparrow^{2/3} + U\bar{n}_\downarrow = \mu, \qquad \frac{\hbar^2}{2m}(6\pi)^{2/3}\bar{n}_\downarrow^{2/3} + U\bar{n}_\uparrow = \mu.$$

Derive an equation for the dimensionless parameter $\zeta = (\bar{n}_\uparrow - \bar{n}_\downarrow)/(\bar{n}_\uparrow + \bar{n}_\downarrow)$ and investigate its solutions.