Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Christian Carbogno
Exercises: Dr. Christian Carbogno, Henrik Kowalski et al.

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http://www.itp.tu-berlin.de/menue/lehre/lv/ss_2017/pflichtveranstaltungen_masterstudium/theoretische_physik_vi_vertiefung_theoretische_festkoerperphysik_i_ii/

Theoretical Material Science: Exercise Sheet 3

Please hand in solutions by: Tuesday, May 16, start of the exercise class

Exercise 7 (8 points): *The Jellium Model*
In the "jellium" model, the many-body Hamiltonian H^e of the periodic (!) solids is treated in a simplified fashion by approximating the electron-nuclear interaction with the constant C^{jellium}:

$$H^e = T^e + V^{e-\text{Nuc}} + V^{e-e} \approx T^e + C^{\text{jellium}} + V^{e-e} = H^{e,j} \ . \tag{1}$$

a) Show that the eigenfunctions of T^e are plane waves $\varphi_{\mathbf{k}}(\mathbf{r}) = \Omega \exp[i(\mathbf{k}\cdot\mathbf{r})]$, determine their eigenvalues ϵ_i as well as the normalization constant Ω.

b) In the N-electron problem, the N single particle states $\varphi_{\mathbf{k}}(\mathbf{r})$ with the lowest eigenvalues ϵ_i are occupied. Derive the definition of the "Fermi radius" k_F by implicitly accounting for the spin: Assume that each state is doubly occupied (spin up and down, respectively).

c) Evaluate the many-body energy $\langle\Psi_H|H^{e,j}|\Psi_H\rangle$: For this purpose, use the Hartree-ansatz for the N-electron problem

$$\Psi_H(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \prod_{i=1}^{N/2} \varphi_{\mathbf{k}_i}(\mathbf{r}_i) \tag{2}$$

that is consistent with the definitions and assumptions made in (a) and (b). *Tip: How does the electron density of* Ψ_H *look?*

d) Evaluate the many-body energy $\langle\Psi_{HF}|H^{e,j}|\Psi_{HF}\rangle$ using a single-determinant Hartree-Fock-ansatz

$$\Psi_{HF}(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\mathbf{k}_1 s_1}(\mathbf{r}_1\sigma_1) \ldots \varphi_{\mathbf{k}_N s_N}(\mathbf{r}_1\sigma_1) \\ \varphi_{\mathbf{k}_1 s_1}(\mathbf{r}_2\sigma_2) \ldots \varphi_{\mathbf{k}_N s_N}(\mathbf{r}_2\sigma_2) \\ \ldots \\ \varphi_{\mathbf{k}_1 s_1}(\mathbf{r}_N\sigma_N) \ldots \varphi_{\mathbf{k}_N s_N}(\mathbf{r}_N\sigma_N) \end{vmatrix} \tag{3}$$

In this case, you have to explicitly account for the spin degree of freedom σ_i. *Tip: How does the electron density of* Ψ_{HF} *look?*

e) How do the solutions in exercise (c) and (d) differ? Which solution is more stable?

Exercise 8 (4 points): *Koopmans' theorem*
Inspect the chapter in the lecture notes, where the relation between the ionization energy I_k and the Lagrange parameters ϵ_{oi} is shown, i.e., the equation

$$I_k := \langle\Phi^{N-1}|H^{e,N-1}|\Phi^{N-1}\rangle - \langle\Phi^N|H^{e,N}|\Phi^N\rangle \approx -\epsilon_{o_k s_k}.$$

Write down and explain the calculation leading to this result. Which assumptions are needed?

Exercise 9 (4 points): *The Hohenberg-Kohn Theorems*
The Hohenberg-Kohn theorems state that for a given external potential $v(\mathbf{r})$ the expectation value of H^e is a functional of the particle density $n(\mathbf{r})$

$$\langle\Phi|H^e|\Phi\rangle = E_v[n] = \int v(\mathbf{r})n(\mathbf{r})d^3\mathbf{r} + F[n] \quad . \tag{4}$$

and that the ground-state density $n_0(\mathbf{r})$ (with the ground-state energy E_0) minimizes this functional. Note that $F[n]$ does not depend explicitly on $v(\mathbf{r})$.

Proof the Hohneberg-Kohn theorems by *reductio ad absurdum* for a non-magnetic system ($n(\mathbf{r}) = 2n_\uparrow(\mathbf{r}) = 2n_\downarrow(\mathbf{r})$) under the assumption that the ground state is non-degenerate.