Prof. Stephan Fritzsche
TPI and HI Jena
— Advanced Quantum Theory —

12. December 2016
Winter Term

Home Work (8)

Task 1: Variational Principle (3 Points)

a) The variational principle can be applied to the first excited state if the orthogonality condition $\langle \phi_1 | \Psi_0 \rangle = 0$ is imposed on the trial wave function ϕ_1, where Ψ_0 is the exact wave function of the ground state.
Show that for a Hamiltonian H with a discrete spectrum the energy of the first excited state is given by

$$E_1 = \min_{|\phi_1\rangle : \langle \phi_1 | \Psi_0 \rangle = 0} \frac{\langle \phi_1 \,|\, H \,|\, \phi_1 \rangle}{\langle \phi_1 \,|\, \phi_1 \rangle}$$

b) Why and how can this be applied to compute the energy of the first excited state $1s2s\,{}^3S$ of helium? Explicitly give the trial wave function for this case.

Task 2: Variational Principle for the Ground State of the Helium Atom (4 Points)

a) Apply the minimization principle to estimate the ground-state energy of helium. We assume that the nuclear charge is partially screened by one of the electrons, such that the other electron, respectively, sees a reduced effective nuclear charge β. Construct the wave function by means of single electron $1s$ wave functions, where the nuclear charge Z has been replaced by the effective nuclear charge β

$$\phi\,(\boldsymbol{r}_i, \beta) = \frac{\beta^{3/2}}{\sqrt{\pi}} \mathrm{e}^{(-\beta r_i)} \,.$$

Calculate the expectation value of the energy, and minimize it with respect to the charge β.
b) Compare your result to the exact value.

Task 3: The Fermi Electron Gas (3 Points)

Consider the system of free electrons whose spatial part of the wave function $\psi(\mathbf{r}) = \mathrm{e}^{i\mathbf{kr}}$ is assumed to be periodic with a period L:

$$\psi(x+L, y, z) = \psi(x, y, z)\,,\ \psi(x, y+L, z) = \psi(x, y, z)\,,\ \psi(x, y, z+L) = \psi(x, y, z)\,.$$

a) Find the total number N_s of individual electronic states for energies up to $E = \hbar^2 k^2/(2m)$.
b) In the ground state (in which the electron gas is at absolute zero temperature) all the individual states of energy less than the Fermi energy E_f are occupied, and all those whose energies are greater than E_f are empty. Find the Fermi energy E_f for the system of N electrons.