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Winter term 2017/18

Problems in Advanced Quantum Mechanics

Blatt ~~2~~43

Problem 7: Thomas-Fermi Atoms (1+1+2)+1+1 = 6 points

We seek the optimal solution for the electron density $n(\boldsymbol{x})$ of a Thomas-Fermi atom within a family of test function. More precisely, we consider the following family of test functions,

$$n(\boldsymbol{x}) = A\,\frac{\mathrm{e}^{-y}}{y^3}, \qquad y = \sqrt{\frac{r}{\lambda}},$$

where λ is a variational parameter and the constant A is fixed by the normalization $\int \mathrm{d}^3x\, n = N$. For a neutral atom we have $N = Z$.

1. Calculate the energy of the atom (ion) as function of λ.
2. Find the minimizing values of the variational parameter.
3. Calculate the corresponding energy as function of N and Z. What do you obtain for an (neutral) atom.

Hints: express the result as function of the TF-parameter γ entering the expression for the kinetic energy. The most demanding part is the calculation of the Coulomb interaction between the electrons,

$$V_{ee} = \frac{e^2}{2}\int \frac{n(\boldsymbol{x})n(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\,\mathrm{d}^3x\mathrm{d}^3y = -\frac{e}{2}\int \varphi(\boldsymbol{x})n(\boldsymbol{x})\mathrm{d}^3x \quad \text{with} \quad \Delta\varphi = -4\pi e n\,.$$

When solving the equation $\Delta\varphi = -4\pi e n$ for φ, for the given ansatz for $n(\boldsymbol{x})$, you arrive at the differential equation

$$\frac{1}{4\lambda^2 y^3}\left(y\frac{\mathrm{d}^2}{\mathrm{d}y^2} + 3\frac{\mathrm{d}}{\mathrm{d}y}\right)\varphi = -4\pi e A\frac{\mathrm{e}^{-y}}{y^3}$$

The solution regular at the origin is

$$\varphi = \frac{\text{const}}{y^2}\left(1 - (1+y)\mathrm{e}^{-y}\right)\,.$$

Check that this is a solution and fix the constant.

Problem 8: Many particle systems and Hartree-Fock 3+1 = 4 points

A systems consists of three identical fermions on the real axis. The Hamiltonian of the system is $H = H^{(1)} + H^{(2)}$, with

$$H^{(1)} = \sum_{i=1}^{3} h_i = \sum_{i=1}^{3}\left(\frac{p_i^2}{2m} + W(x_i^2)\right)$$

being the sum of three one-particle-Hamiltonian, each of which contains the arbitrary potential $W(x^2)$. For simplicity we assume that the particles have no spin (which in reality is not possible).

The two-particle operatorr

$$H^{(2)} = \frac{\lambda}{2} \sum_{i \neq j}^{3} \delta(x_i + x_j).$$

describes the interaction between the particles.

- Calculate within the Hartree-Fock-approximation the energy function (expectation value $\langle H \rangle$) for the anti-symmetric product of arbitrary one-particle wave functions ψ_1, ψ_2, ψ_3.
- Determine the corresponding Hartree-Fock-equation for each factor ψ_i.

Submission date: Thursday, 9. November 2017, before the lecture begins