Mathematical Quantum Mechanics, 2014/15 Homework Problems, LMU

Issued: November 25, 2014; deadline for handing in the solutions: December 2, 2014, 4 pm

23. If the minimization of the Thomas-Fermi functional is constrained by the condition $\int \rho(x)\, d^3x = N$, then a Lagrange multiplier μ has to be introduced into the variations leading to the associated Euler equation, so that for an atomic system and $\rho(x) > 0$ the latter reads

$$\big(3\pi^2 \rho(x)\big)^{2/3} - \frac{Z}{|x|} + \int \frac{\rho(y)}{|x-y|} + \mu = 0. \tag{21}$$

In the sequel, we neglect the repulsion term in the equation (21) and assume that $0 < N \leq Z$.

(i) Solve the equation (21) for the Thomas-Fermi density ρ; set $\mu = Z/R$ and determine R in terms of N by computing

$$N = \int_{|x| \leq R} \rho(x)\, d^3x. \tag{22}$$

(ii) Prove that the corresponding Thomas-Fermi energy

$$E_{\mathrm{TF}}(Z) = \int_{|x|\leq R} \big(\frac{3}{5}(3\pi^2)^{2/3}(\rho(x))^{5/3} - \frac{Z}{|x|}\rho(x)\big)\, d^3x \tag{23}$$

is given by $E_{\mathrm{TF}}(Z) = -(1/2)(3/2)^{1/3} Z^2 N^{1/3} = -(1/2)(3/2)^{1/3} Z^{7/3}$ if $N = Z$.

24. Calculate the series $\sum_{k=1}^{K} k^n$ for the cases $n = 1$ and $n = 2$, $K \geq 1$.

25. Consider a noninteracting hydrogenic atom (i.e., without electron-electron repulsion) with N electrons in K filled shells (i.e., where all the available quantum states with hydrogenic quantum numbers (n, ℓ, m) are occupied up to $n = K$).

(i) By taking into account the degeneracy (including spin) of the hydrogen states, show (by using problem 24) that $N = 2K(K^2/3 + K/2 + 1/6)$.

(ii) Invert this relation to express K as a function of N up to order $o(1)$.

(iii) Compute the energy $E(Z) = -\sum_{n=1}^{K} 2n^2 E_n(Z)$ of this system, where E_n stands for the one-electron hydrogen energy for the quantum number n.

(iv) Compare the result of (iii) with the Thomas-Fermi energy obtained in problem 23.