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Problems in Advanced Quantum Mechanics

Blatt 4

Problem 9: Virial theorem for TF atoms 2+1+4 = 7 points

We consider a atom in the Thomas-Fermi (TF) approximation. The electron density is denoted by $n(\boldsymbol{x})$. The universal function $\chi(s)$ of the dimensionless radial variable s has the properties

$$J \equiv \int_0^\infty \mathrm{d}s \left(\frac{\mathrm{d}\chi}{\mathrm{d}s}\right)^2 = -\frac{2}{7}\chi'(0) \approx 0.454 \quad \text{and} \quad \chi(0) = 1\,.$$

From the information given in the lecture one obtains

$$\gamma n^{2/3} = Ze^2 \frac{\chi(r)}{r}, \quad n = \frac{Z}{4\pi}\frac{\chi''(r)}{r}\,. \tag{1}$$

1. Derive the Virial theorem relating the kinetic and potential energies in the TF approximation.
   Hint: Compute the kinetic, potential and total energies of the TF atom, first for the generic density $n(\boldsymbol{x})$, and then for the rescaled density $n_\lambda(\boldsymbol{x}) = \lambda^3 n(\lambda \boldsymbol{x})$. Then compare the two. Assuming that $n(\boldsymbol{x})$ is a physical solution, according to the variational principle it must correspond to n_λ at the value of λ_* that minimizes the total TF energy. What is λ_*? Write this stationarity condition at λ_*.
2. Use the definition of the screening function χ given in the lecture, as well as the Poisson equation fulfilled by the TF potential ϕ, to prove the second equation in (1).
3. Show that the kinetic energy T, interaction energy between nucleus and electrons V_{ne} and the interaction energy between the electrons are given by

$$T = \alpha\, J, \quad V_{en} = -\frac{7}{3}T, \quad V_{ee} = \frac{1}{3}T$$

   Express the constant α in terms the constant length b in $r = bs$, the charge Ze of the nucleus and the integral J. Assume that the atom is neutral such that the constant ϕ_0 in the treatment of the TF-atom vanishes.
   Hint: observe that $n^{5/3} = n^{2/3} \cdot n$ and use Eq. (1). For the computation of V_{ee} start from the formula

$$V_{ee} = \frac{e^2}{2}\int \mathrm{d}^3x \mathrm{d}^3y \, \frac{n(\boldsymbol{x})n(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|} = -\frac{e}{2}\int \mathrm{d}^3x\, n(\boldsymbol{x})\phi(\boldsymbol{x}) + \frac{Ze^2}{2}\int \mathrm{d}^3x\, \frac{n(\boldsymbol{x})}{|\boldsymbol{x}|}\,,$$

   which follows from

$$\phi(\boldsymbol{x}) = \frac{Ze}{|\boldsymbol{x}|} - e\int \mathrm{d}^3y\, \frac{n(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\,.$$

Problem 10: Two particles with total angular momentum zero 2+2 = 4 points

Given two particles, each with angular momentum j. Prove, that the wave function of the total two-particle system with vanishing total angular momentum (the singlet) can be written as

$$|\Psi_0^0\rangle = \frac{1}{2j+1}\sum_{m=-j}^{j}(-1)^{m+1/2}|\psi_j^m\rangle \otimes |\psi_j^{-m}\rangle, \quad j \in \mathbb{N}_0 + \frac{1}{2},$$

$$|\Psi_0^0\rangle = \frac{1}{2j+1}\sum_{m=-j}^{j}(-1)^{m}|\psi_j^m\rangle \otimes |\psi_j^{-m}\rangle, \qquad j \in \mathbb{N}_0\,.$$

Hint: Recall how the the step operators $J_\pm = J_x \pm \mathrm{i} J_y$ and the component J_z of the total angular momentum $\boldsymbol{J} = \boldsymbol{J}^{(1)} + \boldsymbol{J}^{(2)}$ act on a product state $|\psi_j^m\rangle \otimes |\psi_j^{m'}\rangle$ and use that, for example, $c_{jm}^{+} = c_{jm'}^{+}$ for certain m, m'. It is sufficient to prove the result for an integer (or a half-integer) value of j.

Submission date: Thursday, 16. November 2017, before the lecture begins