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— Theoretical Atomic Physics —

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Summer Term

Home Work (3)

Task 11: Transition energies in hydrogen-like uranium

Calculate the relativistic transition energies of the Ly$-\alpha_1$ ($2p_{3/2} \to 1s_{1/2}$) and Ly$-\alpha_2$ ($2p_{1/2} \to 1s_{1/2}$) lines in hydrogen-like Uranium. Compare to the nonrelativistic energy.

Task 12: Electron-electron interaction

The addition theorem for spherical harmonics is

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_\ell^m(\theta_1, \varphi_1)\, Y_\ell^{m*}(\theta_2, \varphi_2)\ ,$$

where γ is the angle between two vectors in spherical coordinates, whose angular coordinates are θ_1, φ_1 and θ_2, φ_2, respectively. Use the addition theorem, to show that the electron-electron interaction operator can be expanded in terms of spherical harmonics as

$$\frac{1}{r_{12}} = \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} = \frac{4\pi}{r_>} \sum_{\ell,m} \frac{1}{2\ell+1} \left(\frac{r_<}{r_>}\right)^\ell Y^*_{\ell m}(\theta_1, \varphi_1) Y_{\ell m}(\theta_2, \varphi_2)\,,$$

where we use the definitions

$$r_< = \min(r_1, r_2) \qquad\qquad r_> = \max(r_1, r_2)$$

Task 13: Variational principle for the ground-state of the helium atom

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 Construct the wave function by means of single electron $1s$ wave functions, where the nuclear charge Z has been replaced by the effective nuclear charge β

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

Calculate the expectation value of the energy, and minimize it with respect to the charge β. To integrate the exchange term, use the result of the previous task.

b) Compare your result to the exact value.

Task 14: First excited state of the helium atom

The variational principle can also be applied to estimate the energy of some excited states. In this task, we want to estimate the energy of the first excited state of helium ($1s2s\,^3S$). In contrast to the previous problem, the electrons occupy orbitals with different quantum number n. Therefore, we assume that they see a different screened nuclear charge. The inner 1s electron is assumed to see the charge Z_i, whereas the outer 2s electron sees the charge Z_o. The unnormalized one-electron wave functions are then given by

$$\phi_{1s}(r) = \exp\left(-Z_i r\right) ,$$
$$\phi_{2s}(r) = \left(1 - Z_o r/2\right) \exp\left(-Z_o r/2\right) .$$

We will again use these single-electron wave functions to construct the two-electron wave function. After calculating the energy functional, we will minimize the total energy by varying both charges Z_i and Z_o simultaneously.

a) Write down your ansatz for the trial wave function.

b) (optional) Calculate the expectation value of the energy and minimize it with respect to the charges Z_i and Z_o. Do not try to solve the integrals by hand, but use a computer-algebra system like Mathematica instead.

Hint: The orbitals ϕ_{1s} and ϕ_{2s} are not orthogonal if their charges do not equal.

c) (optional) Use your result of the previous task to compare your calculated excitation energy to an experimental value, e.g. from the NIST atomic spectra database.

Task 15: Commutators (3)

Prove that

$$[H, \boldsymbol{L}] = 0\,,$$

where the many-particle Schrödinger Hamiltonian is given by

$$H = \sum_k \left(-\frac{1}{2}\nabla_k^2 - \frac{Z}{r_k}\right) + \sum_{k<i} \frac{1}{r_{ki}}$$

and $\boldsymbol{L} = \sum_k \boldsymbol{l}_k$.