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— Theoretical Atomic Physics —

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Summer Term

Home Work (5)

Task 20: Combinatorics

a) How many possibilities are there to place three electron into an f-shell?

b) Now consider the ^{4}I-term of the f^2-configuration. How many states belong to the ^{4}I-term?

Task 21: Slater Determinant for Lithium

a) Let us consider the ground state $1s^2 2s$ of lithium. Find a possible Slater determinant and explicitly write it in terms of single-electron orbitals.

b) Show that it is an eigenvector of the total angular momentum operator operator $\boldsymbol{J}_z = \sum_i j_z^{(i)}$, and determine its eigenvalue.

Task 22: Matrix Elements of Slater Determinants

Let us consider three electrons in three different radial orbitals, ϕ_a, ϕ_b and ϕ_c. These orbitals are eigenfunctions of the effective one-electron Hamiltonian

$$h_i = -\frac{\nabla_i^2}{2m} + V(\boldsymbol{r}_i)$$

with eigenvalues ϵ_a, ϵ_b and ϵ_c.

a) Determine all Slater determinants, which can be formed such that each orbital is only occupied by one electron.

b) Calculate the expectation value of the total Hamiltonian

$$H = \sum_i h_i + \sum_{i<j} \frac{1}{r_{ij}}$$

for the Slater-determinant belonging to $M_s = 3/2$. Give your result in terms of the Coulomb integrals J_{ab} and exchange integrals K_{ab}.

c) Repeat the same for $M_s = 1/2$

Task 23: Hartree-Fock equations

Write down the radial Hartree-Fock equations for neon.