9.E: The Electronic States of the Multielectron Atoms (Exercises)

Q9.1

In the hydrogen atom, what is the energy of the *[Math Processing Error]* configuration? How many states result from this configuration? What are the term symbols for these states?

Q9.2

Determine the term symbols for the *[Math Processing Error]* electron configuration of carbon.

Q9.3

Determine the term symbol for the ground state of the sodium atom. Write the term symbols for the excited state where the valence electron is in a 3p orbital. Use this information to account for the appearance of the doublet known as the sodium D-line.

Q9.4

A helium atom is in a *[Math Processing Error]* electron configuration. What are the term symbols for the states that result from this configuration? Write antisymmetric (with respect to permutation symmetry) wavefunctions for these states. Show that only a transition from the ground state to one of these states is allowed through the electric-dipole-field interaction.

Q9.5

Rewrite Equation (9-13) so the wavefunction is antisymmetric with respect to permutation of the two electrons. Repeat Exercise 9.6 using your antisymmetric wavefunction to show that the same result is obtained, and, in because the electron-electron interaction is neglected, the energy does not depend on whether the wavefunction is symmetric or antisymmetric.

Q9.6

An ionization energy or ionization potential is the difference in energy between the energy of an atom and the energy of the corresponding ion. It also can be the difference in energy between an ion and the next higher charged ion. These different possibilities are referred to as the first, second, third, etc. ionization energies.

a. Calculate the ground state energy of He^+ and show that the calculated value of 54.4 eV in Table 9.1 for the first ionization energy is correct.
b. Use your insight to explain why the first ionization energy is just half the helium binding energy.

Q9.7

Compute the second ionization energy for Li (*[Math Processing Error]*) neglecting the electron-electron potential energy term in the Hamiltonian. The experimental value is 75.6 eV. Explain why the computed value differs from the experimental value.

Q9.8

For the ground state of hydrogen, the electron is in a 1s orbital where *[Math Processing Error]* so the Hamiltonian operator is *[Math Processing Error]*

Q9.9

Obtain an expression for the energy of the ground state of the hydrogen atom as a function of *[Math Processing Error]*, where *[Math Processing Error]* is an adjustable parameter in the trial wavefunction *[Math Processing Error]*, which is a Gaussian function.

Q9.10

Find the value for that minimizes the energy and calculate a value for the energy.

Q9.11

Compare this minimum energy with the exact value. What is the percent error?

Q9.12

Do you consider this Gaussian function to be a reasonable approximation to the exact hydrogen 1s atomic orbital?

Q9.13

What is the difference between this Gaussian function and the exact hydrogen 1s function? Illustrate the difference with a computer-generated graph.

Q9.14

Consider a one-dimensional anharmonic oscillator for which the potential function is *[Math Processing Error]*

a. Write the full Hamiltonian for this oscillator.
b. What system would serve as the most reasonable zero-order approximation for this oscillator in order to use perturbation theory most efficiently and effectively?
c. Identify the zero and first order perturbation terms in your Hamiltonian.
d. What is the zero order energy of the lowest energy state for this oscillator?
e. Write the integral for evaluating the first order correction to this energy and compute the first order correction to this energy.

Q9.15

Consider the particle in a box. Use first-order perturbation theory to determine how much the energy levels are shifted by an external electric field of V volts/cm.

Q9.16

Consider two electrons in a one-dimensional box.

a. What is the zero order energy of the lowest energy state for these electrons?
b. What is the first order correction to this energy due to the electron-electron interaction?

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