

Problem-set10

32. Polarization of atomic hydrogen in the vicinity of a charged particle.

Consider a hydrogen atom in the vicinity of a charged particle Ze at a fixed distance R from the center of the atom.

- Write down the Hamiltonian for the electron assuming the mass of proton is infinite.
- Assume that R is large, obtain the perturbation H' of the electron due to the charged particle.
- Write down the change to the ground state energy of the atomic hydrogen and show that the correction due to the first order perturbation is zero.
- Write down the general expression for the second-order perturbation and identify all the nonzero matrix elements that will contribute to the sum in the 2nd order perturbation theory. How does the correction to the ground state energy depend on R ?

33. Hermann-Feynmann theorem. This is a famous theorem.

- Prove exercise 18.14 in Merzbacher, p465.
- The most familiar Hermann-Feynmann theorem is actually

$$\langle \Psi_1, \frac{d\Psi_2}{d\lambda} \rangle = \frac{\langle \Psi_1 | \frac{\partial H}{\partial \lambda} | \Psi_2 \rangle}{E_2 - E_1}$$

Prove this equation. Note that the two functions are orthogonal at each fixed parameter λ .

34. Variational and perturbation theory for the ground state of helium atom.

This is the standard textbook problem so I will just ask you to go over yourself following these steps.

- Write down the Hamiltonian for the two electrons in the helium atom, neglecting the spin-orbit interaction.
- Assume that the electron-electron interaction is small, we will treat this term by perturbation. Identify the H_0 and H' where H' is the electron-electron interaction term.
- For the ground state of H_0 , write down the eigenfunction. Include the spin part.
- Evaluate the first order perturbation from H' . From Merzbacher p478 you can see that the correction is 34 eV while the unperturbed energy is -108.8eV. Not that small.
- Next you will use the variational principle to do the calculation. Instead of using $Z=2$ in Merzbacher (18.127) p478, you treat Z as a variational parameter. Confirm the results given at the bottom of this page, i.e., the screening is given by $\sigma = 5/16$.
- Compare the ground state binding energy from experiment, from the first order perturbation theory obtained in (d) and from the variational method in (e), express all the answers in eV.

35. Perturbation theory for the 1s2s singlet and triplet excited states of helium atom.

- Using the same H_0 and H' in the previous problem, consider the 1s2s excited states. Here one of the electrons is in the 1s and the other is in the 2s. We will write the total wavefunction as the product of spin part and the spatial part. For the spin part, construct the spin functions for the two electrons coupled to $S=1$ (the triplet) and $S=0$ (the singlet),

identify whether they are symmetric or antisymmetric under exchange of the two electrons.

(b) The unperturbed wavefunction can be expressed as $\phi_{100}(\vec{r}_1)\phi_{200}(\vec{r}_2)$ where the ϕ 's are hydrogenic 1s and 2s wavefunction respectively. This function is not symmetric or antisymmetric under the exchange of the two electrons. Construct the correct functions which are symmetric or antisymmetric.

(c) Write down explicitly the total wavefunction (spatial part and spin part) for the singlet and the triplet states. What are their energies with respect to H_0 .

(d) Evaluate the matrix elements of H' and identify the so-called direct and exchange integrals.

(e) Identify all the good quantum numbers for your total wavefunction given in (c).