8.421 Fall 2006 Assignment #3 Professor W. Ketterle
Due Friday, March 10, 2006

1. **Ground state energy of the helium atom**

   If we neglect interactions between electrons, the ground state energy of the helium atom is $E = 2Z^2(-\frac{e^2}{2a_0}) = -108.848\text{eV}$ ($Z = 2$). The true (measured) value is -79.006 eV.

   (a) Calculate the interaction energy $< \frac{e^2}{r_{12}} >$ supposing that both electrons are in the $1s$ state and that the spin wavefunction is anti-symmetric. What is the ground state energy?

   (b) The value obtained in (a) is a big improvement, but still several eV off. We can easily get a better value by using a variational method. Use $\psi = \phi(\vec{r}_1)\phi(\vec{r}_2)$

   $$\phi(\vec{r}) = \frac{1}{\sqrt{\pi}}(\frac{Z'}{a_0})^{\frac{3}{2}}e^{-\frac{Z'}{a_0}r}$$

   as a suggested ground state and express the expectation value of the ground state energy in terms of Z'. Provide the physical interpretation of the free parameter Z'.

   (c) Calculate Z' that minimizes the energy. What is the improved ground state energy?

   As long as we use wavefunctions in the form of $\psi = \phi(\vec{r}_1)\phi(\vec{r}_2)$ (one-electron approximation), we cannot reduce discrepancies to less than 1 eV. However, introducing correlations into wavefunctions greatly improve the solutions. For example, minimizing the energy using $\psi \sim e^{-c_1(r_1+r_2)}(1 + c_2r_{12} + c_3(r_1 - r_2)^2)$ gives you a minimum energy only 0.035 eV off from the measured value!

2. **Energy shifts in hydrogen due to the size of the proton**

   (a) Derive the potential produced by a uniformly charged sphere

$$\rho = \begin{cases} \rho_0 & (\mathrm{r} < \mathrm{a}) \\ 0 & (\mathrm{r} > \mathrm{a}) \end{cases}$$

   (b) Calculate the level shift for the $1s$ state of hydrogen due to the finite proton radius. Assume that the proton has a uniform charge distribution over $r_p = 0.9$ fm.

   (c) What frequency accuracy is needed for $1S - 2S$ spectroscopy to measure r_p with 0.010 fm accuracy?

   Recent measurement of the hydrogen $1S-2S$ transition frequency (Th. Udem *et.al.*, PRL **79**, 2646 (1997)) revealed that the rms proton charge radius should be 0.890(14)fm instead of the old value 0.862(12)fm, provided theoretical QED calculations of the Lamb shift are correct.

Help for problem 1 & 2. (Solutions of $[-\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r}]\psi = E\psi$)

$$\psi_{1s} = \frac{1}{\sqrt{\pi}}(\frac{Z}{a_0})^{\frac{3}{2}} e^{-\frac{Z}{a_0}r}, \qquad E_{1s} = -Z^2\frac{e^2}{2a_0}$$

$$(a_0 = \frac{\hbar^2}{m_e e^2} = 5.3 \times 10^{-11}\mathrm{m}, \qquad \frac{e^2}{2a_0} = 13.606\mathrm{eV})$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\exp\left(-\alpha(r_1 + r_2)\right)}{r_{12}} d\vec{r_1} d\vec{r_2} = \frac{20\pi^2}{\alpha^5}$$

3. **Atoms in magnetic fields: the Breit-Rabi formula**

The Hamiltonian for an atom in a magnetic field along $\hat{z}$ may be written

$$H = ah\vec{I} \cdot \vec{J}/\hbar^2 + (g_J \mu_0 m_J - g_I \mu_0 m_I) B_z$$

(a) Restrict attention to the case $J = 1/2$, but arbitrary I. Show the energies of states are given by the Breit-Rabi formula

$$E_m^{\pm} = -\frac{ah}{4} - \mu_0 g_I m B_z \pm \frac{ahF^+}{2}\sqrt{1 + \frac{2mx}{F^+} + x^2}$$

The parameter x is given by $x = (g_I + g_J)\mu_0 B_z / ahF^+$, where $F^+ = I + 1/2$. m is the z component of the total angular momentum.

(b) For the case of $I = 3/2$, make a clear sketch of energies vs. x. Take advantage of the non-crossing rule(levels of the same m do not cross). Be sure to extend your figure to very high field ($1/x \ll g_I/g_J$). Label the lines with quantum numbers at low and high fields and indicate m.

(c) There are some values of magnetic field where the resonance frequency for the (magnetic) dipole transition (selection rules $\Delta m = 0, \pm 1$) is first-order field independent. Show those values for magnetic field and corresponding transitions on your figure.

(d) For Na ($I = 3/2, aF^+ = 1.77\text{GHz}, g_I \mu_0 = 2.22\mu_N$), find the magnetic fields of the first-order field independent transition $(F, m_F) = (1, -1) \rightarrow (2, 0)$.

(e) Atoms in a magnetic trap at 1μK temperature are distributed over a magnetic field range of about 30mG. Calculate the inhomogeneous width of the (1,-1) → (2,0) transition at low B field and at the magnetic field found in question (d).

4. **Atomic g-factors**

Find g-factors for the following states of Na ($I = 3/2$):

$^2P_{\frac{1}{2}}$ $(F = 1, 2)$ $\quad$ $^2P_{\frac{3}{2}}$ $(F = 0, 1, 2, 3)$ $\quad$ $^2S_{\frac{1}{2}}$ $(F = 1, 2)$

- For questions or assistance with this assignment, contact
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