

Homework Assignment #2

Physics 8.421, Spring 2008, Prof. W. Ketterle

Due Monday, March 3rd, 2008

1. Atomic Units

Let the atomic unit of E field be $E_A \equiv e/a_0^2$, the field of the ground state electron at the site of the proton in hydrogen.

- a) (2 points) On the scale of atomic units, the energy of the electrostatic potential balances the energy of quantum confinement. Use this equality to derive the atomic size, a_0 . (Ignore numerical factors.)
- b) (1 point) Find the magnetic field of the electron at the proton, B_N . (Assume a classical orbit for the electron. If factors of 2 arise, ignore them.)
- c) (1 point) Find the magnetic field, B_H , which has an interaction energy of one Hartree with a Bohr magneton.
- d) (1 point) Express these fields in terms of E_A (Gaussian units).
- e) (2 points) Are there strong reasons to prefer B_N or B_H as the atomic unit of magnetic field?

2. Determination of the fine structure constant, α

As was discussed in the class, the fine structure constant (α) determines the maximal ratio of the energy stored in the electromagnetic field produced by a system of charged particles to the total mechanical energy of the system including its rest mass.

Since bound states are quantized, this same ratio together with the rest masses of the particles also determines the minimal energies of the system i.e. the bound states. Atoms consist of bound charged particles and so α , together with the ratios of the masses of elementary particles, becomes responsible for the relative scale of all the observed electromagnetic phenomena in nature. In the words of Richard P. Feynman:

“ $[\alpha]$ has been a mystery ever since it was discovered more than fifty years ago, and all good theoretical physicists put this number up on their wall and worry about it. Immediately you would like to know where this number for a coupling comes from: is it related to? or perhaps to the base of natural logarithms? Nobody knows. It's one of the greatest damn mysteries of physics: a magic number that comes to us with no understanding by man. You might say the "hand of God" wrote that number, and "we don't know how He pushed his pencil." *Richard P. Feynman, QED: The Strange Theory of Light and Matter, Princeton University Press 1985, p. 129.*

If the ratios of masses of the various charged particles in a system are known, α can be measured by comparing the energies of the different bound states. The simplest such system, consisting of a proton and an electron, is hydrogen. Unfortunately, methods based on hydrogen spectra have limited accuracy due to the transition frequencies and linewidths. A better choice are the fine structure splittings of the 2^3P state in helium. The lifetime of 100 ns lifetime and the 40 GHz splitting allow a higher precision compared to 1.6 ns and 10 GHz for hydrogen. However, relating the helium spectrum to α requires precise calculations of the energy levels of the helium atom and, at present unresolved theoretical inconsistencies remain (see Phys. Rev. Lett. 95, 203001 (2005)).

The most precise measurement of α is done by measuring $g - 2$ for a single electron trapped in a Penning trap (G. Gabrielse et al., Phys. Rev. Lett **97**, 030802 (2006)). In this case QED calculations relating $g - 2$ to α can be done to sufficiently high accuracy. However, an independent measurement of α would provide a stringent comparison of the physics behind that measurement with QED. (Ironically, it is the precision of

the *second* most precise experiment that limits the stringency of this comparison.)

An alternative atomic physics method is presented in the problem. It involves the measurement of mass ratios, the Rydberg, and the recoil velocity of an atom after absorbing a photon, which can be done by atom interferometry. This measurement involves several basic physics concepts: structure of hydrogen, cyclotron frequencies, and the momentum of photons and atoms, but does not require QED.

a. (2 points) One of the most precisely known constants in physics is the Rydberg constant R_∞ , which gives us a very accurate measurement of the binding energy of hydrogen in frequency units as $f_\infty = cR_\infty$. Show that α can be expressed simply in terms of f_∞ and the frequency corresponding to the rest energy of an electron $m_e c^2/h$ – “bound” state consisting of a single electron and its electromagnetic field. Show that your result only depends on the experimental values of R_∞ and h/m_e . (Hint: What is c in SI units?)

b. (1 point) Since ratios of masses can be determined very accurately, we don’t have to care for which particle we measure h/m . Show that h/m can be obtained by measuring the velocity and de Broglie wavelength of a neutron beam. (The wavelength is found from a Bragg reflection of the neutrons off a silicon crystal, and the velocity is found from back-reflecting and detecting a modulated neutron beam)

c. (1 point) Show that alternatively h/m can be obtained by measuring the recoil velocity $v_R(\nu)$ of an atom after absorbing a photon of frequency ν .

d. (3 points) Photon frequencies can be accurately determined using optical comb generators. Velocities are much harder to measure so in practice $v_R(\nu)$ is obtained from the Doppler shift of an atomic resonance due to atom recoil. Show that this can be done in the following way:

A well collimated atomic beam is intersected by two counter propagating laser beams at right angles. The first laser beam excited the atom, the second laser beam de-excites the atom. Relate $v_R(\nu_1)$ to the resonance frequencies ν_1 and ν_2 of the two processes. What is h/m_{atom} in terms of these same resonance frequencies? In practice, ultracold clouds of atoms and an atom interferometer are used (Phys. Rev. Lett. 70, 2706 - 2709 (1993)).

e. (1 point) A third method to determine h/m is the following:

Suppose it were possible to precisely measure the mass difference, Δm , of two nuclear energy levels as well as the wavelength, λ (in meters), of the gamma ray emitted in the transition between them. Show that this determines the value of $h/\Delta m$.

This method has been used to directly verify the relation $E = mc^2$ with an accuracy of 0.5ppm (see Nature 438, 1096 - 1097 (21 Dec 2005)), but is not accurate enough to compete for a determination of α .

Note that all those methods depend on accurate measurements of mass ratios using Penning traps. The highest accuracy of such measurements (with 0.01 ppb precision) has been achieved by Dave Pritchard’s group at MIT (S. Rainville et al, *Science*, **303**, pages 334-338, 2004, but for atoms used in atom interferometry the precision was only 0.2 ppb – M.P. Bradley et al., Phys. Rev. Lett. **83**, 4510 (1999)).

3. Ground state energy of the helium atom

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

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

(b) (2 points) 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 $\psi = \phi(\vec{r}_1)\phi(\vec{r}_2)$

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

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) (1 point) 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!

For questions or assistance with this assignment contact:

Marko Cetina
mcetina@mit.edu
617-253-5093

Office hours will be on Friday, Feb 29th at 5:00pm in 26-225, or by e-mail request.