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Spring 2010

Problem Set 6 & 7: Solutions

1. The energies of the stationary states of hydrogen slightly depend on the orbital angular momentum quantum number l. An improved formula for the energy of the state of quantum numbers n and l for nonzero l is

$$\mathsf{E}_{n,l} = \frac{\mathsf{m}_{e} e^{4}}{2 \left(4\pi\epsilon_{o}\right)^{2} \hbar^{2} n^{2}} \left[1 + \frac{e^{4}}{\left(4\pi\epsilon_{o}\right)^{2} \hbar^{2} c^{2} n} \left(\frac{1}{1 + l + \frac{1}{2} \pm \frac{1}{2}} - \frac{3}{4n} \right) \right] \tag{1}$$

where the term $\pm \frac{1}{2}$ corresponds to the spin parallel and antiparallel, respectively, to the orbital angular momentum.

(a) For the case of the first excited state, n=2, l=1, and the spin antiparallel to the orbital angular momentum, find the effective difference *in electron volts* between the energy calculated according to Bohr theory and the energy calculated according to the improved formula above.

(b) For n=2, l=1, find the difference in electron volts between the energies of spin parallel and antiparallel to the angular momentum calculated according to the improved formula above. Which of these states has the lowest energy?

Note: There were two typos in this problem as stated. First, the overall energy should be negative, and the minus sign was missing. Second, there is a spurious 1 in the denominator of the expression above. Here is the correct expression:

$$\mathsf{E}_{n,l} = -\frac{\mathsf{m}_{e} e^{4}}{2 \left(4\pi\epsilon_{o}\right)^{2} \hbar^{2} n^{2}} \left[1 + \frac{e^{4}}{\left(4\pi\epsilon_{o}\right)^{2} \hbar^{2} c^{2} n} \left(\frac{1}{1 + \frac{1}{2} \pm \frac{1}{2}} - \frac{3}{4n}\right)\right]$$
(2)

You will be granted full credit if you solve the problem as stated. However, I will proceed with the corrected energies.

Recall the energy for a level n according to the Bohr model:

$$\mathsf{E}_{\mathsf{n},\mathrm{Bohr}} = \frac{-\mathfrak{m}_{e}e^{4}}{2\left(4\pi\epsilon_{o}\right)^{2}\hbar^{2}\mathfrak{n}^{2}} = \frac{-13.6\,\mathrm{eV}}{\mathfrak{n}^{2}} = \frac{\mathsf{E}_{o,\mathrm{Bohr}}}{\mathfrak{n}^{2}} \tag{3}$$

With this, we can simplify our expression for $E_{n,l}$ above:

$$\mathsf{E}_{n,l} = \frac{\mathsf{E}_{o,\mathrm{Bohr}}}{n^2} \left[1 + \frac{e^4}{(4\pi\epsilon_o)^2 \hbar^2 c^2 n} \left(\frac{1}{l + \frac{1}{2} \pm \frac{1}{2}} - \frac{3}{4n} \right) \right]$$
(4)

If we make a substitution in favor of the fine structure constant, $\alpha = e^2/4\pi\epsilon_0\hbar c$, we could simplify things inside the brackets even further.ⁱ We can also note that $l \pm \frac{1}{2}$ is just the total angular momentum: $l + \frac{1}{2}$ corresponds to the orbital angular momentum l being parallel to the electron's spin angular momentum $(\frac{1}{2})$, whereas $l - \frac{1}{2}$ corresponds to the antiparallel situation. We can clean things up a bit by calling the total angular momentum jⁱⁱ, i.e., $j = l \pm \frac{1}{2}$. This gives us:

$$\mathsf{E}_{\mathbf{n},\mathbf{l}} = \frac{\mathsf{E}_{\mathbf{o},\mathrm{Bohr}}}{\mathfrak{n}^2} \left[1 + \frac{\alpha^2}{\mathfrak{n}^2} \left(\frac{\mathfrak{n}}{\mathfrak{j} + \frac{1}{2}} - \frac{3}{4} \right) \right] \qquad \text{with} \qquad \mathfrak{j} = \mathfrak{l} \pm \frac{1}{2} \tag{5}$$

Thus, the overall energy for states of quantum number n and l can be written as a correction to the Bohr model, whose size depends on the ground state energy in the Bohr model ($E_{0,Bohr}$) relative to the electron's rest energy ($mc^2 = 511 \text{ keV}$), or as the square of the fine structure constant. This is essentially where the name "fine structure constant" comes from – it appears when one attempts to introduce the small corrections of angular momentum and spin into the Bohr model of the hydrogen atom, and correctly predicts the presence of a number of additional spectra lines. The size of the correction is of order $\alpha^2 \approx 1/137^2 \approx 5 \times 10^{-5}$, about 50 parts per million.

In any case, the difference between $E_{n,l}$ and $E_{n,Bohr}$ is now readily found:

$$\mathsf{E}_{n,l} - \mathsf{E}_{n,\mathrm{Bohr}} = \frac{\mathsf{E}_{o,\mathrm{Bohr}}}{n^2} \left[1 + \frac{\alpha^2}{n^2} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right] - \frac{\mathsf{E}_{o,\mathrm{Bohr}}}{n^2} \tag{6}$$

$$=\frac{\mathsf{E}_{\mathsf{o},\mathrm{Bohr}}\alpha^2}{\mathfrak{n}^4}\left(\frac{\mathfrak{n}}{\mathfrak{j}+\frac{1}{2}}-\frac{3}{4}\right)\tag{7}$$

The fractional difference depends only on the fine structure constant and the quantum numbers n and l:

$$\frac{\mathsf{E}_{\mathfrak{n},\mathfrak{l}}-\mathsf{E}_{\mathfrak{n},\mathrm{Bohr}}}{\mathsf{E}_{\mathfrak{n},\mathrm{Bohr}}} = \frac{\alpha^2}{\mathfrak{n}^4} \left(\frac{\mathfrak{n}}{\mathfrak{j}+\frac{1}{2}} - \frac{3}{4} \right) \tag{8}$$

For the particular case n=2, l=1, and antiparallel spin (thus taking $j=l-\frac{1}{2}=\frac{1}{2}$), we have

ⁱThis definition gives the Bohr ground state energy in terms of α as well: $E_{o,Bohr} = -\frac{1}{2}mc^2\alpha^2/n^2$.

ⁱⁱThis is a common thing to do, and you will see it more often.

$$\mathsf{E}_{2,1} - \mathsf{E}_{2,\text{Bohr}} = \frac{\mathsf{E}_{\mathbf{o},\text{Bohr}}\alpha^2}{2^4} \left(\frac{2}{\frac{1}{2} + \frac{1}{2}} - \frac{3}{4}\right) = \alpha^2 \mathsf{E}_{\mathbf{o},\text{Bohr}}\left(\frac{5}{64}\right) \approx -5.66 \times 10^{-5} \,\text{eV} \tag{9}$$

(In the problem as stated, with the erroneous formula, you would have found -1.1×10^{-5} eV.) Since the result is negative, it implies that the antiparallel state is actually lower in energy than the Bohr ground state neglecting angular momentum.ⁱⁱⁱ

We are also asked to find the energy difference between spin parallel and antiparallel to the angular momentum. Parallel corresponds $j=l+\frac{1}{2}$, and antiparallel $j=l-\frac{1}{2}$. Thus,

$$\mathsf{E}_{\mathfrak{n},\mathfrak{l},\uparrow\uparrow} - \mathsf{E}_{\mathfrak{n},\mathfrak{l},\uparrow\downarrow} = \frac{\mathsf{E}_{\mathfrak{o},\mathrm{Bohr}}}{\mathfrak{n}^2} \left[1 + \frac{\alpha^2}{\mathfrak{n}^2} \left(\frac{\mathfrak{n}}{\mathfrak{l}+1} - \frac{3}{4} \right) \right] - \frac{\mathsf{E}_{\mathfrak{o},\mathrm{Bohr}}}{\mathfrak{n}^2} \left[1 + \frac{\alpha^2}{\mathfrak{n}^2} \left(\frac{\mathfrak{n}}{\mathfrak{l}} - \frac{3}{4} \right) \right]$$
(10)

$$= \frac{\alpha^2 \mathsf{E}_{\mathsf{o},\mathrm{Bohr}}}{\mathfrak{n}^4} \left(\frac{\mathfrak{n}}{\mathfrak{l}+1} - \frac{\mathfrak{n}}{\mathfrak{l}} \right) = -\frac{\alpha^2 \mathsf{E}_{\mathsf{o},\mathrm{Bohr}}}{\mathfrak{n}^3 \mathfrak{l} \,(\mathfrak{l}+1)} \tag{11}$$

For the particular case n=2, l=1,

$$\mathsf{E}_{\mathfrak{n},\mathfrak{l},\uparrow\uparrow} - \mathsf{E}_{\mathfrak{n},\mathfrak{l},\uparrow\downarrow} = -\frac{\alpha^2 \mathsf{E}_{\mathbf{o},\mathrm{Bohr}}}{2^4} = \frac{1}{16} \alpha^2 \mathsf{E}_{\mathbf{o},\mathrm{Bohr}} \approx -4.5 \times 10^{-5} \,\mathrm{eV} \tag{12}$$

Again, since the difference is negative, and both energies are negative, it implies the antiparallel state has a lower energy than the parallel state. You can see

http://hyperphysics.phy-astr.gsu.edu/Hbase/quantum/hydfin.html

For a brief discussion of this and the hydrogen-deuterium splitting.

2. The wave function for an electron in the 2p state of hydrogen is given by

$$\psi_{2p} = \frac{1}{\sqrt{3} \left(2a_{o}\right)^{3/2}} \frac{r}{a_{o}} e^{-r/2a_{o}}$$
(13)

where a_o is the Bohr radius, $a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 0.529 \times 10^{-10}$ m. What is the most likely distance from the nucleus to find an electron in the 2p state? Express your answer in terms of a_o .

The most likely distance corresponds to the distance at which the probability of finding the electron is maximum. This is distinct from the expected value of the radius $\langle r \rangle$. The probability of finding an electron at a distance r in the interval [r, r + dr], in spherical coordinates, is the squared magnitude

 $^{^{\}rm iii}{\rm Keep}$ in mind that the energies are all negative when taking their differences \ldots

of the wavefunction times the volume of a spherical shell of thickness dr and radius r:

$$P(\mathbf{r}) d\mathbf{r} = |\psi|^2 \cdot 4\pi \mathbf{r}^2 d\mathbf{r} \qquad \text{or} \qquad P(\mathbf{r}) = |\psi|^2 \cdot 4\pi \mathbf{r}^2 \tag{14}$$

Given $\psi_2 p$ above, we have

$$P(\mathbf{r}) = \left| \frac{1}{\sqrt{3} (2a_o)^{3/2}} \frac{\mathbf{r}}{a_o} e^{-\mathbf{r}/2a_o} \right|^2 \cdot 4\pi \mathbf{r}^2 = \frac{\pi \mathbf{r}^4}{6a_o^5} e^{-\mathbf{r}/a_o}$$
(15)

The most probable radius is when P(r) takes a maximum value, which must occur when dP/dr=0 and $d^2P/dr^2 < 0$. Thus:

$$\frac{\mathrm{dP}}{\mathrm{dr}} = 0 = \left(\frac{\pi}{6a_o^5}\right) \frac{\mathrm{d}}{\mathrm{dr}} \left(r^4 e^{-r/a_o}\right) = \left(\frac{\pi}{6a_o^5}\right) \left(4r^3 e^{-r/a_o} - \frac{r^4}{a_o}e^{-r/a_o}\right) \tag{16}$$

$$0 = \left(\frac{\pi r^3}{6a_o^5} e^{-r/a_o}\right) \left(4 - \frac{r}{a_o}\right) \tag{17}$$

$$\implies \mathbf{r} = \{0, 4\mathbf{a_o}, \infty\} \tag{18}$$

One can either apply the second derivative test or make a quick plot of P(r) to verify that $r=4a_o$ is the sole maximum of the probability distribution, and hence the most probable radius, while r=0 and $r=\infty$ are minima.

3. Repeat the previous problem for an electron in the 2s state, where

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_o}\right)^{3/2} \left(2 - \frac{r}{a_o}\right) e^{-r/2a_o} \tag{19}$$

Repeating our earlier procedure,

$$\mathsf{P}(\mathsf{r}) = \left| \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_{\rm o}} \right)^{3/2} \left(2 - \frac{\mathsf{r}}{a_{\rm o}} \right) e^{-\mathsf{r}/2a_{\rm o}} \right|^2 \cdot 4\pi \mathsf{r}^2 = \frac{1}{8a_{\rm o}^3} \left(4\mathsf{r}^2 - \frac{4\mathsf{r}^3}{a_{\rm o}} + \frac{\mathsf{r}^4}{a_{\rm o}^2} \right) e^{-\mathsf{r}/a_{\rm o}}$$
(20)

The most probable radius occurs when

$$\frac{dP}{dr} = 0 = \left(\frac{1}{8a_o^3}\right) \left(8r - \frac{12r^2}{a_o} + \frac{4r^3}{a_o^2}\right) e^{-r/a_o} - \left(\frac{1}{8a_o^4}\right) \left(4r^2 - \frac{4r^3}{a_o} + \frac{r^4}{a_o^2}\right) e^{-r/a_o}$$
(21)

$$0 = \left(\frac{re^{-r/a_{o}}}{8a_{o}^{3}}\right) \left(8 - 12\frac{r}{a_{o}} + 4\frac{r^{2}}{a_{o}^{2}} - 4\frac{r}{a_{o}} + 4\frac{r^{2}}{a_{o}^{2}} - \frac{r^{3}}{a_{o}^{3}}\right)$$
(22)

At this point, we can already see the trivial solutions r = 0 and $r = \infty$, which just like last time

are uninteresting minima of the probability distribution. The interesting solutions are more easily found if we make a variable substitution $x = r/a_o$:

$$0 = 8 - 16\mathbf{x} + 8\mathbf{x}^2 - \mathbf{x}^3 \tag{23}$$

One can factor this thing by synthetic division and find the roots to be $\{2, 3 \pm \sqrt{5}\}$, but the roots are more easily found on your average graphic calculator to be

$$\mathbf{x} = \frac{\mathbf{r}}{\mathbf{a}_{o}} = \left\{ 0, 3 \pm \sqrt{5} \right\} \approx \{0.764, 2.00, 5.24\}$$
(24)

Direct substitution, or a quick plot of P(r) verifies that $r=0.764a_o$ is a local maximum, $r=2.00a_o$ is a local minimum (zero, actually), and $r=5.24a_o$ is the global maximum we seek.

4. In the quantum theory of diamagnetism, one can write the susceptibility in terms of the mean square distance of electrons from the nucleus $\langle r^2 \rangle$:

$$\chi_{d} = \frac{N\mu}{H} = -\frac{\mu_{0}Ze^{2}n}{6m}\langle r^{2}\rangle$$

where n is the number of atoms per unit volume, Z the atomic number, e and m are the electron charge and mass. The wavefunction of the hydrogen atom in its ground state (1s) is

$$\psi_0 = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

where a_o is the Bohr radius. Show that $\langle r^2 \rangle = 3a_0^2$, and calculate the diamagnetic susceptibility of atomic hydrogen. You may assume that the number of atoms per unit volume is given by Loschmidt's number, $n_0 = 2.687 \times 10^{25} \text{ m}^{-3}$ (*i.e.*, calculate χ_d at STP).

Hint: Remember that the volume element in spherical coordinates is $dV = r^2 \sin \theta \, dr \, d\theta \, d\phi$ when you try to find $\langle r^2 \rangle$. The following integral will be useful:

$$\int_0^\infty x^n e^{-\alpha x} = \frac{n!}{a^{n+1}}$$

First, we must find $\langle \mathbf{r}^2 \rangle$:

$$\langle \mathbf{r}^2 \rangle = \int \mathbf{r}^2 |\psi|^2 \, \mathrm{d}\mathbf{V} = \int_0^\pi \mathrm{d}\theta \, \int_0^{2\pi} \mathrm{d}\varphi \, \int_0^\infty \mathbf{r}^2 \left(\frac{1}{\pi a_o^3}\right) e^{-2\mathbf{r}/a_o} \, \mathbf{r}^2 \sin\theta \, \mathrm{d}\mathbf{r} \, \mathrm{d}\theta \, \mathrm{d}\varphi \tag{25}$$

$$= \frac{4}{\mathfrak{a}_{o}^{3}} \int_{0}^{\infty} r^{4} e^{-2r/\mathfrak{a}_{o}} \, \mathrm{d}r = \frac{4}{\mathfrak{a}_{o}^{3}} \frac{4!}{(2/\mathfrak{a}_{o})^{5}} = 3\mathfrak{a}_{o}^{2}$$
(26)

Substituting this, $n = n_0$, Z = 1, and $a_o = 5.29 \times 10^{-11}$ m in our formula for χ_d ,

$$\chi_{d} = \frac{N\mu}{H} = -\frac{\mu_{0}Ze^{2}n}{6m} \langle r^{2} \rangle \approx -1.33 \times 10^{-9} \, \mathrm{m}^{3}/\mathrm{mol}$$

If we use Avogadro's number for the number of atoms per mole rather than Loschmidt's number, we obtain $\chi_d \approx 3 \times 10^{-11}\,\rm m^3/mol$

5. (a) Evaluate the expectation values of the position $\langle x \rangle$ for a particle in the ground state of the one-dimensional simple harmonic oscillator, where:

$$\psi_0 = \sqrt{\frac{1}{a\sqrt{\pi}}} e^{-x^2/2a^2} \tag{27}$$

(b) Evaluate the expectation value of the position $\langle x \rangle$ for a particle in the first excited state of the one-dimensional simple harmonic oscillator. The wave function is:

$$\psi_1 = \sqrt{\frac{1}{2a\sqrt{\pi}}} \left(\frac{2x}{a}\right) e^{-x^2/2a^2} \tag{28}$$

where $a = \sqrt{\frac{\hbar}{m\omega_o}}$ and $\omega_o = \sqrt{k/m}$.

(c) Evaluate $\langle x^2 \rangle$ for the ground state and first excited states of the simple harmonic oscillator in one dimension. What is the expectation value of the potential energy of the particle in each state? (d) Find the uncertainty in position, $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ for the ground state and first excited state.

The following integrals may be useful:

$$\int_{0}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{4} \sqrt{\frac{\pi}{\alpha^3}}$$
(29)

$$\int_{-\infty}^{\infty} x^3 e^{-ax^2} dx = \int_{-\infty}^{\infty} x e^{-ax^2} dx = 0$$
(30)

$$\int_{0}^{\infty} x^4 e^{-\alpha x^2} \, \mathrm{d}x = \frac{3}{8} \sqrt{\frac{\pi}{\alpha^5}} \tag{31}$$

For the ground state, we have

$$\langle \mathbf{x} \rangle_{\mathbf{o}} = \int \mathbf{x} |\psi_0|^2 \, \mathrm{d}\mathbf{x} = \frac{1}{a\sqrt{\pi}} \int_{-\infty}^{\infty} \mathbf{x} e^{-\mathbf{x}^2/a^2} \, \mathrm{d}\mathbf{x} = 0$$
 (32)

The integral vanishes by symmetry, since the integrand is an odd function of x (and, it was given above).

Classically, a harmonic oscillator is something like a mass on a spring, which oscillates uniformly about its equilibrium point at x=0. This means that its average position, over a full cycle of motion, is just x=0. The quantum version is no different: if we made many repeated measurements of the particle's position, we would find the average position to be x=0. The same will be true of the first excited state:

$$\langle \mathbf{x} \rangle_1 = \int \mathbf{x} |\psi_1|^2 \, \mathrm{d}\mathbf{x} = \frac{2}{a^3 \sqrt{\pi}} \int_{-\infty}^{\infty} \mathbf{x}^3 e^{-\mathbf{x}^2/a^2} \, \mathrm{d}\mathbf{x} = 0 \tag{33}$$

Evaluating $\langle x^2 \rangle$ proceeds similarly, except that the integrals will *not* vanish, since the integrands will be *even* functions of x

$$\langle x^{2} \rangle_{\mathbf{o}} = \int x^{2} |\psi_{\mathbf{o}}|^{2} \, \mathrm{d}x = \frac{1}{a\sqrt{\pi}} \int_{-\infty}^{\infty} x^{2} e^{-x^{2}/a^{2}} \, \mathrm{d}x = \frac{1}{a\sqrt{\pi}} \cdot 2 \cdot \frac{1}{4} \cdot \sqrt{\frac{\pi}{(1/a^{2})^{3}}} = \frac{1}{2}a^{2} \tag{34}$$

Here the factor of 2 comes from doubling the given integral, with limits of 0 and ∞ , since the desired integral is symmetric about x=0 with limits of $-\infty$ and ∞ . The expectation value of the potential energy can then be found by noting $U=\frac{1}{2}kx^2$, and thus

$$\langle \mathbf{U} \rangle_{\mathbf{o}} = \frac{1}{2} \mathbf{k} \langle \mathbf{x}^2 \rangle_{\mathbf{o}} = \frac{1}{4} \mathbf{k} \mathbf{a}^2 = \frac{1}{4} \mathbf{m} \boldsymbol{\omega}_{\mathbf{o}}^2 \left(\frac{\hbar}{\mathbf{m} \boldsymbol{\omega}} \right) = \frac{1}{4} \hbar \boldsymbol{\omega} = \frac{1}{2} \mathbf{E}_{\mathbf{o}}$$
(35)

As expected, the potential energy is one half the total ground state energy of $E_o = \frac{1}{2}\hbar\omega_o$.

Since we need $\langle x^2 \rangle$ for the first excited state in the last part of the problem, we may as well repeat the preceding calculation for the first excited state:

$$\langle x^2 \rangle_1 = \int x^2 |\psi_1|^2 \, \mathrm{d}x = \frac{2}{a^3 \sqrt{\pi}} \int_{-\infty}^{\infty} x^4 e^{-x^2/a^2} \, \mathrm{d}x = \frac{2}{a^3 \sqrt{\pi}} \cdot 2 \cdot \frac{3}{8} \cdot \sqrt{\frac{\pi}{(1/a^2)^5}} = \frac{3}{2} a^2 \tag{36}$$

This yields $\langle U \rangle_1 = \frac{3}{4} \hbar \omega = \frac{3}{2} E_o$. Finally, we can find the uncertainty in position for both the ground state and first excited state:

$$\Delta \mathbf{x}_{\mathbf{o}} = \sqrt{\langle \mathbf{x}^2 \rangle_{\mathbf{o}} - \langle \mathbf{x} \rangle_{\mathbf{o}}^2} = \sqrt{\langle \mathbf{x}^2 \rangle_{\mathbf{o}}} = \frac{\mathbf{a}}{\sqrt{2}}$$
(37)

$$\Delta x_1 = \sqrt{\langle \mathbf{x}^2 \rangle_1 - \langle \mathbf{x} \rangle_1^2} = \sqrt{\langle \mathbf{x}^2 \rangle_1} = \mathfrak{a} \sqrt{\frac{3}{2}}$$
(38)

6. Electromagnetic radiation of wavelength 20 nm is incident on atomic hydrogen. Assuming that an electron in its ground state is ionized, what is the maximum velocity at which it may be emitted?

We need only analyze conservation of energy: the electron's initial energy E_o plus the photon's energy must give the electron's kinetic energy:

$$\mathsf{E}_{\mathsf{o}} + \frac{\mathsf{h}\mathsf{c}}{\lambda} = (\gamma - 1)\,\mathsf{m}\mathsf{c}^2\tag{39}$$

$$\gamma = \frac{1}{\sqrt{1 - \nu^2/c^2}} = \frac{E_o}{mc^2} + \frac{h}{mc\lambda} + 1$$
(40)

$$1 - \frac{\nu^2}{c^2} = \frac{1}{\left(\frac{E_o}{mc^2} + \frac{h}{mc\lambda} + 1\right)^2} \tag{41}$$

$$\frac{\nu}{c} = \sqrt{1 - \frac{1}{\left(\frac{E_o}{mc^2} + \frac{h}{mc\lambda} + 1\right)^2}}$$
(42)

Given $E_o = -\frac{1}{2}mc^2\alpha^2$ (where $\alpha \approx 1/137$ is the fine structure constant and $\lambda_c = h/mc \approx 0.00243$ nm is the Compton wavelength, we can simplify this somewhat:

$$\frac{\nu}{c} = \sqrt{1 - \frac{1}{\left(\frac{\lambda_c}{\lambda} - \frac{1}{2}\alpha^2 + 1\right)^2}} \approx 0.0138$$
(43)

The dominant contribution is from the photon's initial energy ($\approx 62 \text{ eV}$, compared to $E_o \approx -13.6 \text{ eV}$), so one incurs only a small error in neglecting the electron's binding energy in the ground state.

7. An excited argon ion in a gas discharge radiates a spectral line of wavelength 450 nm. The transition from the excited to the ground state that produces this radiation takes an average time of 10^{-8} s. What is the inherent width of the spectral line $\Delta\lambda/\lambda$? *Hint: uncertainty principle.*

The energy-time uncertainty principle gives us

$$\Delta E \Delta t \ge \frac{h}{4\pi} \qquad \Longrightarrow \qquad \Delta E = \frac{h}{4\pi\Delta t} \tag{44}$$

How do we get from energy uncertainty to wavelength uncertainty? What you cannot do is this:

$$\Delta E = \frac{hc}{\Delta \lambda} \qquad \text{WRONG} \tag{45}$$

Rather, since ΔE is an uncertainty, we must use propagation of uncertainty to find $\Delta \lambda$. First, we can write the energy-wavelength relationship $E = hc/\lambda$ in terms of differentials:

$$\frac{\mathrm{dE}}{\mathrm{d\lambda}} = \frac{-\mathrm{hc}}{\lambda^2} \tag{46}$$

$$d\mathsf{E} = -\frac{\mathsf{h}c}{\lambda^2} \, d\lambda = -\frac{\mathsf{E} \, d\lambda}{\lambda} \tag{47}$$

$$\frac{\mathrm{dE}}{\mathrm{E}} = -\frac{\mathrm{d\lambda}}{\lambda} \tag{48}$$

For small^{iv} but not infinitesimal differences, we may write $|\Delta E/E| \approx \Delta \lambda/\lambda$. This is something you will encounter in your laboratory classes if you have not already; if it is unfamiliar, see, for example,

http://en.wikipedia.org/wiki/Propagation_of_uncertainty

Particularly, the section on "Example formulas" is worth noting. In any event, we may use this result to find the relative uncertainty in wavelength:

$$\frac{\Delta\lambda}{\lambda} = \left|\frac{\Delta E}{E}\right| = \frac{h}{4\pi\Delta t}\frac{\lambda}{hc} = \frac{\lambda}{4\pi c\Delta t} \approx 1 \times 10^{-8}$$
(49)

This gives an absolute uncertainty in wavelength of $\Delta\lambda \approx 5 \times 10^{-6}$ nm.

8. The typical operating voltage for an electron microscope is $\Delta V = 50$ kV. (a) What is the smallest feature one could hope to resolve? (b) What is the equivalent resolution if neutrons are used? (c) Explain in words why electrons are used, and not protons or neutrons.

 $^{^{\}rm iv} {\rm Where}$ "small" means we still only need first-order terms in $\Delta \lambda$ and $\Delta E.$

The smallest feature one could hope to resolve would be of the order of the wavelength of the electron, in analogy to microscopy with light waves. For massive objects, de Broglie first related an objects wavelength λ to its momentum $|\vec{p}|$:

$$\lambda = \frac{h}{|\vec{p}|}$$

where h is Planck's constant as usual. If we can find the particle's momentum, we can find its wavelength, and hence estimate the microscope's resolution. If the electron is accelerated by a $\Delta V = 50 \text{ kV}$ electric potential, we know that it starts with a relative potential energy $e\Delta V$ which is wholly converted into kinetic energy. From the accelerating voltage, we can get kinetic energy, from which we can get velocity, which gives us momentum and finally wavelength.

Somewhat shorter is to use an alternative formula for kinetic energy, which you can readily verify is correct, and add conservation of energy as described above:

$$\mathsf{KE} = \frac{|\vec{\mathbf{p}}|^2}{2\mathsf{m}} = e\Delta \mathsf{V}$$

Solving this equation for momentum ...

$$|\vec{p}|^2 = 2me\Delta V$$

 $|\vec{p}| = \sqrt{2me\Delta V}$

Now plugging that into the de Broglie relationship, and using the requisite constants and electron mass:

$$\begin{split} \lambda &= \frac{h}{|\vec{p}|} = \frac{h}{\sqrt{2me\Delta V}} \\ &= \frac{6.63 \times 10^{-34} \,\mathrm{J} \cdot \mathrm{s}}{\sqrt{2 \cdot 9.11 \times 10^{-31} \,\mathrm{kg} \cdot 1.60 \times 10^{-19} \,\mathrm{C} \cdot 50.0 \times 10^3 \,\mathrm{V}}} = 5.49 \times 10^{-12} \, \frac{\left[\mathrm{kg} \cdot \frac{\mathrm{m}^2}{\mathrm{s}^2} \cdot \mathrm{s}\right]}{\sqrt{\left[\mathrm{kg} \cdot \mathrm{C} \cdot \mathrm{V}\right]}} \\ &= 5.49 \times 10^{-12} \, \frac{\left[\mathrm{kg} \cdot \mathrm{m}^2\right]}{\left[\mathrm{s}\sqrt{\mathrm{kg} \cdot \mathrm{C} \cdot (\mathrm{N/C}) \cdot \mathrm{m}}\right]} = 5.49 \times 10^{-12} \, \frac{\left[\mathrm{kg} \cdot \mathrm{m}^2\right]}{\left[\mathrm{s}\sqrt{\mathrm{kg} \cdot (\mathrm{kg} \cdot \mathrm{m/s}^2) \cdot \mathrm{m}}\right]} \\ &= 5.49 \times 10^{-12} \, \frac{\left[\mathrm{kg} \cdot \mathrm{m}^2\right]}{\left[\mathrm{s} \cdot \mathrm{kg} \cdot \mathrm{m/s}\right]} = 5.49 \times 10^{-12} \, \mathrm{m} = 5.49 \,\mathrm{pm} \end{split}$$

The units are a bit ugly here, which is why we worked them out explicitly for a change ... for the units to come out properly, it is easiest to remember that the entire bit under the radical above must have units of momentum, or kg \cdot m/s (which avoids much of the manipulation above), or at

least to remember that 1 N/C = 1 V/m to do it the hard way. Anyway: this is a decent estimate of the *fundamental* resolution of an electron microscope operating at 50 kV accelerating potential. In reality, the resolution limit is a few orders larger most of the time – the electromagnetic lenses aren't perfect, and we have thermal motion to worry about besides.

What about if we use neutrons? The answer is far simpler in this case: since neutrons have no charge, they can't be accelerated by electric potentials like electrons. The microscope simply won't work like this, there is no resolution! Why not protons, though, since they can be accelerated by potentials? Electrons, we found, are bound to their atomic nuclei with energies on the order of a few or a dozen electron volts - they are easy enough to remove from atoms for acceleration and focusing. Protons, being bound within the nucleus, are much, much harder to separate from their constituent atoms - their binding energy is more like a million electron volts (MeV). We use electrons because they are relatively easily isolated and pushed around.

9. The neutral hydrogen atom in its normal state behaves in some respects like an electric charge distribution which consists of a point charge of magnitude e surrounded by a distribution of negative charge whose density is given by

$$-\rho(\mathbf{r}) = Ce^{-2\mathbf{r}/a_o}$$

Here a_o is the *Bohr radius*, 0.53×10^{-10} m, and C is a constant with the value required to make the total amount of negative charge exactly e.

- (a) What is the net electric charge inside a sphere of radius a_0 ?
- (b) What is the electric field strength at this distance from the nucleus?
- (c) What is C?

Charge is charge density integrated through a volume, just as mass is density integrated through volume:

$$q = \int \rho \, dV \tag{50}$$

If we want the charge contained in a radius a_o from the origin, we simply perform the integral over the interval $r: 0 \to a_o$ and over the full range of θ and φ . Performing the integral over all space (i.e., $r: 0 \to \infty$) would give us the whole charge of an electron, which must be -e. We'll use this fact in part c.

The first question is: how to perform the volume integral? Our function is radially symmetric, and this strongly suggests – no, *insists* – that we use spherical coordinates. Let's try setting it up in

cartesian coordinates to see why. In cartesian coordinates, a volume element is dV = dx dy dz, and our radius is $r = \sqrt{x^2 + y^2 + z^2}$. Thus,

$$q = -\int dx \int dy \int dz \ C e^{-\frac{2}{a_o}\sqrt{x^2 + y^2 + z^2}}$$
(51)

where the limits of integration correspond to $\sqrt{x^2 + y^2 + z^2}$ running from 0 to a_o . This integral puzzles even the Wolfram Integrator ... which is not a good sign. In spherical coordinates, our volume element is

$$d\mathbf{V} = \mathbf{r}^{2}\sin\theta \,d\mathbf{r} \,d\theta \,d\varphi \qquad \text{where} \quad \begin{cases} \mathbf{r}: 0 \to \mathbf{a}_{o} \\ \theta: 0 \to \pi \\ \varphi: 0 \to 2\pi \end{cases}$$
(52)

where we have also indicated the appropriate ranges for the integration. What is nice about this? First, there are no θ or ϕ terms in our function, so those integrals are trivial. Second, the integral over r is tractable. Let's grind through it:

$$q(a_{o}) = \int_{0}^{\pi} \sin\theta \, d\theta \int_{0}^{2\pi} d\phi \int_{0}^{a_{o}} \rho(\mathbf{r}) \mathbf{r}^{2} \, d\mathbf{r}$$
(53)

note
$$\int_{0}^{\pi} \sin \theta d\theta = -\cos \theta \Big|_{0}^{\pi} = 2 \quad \text{and} \quad \int_{0}^{2\pi} d\phi = \phi \Big|_{0}^{2\pi} = 2\pi$$
(54)

$$q(\mathbf{a}_{o}) = 4\pi \int_{0}^{\mathbf{a}_{0}} \rho(\mathbf{r})\mathbf{r}^{2} \, \mathrm{d}\mathbf{r}$$
(55)

The last integral is doable. You can integrate by parts twice, starting with u=r and $dv=e^{-2r/a_0}$. Also, Wolfram is all over it. The result is

$$q(a_{o}) = -4\pi C \int_{0}^{a_{0}} r^{2} e^{-2r/a_{o}} dr = -4\pi C \left[\frac{-1}{4} e^{-2r/a_{o}} \left(a_{o}^{3} + 2ra_{o}^{2} + 2a_{o}r \right) \right]_{0}^{a_{o}}$$
(56)

$$q(\mathbf{a}_{\mathbf{o}}) = \pi \mathbf{C} \mathbf{a}_{\mathbf{o}}^3 \left(\frac{5}{e^2} - 1\right) \approx -0.32\pi \mathbf{C} \mathbf{a}_{\mathbf{o}}^3 \tag{57}$$

Note that here e is the base of the natural logarithm, *not* the electron charge!

What is the field at $r = a_o$? If the charge distribution is spherically symmetric, we can apply Gauss'

law: it looks just like a point charge of magnitude $q(a_o)$. Thus,

$$\vec{\mathbf{E}} = \frac{\mathbf{kq}}{\mathbf{a}_{\mathbf{o}}^2}\,\hat{\mathbf{r}} = \pi \mathbf{k} \mathbf{C} \mathbf{a}_{\mathbf{o}} \left(\frac{5}{e^2} - 1\right)\,\hat{\mathbf{r}}$$
(58)

Finally, we need the normalization constant C. We can find this by noting that the charge distribution integrated over all space must give the net charge for one electron, viz., -e. Rather than performing the integration over $r: 0 \rightarrow a_o$, we perform it over $r: 0 \rightarrow \infty$ and note $\lim_{r\to\infty} e^{-r}r^n = 0$.

$$q_{tot} = -e = -4\pi C \int_{0}^{\infty} r^2 e^{-2r/a_o} dr = -4\pi C \left[\frac{-1}{4} e^{-2r/a_o} \left(a_o^3 + 2ra_o^2 + 2a_o r \right) \right]_{0}^{\infty}$$
(59)

$$-\mathbf{e} = -4\pi C \left(-\frac{1}{4}a_{o}^{3}\right) = \pi C a_{o}^{3} \tag{60}$$

$$\implies C = \frac{e}{\pi a_o^3} \tag{61}$$

Note that here e is the electron charge ... and thus about 32% of the electron's total charge is contained within a radius a_o in this model based on our earlier result.