6.055J / 2.038J The Art of Approximation in Science and Engineering Spring 2008

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Let *A* be the atomic mass of the atom; it is (roughly) the number of protons and neutrons in the nucleus. Although *A* is called a mass, it is dimensionless. Each atom occupies a cube of side length  $a \sim 3$  Å, and has mass  $Am_{proton}$ . The density of the substance is

$$\rho = \frac{\text{mass}}{\text{volume}} \sim \frac{Am_{\text{proton}}}{(3 \text{ Å})^3}.$$

You do not need to remember or look up  $m_{\text{proton}}$  if you multiply this fraction by unity in the form of  $N_A/N_A$ , where  $N_A$  is Avogadro's number:

$$\rho \sim \frac{Am_{\rm proton}N_{\rm A}}{(3\,{\rm \AA})^3 \times N_{\rm A}}$$

The numerator is A g, because that is how  $N_A$  is defined. The denominator is

$$3 \cdot 10^{-23} \,\mathrm{cm}^3 \times 6 \cdot 10^{23} = 18.$$

So instead of remembering  $m_{\text{proton}}$ , you need to remember  $N_A$ . However,  $N_A$  is more familiar than  $m_{\text{proton}}$  because  $N_A$  arises in chemistry and physics. Using  $N_A$  also emphasizes the connection between microscopic and macroscopic values. Carrying out the calculations:

$$\rho \sim \frac{A}{18} \,\mathrm{g} \,\mathrm{cm}^{-3}.$$

The table compares the estimate against reality. Most everyday elements have atomic masses between 15 and 150, so the density estimate explains why most densities lie between 1 and 10 g cm<sup>-3</sup>. It also shows why, for materials physics, cgs units are more convenient than SI units are. A typical cgs density of a solid is 3 g cm<sup>-3</sup>, and 3 is a modest number and easy to remember and work with. However, a typical SI density of a solid 3000 kg m<sup>-3</sup>. Numbers such as 3000 are unwieldy. Each time you use it, you have to think, 'How many powers of ten were there again?' So the table tabulates densities using the cgs units

of  $g \text{ cm}^{-3}$ . I even threw a joker into the pack – water is not an element! – but the density estimate is amazingly accurate.

## 7.4.3 Physical interpretation

The previous method, dimensional analysis, is mostly mathematical. As a second computation of  $a_0$ , we show you a method that is mostly physics. Besides checking the Bohr radius, it provides a physical interpretation of it. The Bohr radius is the radius of the orbit with the lowest energy (the ground state). The energy is a sum of kinetic and potential energy. This division suggests, again, a divide-and-conquer approach: first the kinetic energy, then the potential energy.



Element	$ ho_{ ext{estimated}}$	$ ho_{ m actual}$
Li	0.39	0.54
H <sub>2</sub> O	1.0	1.0
Si	1.56	2.4
Fe	3.11	7.9
Hg	11.2	13.5
Au	10.9	19.3
U	13.3	18.7

## 6.055 / Art of approximation

What is the origin of the kinetic energy? The electron does not orbit in any classical sense. If it orbited, it would, as an accelerating charge, radiate energy and spiral into the nucleus. According to quantum mechanics, however, the proton confines the electron to a region of size r – still unknown to us – and the electron exists in a so-called stationary state. The nature of a stationary state is mysterious; no one understands quantum mechanics, so no one understands stationary states except mathematically. However, in an approximate estimate you can ignore details such as the meaning of a stationary state. The necessary information here is that the electron is, as the name of the state suggests, stationary: It does not radiate. The problem then is to find the size of the region to which the electron is confined. In reality the electron is smeared over the whole universe; however, a significant amount of it lives within a typical radius. This typical radius we estimate and call  $a_0$ .

For now let this radius be an unknown *r* and study how the kinetic energy depends on *r*. Confinement gives energy to the electron according to the **uncertainty principle**:

$$\Delta x \Delta p \sim \hbar,$$

where  $\Delta x$  is the position uncertainty and  $\Delta p$  is the momentum uncertainty of the electron. In this model  $\Delta x \sim r$ , as shown in the figure, so  $\Delta p \sim \hbar/r$ . The kinetic energy of the electron is

$$E_{\text{Kinetic}} \sim \frac{(\Delta p)^2}{m_{\text{e}}} \sim \frac{\hbar^2}{m_{\text{e}}r^2}$$

This energy is the **confinement energy** or the **uncertainty energy**. This idea recurs in the book.

The potential energy is the classical expression

$$E_{\text{Potential}} \sim -\frac{e^2}{4\pi\epsilon_0 r}.$$

The total energy is the combination

$$E = E_{\text{Potential}} + E_{\text{Kinetic}} \sim -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{m_e r^2}.$$

The two energies compete. At small r, kinetic energy wins, because of the  $1/r^2$ ; at large r, potential energy wins, because it goes to zero less rapidly. Is there a minimum combined energy at some intermediate value of r? There has to be. At small r, the slope dE/dr is negative. At large r, it is positive. At an intermediate r, the slope crosses between positive and negative. The energy is a a minimum there. The location would be easy to estimate if the energy were written in dimensionless form. Such a rewriting is not mandatory in this example, but it is helpful in complicated examples and is worth learning in this example.

In constructing the dimensionless group containing  $a_0$ , we constructed another length:

$$l = \frac{\hbar^2}{m_{\rm e}(e^2/4\pi\epsilon_0)}$$



To scale any length – to make it dimensionless – divide it by l. So in the total energy the scaled radius

$$\bar{r}\equiv \frac{r}{l}.$$

The other unknown in the total energy is the energy itself. To make it dimensionless, a reasonable energy scale to use is  $e^2/4\pi\epsilon_0 l$  by defining scaled energy as

$$\bar{E} \equiv \frac{E}{e^2/4\pi\epsilon_0 l}.$$

Using the dimensionless length and energy, the total energy

$$E = E_{\text{Potential}} + E_{\text{Kinetic}} \sim -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{m_{\text{e}}r^2}$$

becomes

$$\bar{E} \sim -\frac{1}{\bar{r}} + \frac{1}{\bar{r}^2}.$$

The ugly constants are placed into the definitions of scaled length and energy. This dimensionless energy is easy to think about and to sketch.

Simple calculus: minimizing scaled energy  $\bar{E}$  versus scaled bond length  $\bar{r}$ . The scaled energy is the sum of potential and kinetic energy. The shape of this energy illustrates Feynman's explanation of the atomic hypothesis. At a 'little distance apart' – for large  $\bar{r}$  – the curve slopes upward; to lower their energy, the proton and electron prefer to move closer, and the resulting force is attractive. 'Upon being squeezed into one another' – for small  $\bar{r}$  – the potential rapidly increases, so the force between the particles is repulsive. Somewhere between the small and large regions of  $\bar{r}$ , the force is zero.



Calculus (differentiation) locates this minimum-energy  $\bar{r}$  at  $\bar{r}_{min} = 2$ . An alternative method is **cheap minimization**: When two terms compete, the minimum occurs when the terms are roughly equal. This method of minimization is familiar from **Section 6.2.2**.

Equating the two terms  $\bar{r}^{-1}$  and  $\bar{r}^{-2}$  gives  $\bar{r}_{min} \sim 1$ . This result gives a scaled length. In actual units, it is

$$r_{\min} = l\bar{r}_{\min} = \frac{\hbar^2}{m_{\rm e}(e^2/4\pi\epsilon_0)},$$

which is the Bohr radius computed using dimensional analysis. The sloppiness in estimating the kinetic and potential energies has canceled the error introduced by cheap minimization!

Here is how to justify cheap minimization. Consider a reasonable general form for E:

$$E(r)=\frac{A}{r^n}-\frac{B}{r^m}.$$

This form captures the important feature of the combined energy

$$E = E_{\text{Potential}} + E_{\text{Kinetic}} \sim -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{m_e r^2},$$

that two terms represent competing physical effects. Mathematically, that physical fact is shown by the opposite signs.

To find the minimum, solve  $E'(r_{\min}) = 0$  or

$$-n\frac{A}{r_{\min}^{n+1}} + m\frac{B}{r_{\min}^{m+1}} = 0.$$

The solution is

$$\frac{A}{r_{\min}^n} = \frac{n}{m} \frac{B}{r_{\min}^m} \qquad \text{(calculus)}.$$

This method minimizes the combined energy by equating the two terms  $A/r^n$  and  $B/r^m$ :

$$\frac{A}{r_{\min}^n} = \frac{B}{r_{\min}^m}.$$

This approximation lacks the n/m factor in the exact result. The ratio of the two estimates for  $r_{\min}$  is

$$\frac{\text{approximate estimate}}{\text{calculus estimate}} \sim \left(\frac{n}{m}\right)^{1/(m-n)},$$

which is smaller than 1 unless n = m, when there is no maximum or minimum. So the approximate method underestimates the location of minima and maxima.

To judge the method in practice, apply it to a typical example: the potential between nonpolar atoms or molecules, such as between helium, xenon, or methane. This potential is well approximated by the so-called Lennard–Jones potential where m = 6 and n = 12:

$$U(r) \sim \frac{A}{r^{12}} - \frac{B}{r^6}$$

The approximate result underestimates  $r_{\min}$  by a factor of

$$\left(\frac{12}{6}\right)^{1/6} \sim 1.15.$$

An error of 15 percent is often small compared to the other inaccuracies in an approximate computation, so this method of approximate minimization is a valuable time-saver.

Now return to the original problem: determining the Bohr radius. The approximate minimization predicts the correct value. Even if the method were not so charmed, there is no point in doing a proper, calculus minimization. The calculus method is *too accurate* given the inaccuracies in the rest of the derivation.

Engineers understand this idea of not over-engineering a system. If a bicycle most often breaks at welds in the frame, there is little point replacing the metal between the welds with expensive, high-strength aerospace materials. The new materials might last 100 years instead of 50 years, but such a replacement would be overengineering. To improve a bicycle, put effort into improving or doing without the welds.

In estimating the Bohr radius, the kinetic-energy estimate uses a crude form of the uncertainty principle,  $\Delta p \Delta x \sim \hbar$ , whereas the true statement is that  $\Delta p \Delta x \geq \hbar/2$ . The estimate also uses the approximation  $E_{\text{Kinetic}} \sim (\Delta p)^2/m$ . This approximation contains *m* instead of 2m in the denominator. It also assumes that  $\Delta p$  can be converted into an energy as though it were a true momentum rather than merely a crude estimate for the root-mean-square momentum. The potential- and kinetic-energy estimates use a crude definition of position uncertainty  $\Delta x$ : that  $\Delta x \sim r$ . After making so many approximations, it is pointless to minimize the result using the elephant gun of differential calculus. The approximate method is as accurate as, or perhaps more accurate than the approximations in the energy.

This method of equating competing terms is **balancing**. We balanced the kinetic energy against the potential energy by assuming that they are roughly the same size. The consequence is that

$$a_0 \sim \frac{\hbar^2}{m_{\rm e}(e^2/4\pi\epsilon_0)}$$

Nature could have been unkind: The potential and kinetic energies could have differed by a factor of 10 or 100. But Nature is kind: The two energies are roughly equal, except for a constant that is nearly 1. 'Nearly 1' is also called **of order unity**. This rough equality occurs in many examples, and you often get a reasonable answer by pretending that two energies (or two quantities with the same units) are equal. When the quantities are potential and kinetic energy, as they often are, you get extra safety: The so-called virial theorem protects you against large errors (for more on the virial theorem, see any intermediate textbook on classical dynamics).

## 7.5 Bending of light by gravity

Rocks, birds, and people feel the effect of gravity. So why not light? The analysis of that question is a triumph of Einstein's theory of general relativity. I can calculate how gravity bends light by solving the so-called geodesic equations from general relativity:

$$\frac{d^2 x^\beta}{d\lambda^2} + \Gamma^\beta_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda} = 0.$$