Tuesday 17th May 2005

Answer to Quantum Physics Classwork 5

The Quantum Mechanics of Bricks

1. The density is the mass per atom divided by the volume per atom. We are given an atomic radius $a \approx 1$ Å. Since it is impossible to pack spheres perfectly, the volume per atom must be greater than $4\pi a^3/3$. And since most crystal structures are denser than the simple cubic structure, the volume per atom is probably less than $(2a)^3$.

   Hence:
   $$\frac{20 \times 1.66 \times 10^{-27}}{\frac{4}{3}\pi(10^{-10})^3} > \rho > \frac{20 \times 1.66 \times 10^{-27}}{(2 \times 10^{-10})^3} \ ,$$
   yielding (very roughly)
   $$8000\,\mathrm{kg\,m^{-3}} > \rho > 4000\,\mathrm{kg\,m^{-3}} \ .$$
   (An estimate made using a brick I found in the garden, a ruler and my bathroom scales suggests that the real answer is less than $2000\,\mathrm{kg\,m^{-3}}$.)

2. $\langle x \rangle = 0$ because the atom is sitting at the origin; $\langle p_x \rangle = 0$ because the atom is stationary.

3. We are told that
   $$\langle r^2 \rangle = \langle x^2 + y^2 + z^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = a^2 \ .$$
   Since the atom is spherical, $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle$, this gives
   $$3\langle x^2 \rangle = a^2 \ .$$
   Remembering that $\langle x \rangle = 0$, we obtain
   $$(\triangle x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle = a^2/3 \ ,$$
   or
   $$\triangle x = a/\sqrt{3} \ ,$$
   as required.

4. Since $\langle p_x \rangle = 0$, it follows that $(\triangle p_x)^2 = \langle (p_x - \langle p_x \rangle)^2 \rangle = \langle p_x^2 \rangle$. Assuming minimum uncertainty (the equality in the uncertainty principle) and setting $\triangle x = a/\sqrt{3}$, we obtain:

$$\langle p_x^2 \rangle = (\triangle p_x)^2 \approx \frac{3\hbar^2}{4a^2} \, .$$

Substituting for p_x using $p_x = mv_x$ then gives:

$$\langle \frac{1}{2} m v_x^2 \rangle = \frac{\langle p_x^2 \rangle}{2m} \approx \frac{3\hbar^2}{8ma^2} \, .$$

5. The outermost electron sees the charge $+Ze$ of the nucleus, but also the charge $-(Z-1)e$ of all the inner electrons. The effective charge is $+e$ regardless of the value of Z.

6. The total energy is the sum of the KE (x, y and z components) and the PE:

$$E \approx \frac{9\hbar^2}{8ma^2} - \frac{e^2}{4\pi\varepsilon_0 a} \, .$$

Differentiating gives

$$\frac{dE}{da} \approx -\frac{18\hbar^2}{8ma^3} + \frac{e^2}{4\pi\varepsilon_0 a^2} \, ,$$

and solving the equation $dE/da = 0$ gives

$$a \approx \frac{9\pi\varepsilon_0 \hbar^2}{me^2} \approx 1.18 \times 10^{-10}\,\mathrm{m} = 1.18\,\text{Å} \, .$$

The total energy of an electron in this orbit is:

$$E \approx \frac{9\hbar^2}{8ma^2} - \frac{e^2}{4\pi\varepsilon_0 a} \approx -9.73 \times 10^{-19}\,\mathrm{J} \approx -6.08\,\mathrm{eV} \, .$$

The estimate of the ionisation energy is thus 6.08 eV.

Both estimates are pretty good bearing in mind the rough and ready method used.

7. In the expression for the total energy of the atom, the PE term is negative and proportional to $1/a$, while the KE term is positive and proportional to $1/a^2$. To lower the PE, the atom would like to be as small as possible, while to lower the KE, it would like to be as large as possible. The sum of the two terms has a minimum at the actual atomic radius.

   If the electrons were replaced by muons, the PE term would not be affected, but the KE term, which is proportional to $1/m$, would decrease. The PE term would therefore dominate and the atom would be smaller. From the expression for a derived in (6), we can see that the radius is proportional to $1/m$.

   The expression for the atomic radius a derived in (6) does not involve the atomic number because, for reasons explained in (5), the PE of the outermost electron does not depend on the atomic number. In practice, atomic sizes do vary somewhat, partly because the assumption of (5) is only approximate and partly because of shell filling effects.