CHEM 2C

Instructor:

Ram Seshadri, Professor of Materials, and Chemistry and Biochemistry
MRL Rm 3008, x6129, seshadri@mrl.ucsb.edu

Some notes on the Heisenberg uncertainty principle

The Heisenberg Uncertainty Principle relates the uncertainty Δx in the position x of a particle, to the uncertainty Δp_x in the momentum of the particle in the x direction according to

$$\Delta x \Delta p_x \geq \frac{1}{2}\hbar$$

where $\hbar = h/(2\pi)$.

The uncertainty Δx is the *standard deviation* determined from a number of different measurements of the value of x, and likewise, the uncertainty in the momentum Δp_x, is the standard deviation of the momentum p_x. The formal definition is

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \text{ and } \Delta p_x = \sqrt{\langle (p_x - \langle p_x \rangle)^2 \rangle}$$

where the $\langle\,\rangle$ indicate average average values. We can use the equality $\Delta x \Delta p_x \approx \frac{1}{2}\hbar$ to estimate various aspects of atoms, nucleii, and other objects whose behavior is controlled by quantum mechanics.

Energetics of atoms For example, consider that the diameter of a typical atoms is 1 Å or 1×10^{-10} m. This means electrons are trapped in 1D within objects this size. What is the typical energy scale holding electrons together in atoms and giving atoms their structure ?

To answer this, let us set $\Delta x \approx 1 \times 10^{-10}$ m. In effect, we are saying that the electron is somewhere within the atom, and that is the most we know about it. Then the uncertainty in the momentum is obtained:

$$\Delta p_x \approx \frac{1}{2}\hbar/\Delta x \approx \frac{1}{2} \times \frac{1}{2\pi} \times 6.626 \times 10^{-34}\,\text{kg}\,\text{m}^2\text{s}^{-1}/1 \times 10^{-10}\text{m} \approx 5.27 \times 10^{-25}\,\text{kg}\,\text{ms}^{-1}$$

Let us simply guess that the uncertainty in the momentum of the electron is in the typical range of electron momenta, $p_x \approx \Delta p_x$, and use this to calculate the kinetic energy of electrons in atoms. So $p_x = 5.27 \times 10^{-25}\,\text{kg}\,\text{ms}^{-1}$. The kinetic energy (still in 1D) is given by

$$E_K = \frac{1}{2}mv_x^2 = p_x^2/(2m)$$

using $m = m_e$, the mass of the electron ($m_e = 9.109 \times 10^{-31}$ kg), we determine $p_x^2/(2m_e)$:

$$E_K = p_x^2/(2m_e) = (5.27 \times 10^{-25})^2\,\text{kg}^2\,\text{m}^2\,\text{s}^{-2}/2 \times 9.109 \times 10^{-31}\,\text{kg} = 1.52 \times 10^{-19}\,\text{J}$$

We convert this to units that are familiar to people dealing with electrons, notably electron volts (eV). 1 eV is the energy gained by an electron when it experiences an electric field of 1 V (1 volt). The conversion is 1 eV = 1.602×10^{-19} J, so in the case above

$$E_K = 1.52 \times 10^{-17}\,\text{J}/(1.602 \times 10^{-19}\,\text{JeV}^{-1}) = 0.95\,\text{eV} \approx 1\,\text{eV}$$

This is the typical energy scale for electrons in atoms !

Energetics of nucleii Lets now consider that the diameter of a typical nucleus is 1×10^{-15} m. This means protons and neutrons are trapped in 1D within objects this size. What is the typical energy scale holding nucleii together?

To answer this, we set $\Delta x = 1\times10^{-15}$ m. We are saying that a proton is somewhere within the nucleus, and that is the most we know about it. Then the uncertainty in the momentum is obtained:

$$\Delta p_x \approx \frac{1}{2}\hbar/\Delta x \approx \frac{1}{2}\times\frac{1}{2\pi}\times 6.626\times10^{-34}\,\text{kg}\,\text{m}^2\text{s}^{-1}/1\times10^{-15}\text{m} \approx 5.27\times10^{-20}\,\text{kg}\,\text{ms}^{-1}$$

Let us again guess that the uncertainty in the momentum of the proton is in the typical range of proton momenta, $p_x \approx \Delta p_x$, and use this to calculate the kinetic energy of electrons in atoms. So $p_x = 5.27\times10^{-20}\,\text{kg}\,\text{ms}^{-1}$ and $m_p = 1.673\times10^{-27}$ kg. The corresponding scale of the velocity, v_x (along the x direction) is obtained from

$$v_x = p_x/m_p = 5.27\times10^{-20}\,\text{kg}\,\text{m}\,\text{s}^{-1}/1.673\times10^{-27}\,\text{kg} = 3.15\times10^{-7}\,\text{ms}^{-1}$$

Note that the velocity is more than 10% the speed of light, c, so we should properly use relativistic mechanics,[1] but lets just pretend that classical expressions for the energy work.

$$E_K = p_x^2/(2m_p) = (5.27\times10^{-20})^2\,\text{kg}^2\,\text{m}^2\,\text{s}^{-2}/2\times1.673\times10^{-27}\,\text{kg} = 8.30\times10^{-13}\,\text{J}$$

Converting this to eV, we have

$$E_K = 8.30\times10^{-13}\,\text{J}/(1.602\times10^{-19}\,\text{J}\,\text{eV}^{-1}) = 5.2\times10^{6}\,\text{eV} = 5.2\,\text{MeV}$$

Energies associated with the nucleus are a million times larger than energies associated with electrons!

[1]Look at the wikipedia entry on kinetic energy to see what sort of corrections are necessary when velocities start approaching c.