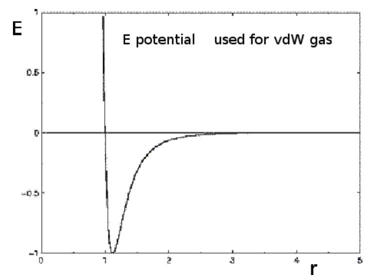
1 Session 1 Week 3 Day 1: potential energy and electrons

1. In addition to the kinetic energy, (for a spherical atom or for an electron, $E_{kinetic} = E_{trans} = \frac{1}{2}mv^2$), molecules and atoms can have a *potential energy.* Kinetic energy is based on how fast the atoms are travelling. In Chem 2070, all potential energy is based on where the atoms are located.

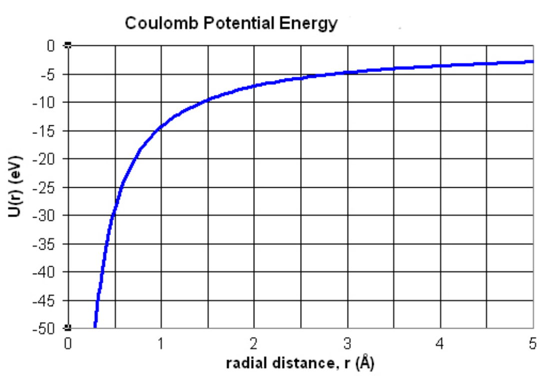
   Potential energy is important because energy is conserved: for a group of molecules which are only in contact with one another, their kinetic energy *plus* their potential energy is invariant. Over time, total energy doesn't change. If the potential energy decreases, the kinetic energy must increase an equal amount.

2. While ideal gas molecules do not have potential energy, van der Waals molecules do. The curve below shows the potential energy between two van der Waals molecules. In this graph, the horizontal axis gives the distance between the two gas molecules, while the vertical axis shows their combined potential energy. Where the potential energy has a *positive* slope, the molecules are attracted to one another. Where it has a *negative* slope, the two gas molecules are repelled.



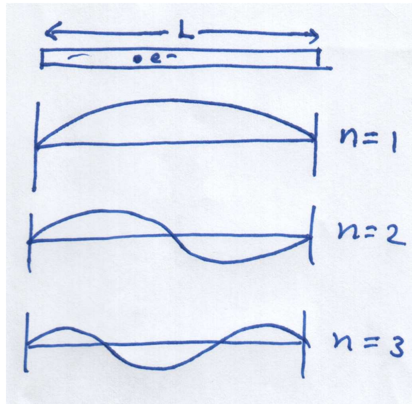
3. Assume two van der Waals gas molecules start a fair distance apart. Assume, initially, neither of the molecules are moving. A movie is made showing the positions and the velocities of the two atoms. Describe in as much detail as you can, what this movie would look like.

4. Shown below is the kinetic and potential energy of an electron and a proton (called the Coulomb or Coulombic energy). Assuming electrons and protons behave as normal objects (Electrons are actually not all that normal: electrons obey the laws of quantum not classical physics), describe what a movie would look like of an electron and a proton, which are initially a fair distance apart from one another and which initially are both not moving, but which, over time, experience a Coulombic attraction to one another.



5. **An electron in a box:** Illustrated below is a very narrow box. It provides one of the simplest quantum mechanical (or wave) models for electrons. The length of the box is L. The box is totally narrow in its other two dimensions. Electrons confined to boxes like these are always waves. These

waves always equal zero at the two ends of the box. Three of the most important waves which meet these conditions are shown in the picture below.



(a) The three waves have each of them a number assigned to them, their quantum number. The letter n is typically chosen to designate the quantum numbers. See picture.
(b) State an equation (with an equal sign) expressing the wavelength, λ, for the $n = 1$ state in terms of L.
(c) State an equation (with an equal sign) expressing the wavelength, λ, for the $n = 2$ state in terms of L.
(d) State an equation (with an equal sign) expressing the wavelength, λ, for the $n = 3$ state in terms of L.
(e) Based on your previous three answers deduce an equation (with an equal sign) expressing the wavelength, λ, in terms of L and n.
(f) In the last problem set, based on the three equations, $E_{trans} = \frac{1}{2}mv^2$, $p = mv$, and $p = \frac{h}{\lambda}$, state again the equation expressing E_{trans} in terms of λ, h, and m.
(g) Based on the previous two problems, please state an equation (with an equal sign) expressing E_{trans} in terms of m, h, n, and L.
(h) Examine your answer to the last question. If the length of the box is doubled, what happens to E_{trans}?
(i) If n is doubled, what happens to E_{trans}?

6. **Bohr model for an atom:** The Bohr model for an atom gives the energy of an electron for atoms or atomic ions with just a single electron: H, He^+, Li^{2+}, Be^{3+}, etc... In this model,

$$E_{total} = -R_H \frac{Z^2}{n^2},$$

where $R_H = 2.179 \times 10^{-18}$ J, Z is the number of protons for the element, and n is the principal quantum number with possible values of 1, 2, 3, 4 .... In the Bohr model, and in fact for the electrons in all stable molecules, $E_{potential} = -2 \times E_{kinetic}$. This last relation is part of the *virial theorem.*

(a) By what factor is the H^+ $n = 1$ electron lower in energy than the H^+ $n = 3$ electron?
(b) By what factor is the Li^{2+} $n = 1$ electron lower in energy than the Li^{2+} $n = 3$ electron?
(c) By what factor is the Li^{2+} $n = 2$ electron lower in energy than the He^+ $n = 5$ electron?
(d) What is the highest possible energy of a He^+ electron?
(e) For what value of n does the Li^{2+} ion have exactly the same energy as the H^+ $n = 3$ electron.