Chem 442: Homework for lecture 2

Bold "Turn in" problem is due at beginning of first lecture next week.

1. A spring has restoring force F=-kx, where k is the spring constant. x=0 when the spring is not stretched or compressed. Assume that x(t=0) = 0 and v(t=0)=0 initially. Plug into the Verlet algorithm to show that x(t=Δt) = 0 also. If the spring is initially unstretched and not moving, it will remain still and do nothing!

Turn in: 2. Now do the same, but let x(t=0) = x_0>0, and v(t=0) = 0. What is x(t=Δt)? Is x(t) bigger or smaller than x(t=0), and why?

3. Starting with V(r) for the Lennard-Jones potential, calculate F(r)=-∂V/∂r. Show that F approaches 0 as r approaches ∞: when two argon atoms are far apart, they do not exert a force on one another.

4. If I move two electrons closer to one another by a factor of 2 in distance, by what factor does the potential energy change? Does it go up or down? Draw a sketch of V(r) as a function of r and mark two distances consistent with the problem.