Homework 1. Dimensions Exercises PH3110 Fall 2006 Due 9/13/06

1. The Lennard-Jones 6-12 interatomic potential is given by:

$$V(r) = -4\varepsilon\left[\left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12}\right],$$

where *V(r)* is the potential energy of a pair of atoms, ε is a parameter with dimensions of energy, and σ is a parameter with dimensions of length.

(a) Plot the dimensionless form for the Lennard-Jones 6-12 potential using a computer or graph paper. (Plot, don't sketch. Make sure your axes are labeled.) You may use a reasonable range of $r'=r/\sigma$ from 0 to 5 or 0 to 10, as you find appropriate.

(b) Analytically find the minimum of the potential (i.e. find V_{min} and at what $r=r_{mi}$) and compare to your plot.

2. The Lennard-Jones potential is commonly used to perform Molecular Dynamics simulations. The natural time scale for the potential is given by ε, σ and also the particle mass, *m*.

(a) Using the method we used in class to find a relationship for Keppler's 3rd law, find the combination of ε, σ and *m* that gives the dimensions of time. Start with $[T] = [\varepsilon]^a[\sigma]^b[m]^c$ and find the exponents a, b, c.

(b) Taking order of magnitude parameters like ε = 1 eV, $\sigma = 10^{-10}$ m and $m = 40\times10^{-26}$ kg, what is the natural time scale for a resulting simulation?