PH: 322 Molecular Simulation Homework 2 **Due date: 2nd March**

1. Consider the angle bending potential of the following form

$$E_\theta = \tfrac{1}{2} \sum_{angles} K_\theta \left(\theta - \theta_o\right)^2$$

Derive the expression for force on the three atoms making the angle bending term. Compare this with the force obtained for the cos-harmonic bending potential give as

$$E_\theta = \tfrac{1}{2} \sum_{angles} K_\theta^{'} \left(\cos\theta - \cos\theta_o\right)^2$$

2. Consider the exponential-6 potential given by following form

$$V_{vdw} = Ae^{-\alpha r} - \left(\frac{C}{r}\right)^6$$

Plot this potential as a function of *r* (inter-particle separation) and discuss its behavior for very small values of *r*

3. For a Lennard-Jones system in NVE ensemble plot the RMS fluctuation in energy as a function of time step (δt) of integration. From this comment on how large time step one can choose for simulation.

4. Remember we discussed the use of switching functions in the context of truncating and shifting the non-bond potential. We discussed the use spline functions as well as various order polynomial switching functions. For non-bond LJ interactions please compare the energy accuracy and RMS fluctuation in force for cubic spline as well as higher order (5th) polynomial switching functions.

5. Show that the heat capacity is related to the fluctuation in total energy through the following relation

$$C_V = \frac{\langle U^2 \rangle - \langle U \rangle^2}{k_B T^2}$$

From your NVT MD simulation calculate the specific heat of the Lennard-Jones system at two densities (one in gas phase and another in liquid phase).

6. Using the MD code (supplied or written by you) compute the equation of state for LJ fluid at T=1.0, T=2.0 and T=0.9. Take a system of 1000 LJ particles.