PH: 322 Molecular Simulation Homework 1 **Due 12th Feb, 2010**

1. Show that volume in phase space is preserved under Hamiltonian dynamics.
2. Show that Liouville operator (L) is hermitian : $L = L^\dagger$
3. Define the propagator $U(t) = exp(iLt)$
(a) Show that it is a unitary operator

$$U^\dagger(t)U(t) = I$$

(b) Show that determinant of U(t) is 1
(c) Define propagator $U(\delta t)$ for small time step δt . Show $U^\dagger(\delta t) = U(-\delta t) = U^{-1}(\delta t)$
and $U(-\delta t)\, U(\delta t) = I$

4. Write the Liouville operator as follows

$$iL = \frac{p}{m}\frac{\partial}{\partial x} + F(x)\frac{\partial}{\partial p} = iL_1 + iL_2$$

$$iL_1 = \frac{p}{m}\frac{\partial}{\partial x} \qquad iL_2 = F(x)\frac{\partial}{\partial p}$$

Show that iL_1 and iL_2 do not commute: $[iL_1, iL_2] \neq 0$.

5. Consider the case of simple harmonic oscillator

$$F(x) = -\omega^2 x$$

Using the position Verlet scheme do the linear stability analysis of the equation of motion. The stability analysis will give you limit on the time step δt to be used in the simulation.

6. Derive the classical propagator for a multiple time step (MTS) integration scheme. Also derive Verlet like equation for the MTS integration scheme.