

Chem. 550

Instructor: Nancy Makri

CLASSICAL – COMPUTER ASSIGNMENT 1

- (a) Write a computer code that implements the Verlet algorithm to integrate Hamilton's equations for a one-dimensional system.
- (b) Use your code to compute classical trajectories in a one-dimensional harmonic system of unit frequency and mass, starting from various initial conditions q_0, p_0 . Plot the trajectories for at least three periods of motion. Verify that your solutions agree with the analytical expression. Check the energy conservation along each trajectory.
- (c) Now set $x_0 = 0$ and plot the trajectories for various values of p_0 . What do you observe?