PHYS-552: Advanced Statistical Mechanics

March 23, 2012

Due date: 29th of March, 2012

1 Reversible Multiple Time Step Molecular Dynamics via the Liouville Operator

Suppose a system has two particles, one with mass M_A the other with mass M_B, and that $M_B >> M_A$. The Hamiltonian can be written as

$$H(p_a, p_B, q_A, q_B) = \frac{p_A^2}{2M_A} + \frac{p_B^2}{2M_B} + V(q_A, q_B). \tag{1}$$

Under these circumstances one expects that the time scales of motion of the two atoms are very different. Construct a multiple time-scale molecular dynamics algorithm in which the Liouville operator is used to derive the equations of motion. The algorithm should be such that the time steps associated with the smaller mass should be smaller than that associated with the larger mass. (Hint: see Frenkel and Smit: Understanding Molecular Simulation, http://www.sciencedirect.com/science/book/9780122673511)

2 Pathria & Beale: Problem 5.1

3 Pathria & Beale: Problem 5.2

4 Pathria & Beale: Problem 5.4