Physics 371: Problem Set 3

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Due date: 8th of March, 2013.

Liouvillian derivation of reversible molecular dynamics algorithms

a.) Using the Liouville formalism derive the Verlet algorithm for a particle in one dimension moving in a potential $V(x)$.

b.) Given a system with two particles, one with mass m the other with mass M $(m<<M)$, interacting via a potential $V(x,X)$, derive an MD algorithm in which the time step used to propagate the particle with the smaller mass is δt, that for the larter mass is Δt, where ($\Delta t = n\delta t$, with n integer).

Metropolis Monte Carlo algorithm and detailed balance

Given a probability distribution $P(x)$ and a transition matrix $T(x|x')$, representing the probability to move to position x' from the position x. In the Metropolis Monte Carlo method a random move is proposed which is accepted or rejected according to some acceptance probability. In this case the transition matrix can be represented as the product of two matrices $T(x|x')=M(x|x')A(x|x')$, where $M(x|x')$ denotes the transition probability of the random move, $A(x|x')$ denotes the acceptance probability given that the system moved from position x to x'.

Using the detailed balance relation, which can be written $P(x)T(x|x') = P(x')T(x'|x)$, derive an explicit form for the acceptance ratio $A(x|x')$ assuming that
a.) $M(x|x')$ is symmetric.
b.) $M(x|x')$ is *not* symmetric.