Problem set 3: Molecular Dynamics

1. In Quantum Mechanics we can assign wave lengths to moving particles. The average velocity of a particle is given by the Maxwell-Boltzmann distribution $(8k_BT/m\Pi)^{0.5}$.
   a. Determine the corresponding DeBroglie wave length $\lambda=h/p$.
   b. You would like to study the glass transition of SiO_2 (T_c=1450K) with Molecular dynamics simulations. The length of a Si-O-bond is 1.6 Angström (h=6.63 10^{-34}JS, k_B=1.38 10^{-23}J/K, m(Si)=28u). Can we describe the system with a classical potential or do we need to consider quantum effects?

2. a. Derive $r(t+\Delta t)$ for the Verlet algorithm.
   b. Demonstrate that velocity Verlet and the Verlet algorithm are equivalent.
   c. If the time step in microcanonical MD is too big, energy drifts. Does the energy drift to higher or lower values? Why?
   d. The equation of motion for the Langevin thermostat is given by:
   $$ma(t) = -\xi v(t) + f(r,t) + f'(t)$$
   Apart from the conservative force f(r,t), there is a friction term $(-\xi v)$ and an additional Gaussian distributed random force (f'), which couples the system to a stochastic heat bath.
   You would like to integrate the equations of motions with the velocity Verlet algorithm. Which problem occurs?
   (Hint: Which terms are needed to derive $v(t+\Delta t)$ and $a(t+\Delta t)$?)
   Is momentum conserved? What happens to the center of mass?

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