Homework assignment #3 for CCB 422/522, Spring 2021

Please show your work for all problems!

1. Start with the Langevin equation:

$$\frac{dv(t)}{dt} = -\zeta v(t) + f(t) \tag{1}$$

(Here, $\zeta = \xi/m$, compared to what was in the notes.) If the velocity at time $t = 0$ is v_0, show that the following is a formal solution:

$$v(t) = v_0 e^{-\zeta t} + e^{-\zeta t} \int_0^t e^{\zeta t'} f(t') dt' \tag{2}$$

Hint: substitute the second equation into the first.

2. Continuing from problem 1: Assuming that the ensemble average of the stochastic force is zero (i.e. $\langle f(t) \rangle = 0$), derive an equation for the ensemble average $\langle v^2 \rangle (t)$. Next, take the limit as $t \to \infty$.

3. Intermolecular interactions that don't involve charges are often approximated by a Lennard-Jones potential:

$$V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

Here r is the separation between atoms and ε and σ are parameters. At low temperatures, entropy is relatively unimportant, and the free energy is minimized when $V(r)$is minimized.

   a) At what separation does that occur?

   b) What is the energy of that state?

   c) What are units of ε and σ ?

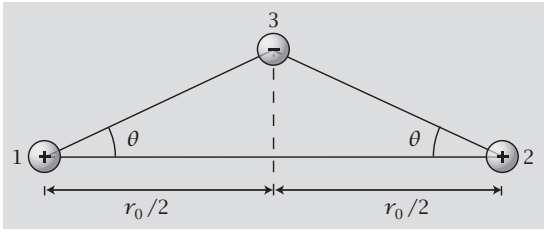
4. Consider two fixed unit positive charges separated by a distance r_0, and a unit negative charge that is free to move along a dividing line (see the figure below).

   a) For fixed r_0, how does the Coulombic energy depend on r_0 and θ?

   b) For what angle θ is the Coulombic energy a minimum?

   c) What is the energy at its minimum value?

   d) At what angle θ is the energy equal to zero?



Two positive charges (1 and 2) at a fixed separation r_0, with a minus charge (3) that is free to move vertically between them.