Homework 5: Langevin Dynamics, NPT, and grand canonical ensembles

Glen Hocky

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1. (Computational) Follow the instructions in the Langevin Dynamics notebook under molecular-dynamics/ at: https://github.com/hockyg/chem-ga-2600/
   You don’t have to turn in anything for this part

2. Ideal gas law at constant pressure. Derive the equivalent of the ideal gas law in the (N,P,T) ensemble. See Tuckerman Chapter 5.5.

3. Volume fluctuations at constant pressure. Derive the relationship between the isothermal compressibility $\kappa = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_{N,T}$ and the variance in the volume $\text{Var}(V) = \langle V^2 \rangle - \langle V \rangle^2$.
   You should be able to do this starting by plugging $V = -k_B T \left( \frac{\partial \ln \Delta}{\partial p} \right)_{N,T}$ into the definition of $\kappa$.

4. Sackur-Tetrode equation for the grand canonical ensemble. Write the entropy of an ideal gas in the ($\mu,V,T$) ensemble. See Tuckerman Chapter 6.5.