PHYS 305 - Assignment #8

Make sure your name is listed as a comment at the beginning of all your work.

Purpose: Develop and explore a simple model using Monte-Carlo sampling.

Monte-Carlo

Sometimes when solving a physical system, the kinetics (dynamics) are unnecessary; you may only be interested in *average* properties of the system. It may be the case that the system is *impossible* to solve analytically or perhaps computational intractable (c.f. many Biophysical systems like protein folding). In this case you'll want to sample the system and tabulate the macrostate quantities. The standard technique for doing this is known as Monte-Carlo, named for the connection to the real-world gambling city counterpart.

For a one-dimensional system with a potential $V(x)$ the most common Monte-Carlo scheme is the Metropolis-Hastings which says

$$P(x_a \to x_b) = \frac{P(x_b)}{P(x_a)} = \exp\left(-\frac{V(x_b) - V(x_a)}{kT}\right) \tag{1}$$

Where k is the Boltzmann's constant and T is the temperature of the system. The idea is to select a random new state x_b, calculate the energy and $P(x_a \to x_b)$. Choose a random number $r \in [0, 1]$ and if $r < P(x_a \to x_b)$ move to state x_b, otherwise stay at the original state x_a.

Double-well Potential

- Set $k = 1$ and use the potential

$$V(-2 \leq x \leq 2) = x^4 - 3x^2 + (1/2)x \tag{2}$$
$$V(x < -2) = \infty \tag{3}$$
$$V(x > 2) = \infty \tag{4}$$

- Subdivide the finite region of the potential into $m = 30$ intervals. Create a vector that records the number of times you visit interval, (g_i would be the number of times you visited the ith interval).

- Starting at $x = 0$ run the Monte-Carlo algorithm $N = 10^6$ times at $T = 1.0$, keeping track at each step which interval you are in.

- Compute the sum-over-all-states (partition function)

$$\mathcal{Z} = \sum_{i}^{m} g_i \tag{5}$$

- Plot the probability of being in each interval ($P(x)$ vs x)

$$P(x_a) = \frac{g_a}{\mathcal{Z}} \tag{6}$$

- Repeat the above procedure with $T \in [0.1, 2.0]$ over $h = 10$ temperature intervals on a single plot with axis labels and a legend. Overlay the potential $V(x)$ onto this plot (you may scale the potential by a constant factor for clarity).
- What happens at high-temperatures? Low temperatures?
- Compute and plot $\langle E \rangle$ vs T, the average energy as a function of temperature over $h = 50$ intervals

$$\langle E \rangle = \sum_{i}^{m} P(x_i) V(x_i) = \frac{1}{\mathcal{Z}} \sum_{i}^{m} g_i V(x_i) \tag{7}$$

$$\tag{8}$$

- Compute and plot the specific heat C_V vs T and identify which temperature the system 'melts' (this is the peak of the specific heat). Mark this temperature on your plot.

$$\left\langle E^2 \right\rangle = \sum_{i}^{m} P(x_i) V(x_i)^2 = \frac{1}{\mathcal{Z}} \sum_{i}^{m} g_i V(x_i)^2 \tag{9}$$

$$C_V = (1/T^2)(\left\langle E^2 \right\rangle - \langle E \rangle^2) \tag{10}$$