24-623/12-623 2017 HW#5

Total points: 50
Assigned: October 25, 2017.
Due: November 9, 2017, midnight to Canvas. Please use the Canvas discussion board to ask questions of the instructor, the course assistant, or the other students.

1. (25 points) In this problem, you will use Monte Carlo simulations to study the properties of the single oscillators from HW#2, which had potential energies (i) $U = x^2/2$ and (ii) $U = x^4 - 2x^2 + 1$.

(a) Determine $\langle U \rangle$, $\langle x \rangle$, and $\langle x^2 \rangle$ for $\beta = 0.1$, 1, 5, and 10 for oscillator (i) by directly evaluating the appropriate integrals (either analytically or numerically).

(b) Write a C++ code that uses the Metropolis Monte Carlo algorithm to compute $\langle U \rangle$, $\langle x \rangle$, and $\langle x^2 \rangle$ for $\beta = 0.1$, 1, 5, and 10 for (i). Discuss the following: How did you specify the trial move? How did you specify the maximum step size? How did you specify the initial condition and does it matter? How many trial moves do you need to get convergence of $\langle U \rangle$, $\langle x \rangle$, and $\langle x^2 \rangle$?

(c) Present all of your direct evaluation and Monte Carlo results in a single table and compare them.

(d) Compare your results to the behavior you observed in HW#2.

(e) Repeats part (a)-(d) for oscillator (ii).

2. (25 points) Consider a two-particle system, where each particle can be in one of two states. The potential energy is $U = U_1 + U_2 + U_1 U_2$, where U_1 and U_2 are the potential energies of the two particles and can take on values of γ or μ.

(a) List all microstates of this system. Develop an expression for $\langle U \rangle$ in terms of β, γ, and μ.

(b) For $\gamma = 0$ and $\mu = 1$, plot $\langle U \rangle$ vs. β for $0.01 \leq \beta \leq 100$. Make the β axis logarithmic. Interpret the limit of $\langle U \rangle$ as $\beta \to 0$ from a physical perspective.

(c) Write a C++ code that uses Metropolis Monte Carlo algorithm to compute $\langle U \rangle$. Discuss the following: How did you specify the trial move? How did you specify the initial condition and does it matter?

(d) For $\gamma = 0$ and $\mu = 1$, plot $\langle U \rangle$ from your MC code vs. β on the same graph as (b) for $\beta = 0.01$, 0.1, 1, 10, and 100. Present all the data from (b) (for appropriate β) and the MC simulations in a single table. Discuss the following: How many trial moves do you need to get convergence of $\langle U \rangle$? How do the results compare to those from (b)?

BONUS WORK:

(5 points) The Metropolis acceptance/rejection criterion is not unique. There are other acceptance/rejection criteria that can be used to perform Monte Carlo calculations in the NVT ensemble. Repeat 1(e) by computing the acceptance probability for all moves as

$$acc(old \rightarrow new) = \frac{\exp(-\beta\delta E/2)}{\exp(-\beta\delta E/2) + \exp(\beta\delta E/2)},$$

where $\delta E = U(new) - U(old)$. Simulations performed using this criterion are called Kawasaki Monte Carlo. In addition to implementing Kawasaki Monte Carlo in your C++ code, show analytically that this criterion satisfies detailed balance. Compare your results to those from 1(e).