PHYS516 ASSIGNMENT 3—MC SIMULATION OF THE ISING MODEL

Due: Wednesday, February 10, 2021

Submit to Blackboard by 11:59 pm. Please create a single file (*e.g.*, in PDF format) that has all materials (source code, plots, and explanation) and your name in it.

Part I—Theoretical Foundation

(**Metropolis algorithm**) Consider a set of N states, $\{\Gamma_1, \Gamma_2, ..., \Gamma_N\}$, and let the probability to find the system in the m-th state, Γ_m, be ρ_m. Prove that the probability distribution is a fixed point of the Metropolis transition matrix defined below, *i.e.*, $\Pi\rho = \rho$.

$$\left(\text{Metropolis transition matrix}\right) \quad \pi_{mn} = \begin{cases} \alpha_{mn} & \rho_m \geq \rho_n \quad m \neq n \\ \left(\rho_m/\rho_n\right)\alpha_{mn} & \rho_m < \rho_n \quad m \neq n \\ 1 - \sum_{m' \neq n} \pi_{m'n} & m = n \end{cases}$$

Here, π_{mn} are elements of matrix Π, ρ_m are elements of vector ρ, and α_{mn} are elements of a symmetric attempt matrix, *i.e.*, $\alpha_{mn} = \alpha_{nm}$.

Submission: Submit your answer, including all algebra and proof steps explained in your own words.

Part II—Computer Simulation

1. Write a program that performs Monte Carlo (MC) simulations of the $L \times L$ two-dimensional Ising model following the discussion in the lecture note.

2. Run MC simulations for 2 million steps, where $L = 20$, $H = 0.0$, and $J/k_BT = 0.2$, 0.3, 0.4, 0.5, 0.6, 0.7, and 0.8. Plot the absolute value of the mean magnetization and its standard deviation as a function of J/k_BT.

3. For the case of $J/k_BT = 0.2$, plot the histogram of magnetization M, *i.e.*, the number of MC samples whose summed spin values is M for each value of $M \in [-L^2, L^2]$.

Submission: Submit your source code along with the two plots.