PH4074: Computational Physics Lab

Prof. Mithun Biswas

August 14, 2024

1. Using the Monte Carlo method,

   (a) Find out the area of a circle of radius 4 meters.

   (b) Compute the value of π.

   (c) Solve the integrations, (i) $\int_{-2}^{2} x^2 dx$, (ii) $\int_0^\pi sin(x)dx$, and (iii) $\int_{-2}^{2} e^{-x^2/2} dx$.

2. Using the Metropolis Monte Carlo method, compute various thermodynamical properties of the Ising model in two dimensions.

   Ising Model is a simple model for magnetic system. In 2D, it consists of spins on a square lattice, where the spins at each site s_i can take values $+1$ or -1. The Hamiltonian in such a system is

   $$H = -J \sum_{\langle ij \rangle} s_i s_j - B \sum_i s_i \tag{1}$$

   where $\langle ij \rangle$ denotes a sum over the nearest neighbours (horizontal and vertical) on the lattice. B is the external magnetic field. $J > 0$ favors ferromagnetism (spins wants to line up) and $J < 0$ favors antiferromagnetism.

   Consider a 100×100 square lattice and $J = 1$. In case of no effect of external magnetic field, calculate and plot the following.

   (a) Variation of average magnetization, specific heat per spin, and susceptibility per spin with Monte Carlo time steps.

   (b) Variation of average magnetization, specific heat per spin, and susceptibility per spin with temperature

   (c) Comment on your observations about the critical temperature for phase transition from paramagnetic to ferromagnetic.

   (d) Average magnetization, $\langle |M| \rangle = \frac{1}{N} \langle | \sum_i s_i | \rangle$ (order parameter for ordered/disordered state or ferromagnetic/paramagnetic phase), specific heat per spin, $c = \frac{\beta}{T\ N} \Big[\langle E^2 \rangle - \langle E \rangle^2 \Big]$, and susceptibility per spin, $\chi = \beta\ N \Big[\langle M^2 \rangle - \langle M \rangle^2 \Big]$. (*Use your thermodynamics knowledge to prove these formulas.)