

Phase behaviour of the PSM GCM and GEM- n models

Studied the softmatter physics with Monte Carlo

Yun-Hsuan Chou

¹Department of Pysics
National Taiwan University

Final Porject, 2016, 06, 26

1 Introduction to the Monte Carlo Method

- Demo - calculate π
- Demo - calculate 2-D classical Ising model
- Calculate L-J particles in the NVT-ensemble

2 Introduction to the models for describing the phase behaviour

- Penetrable Sphere Model (PSM)
- Gaussian core Model (GCM)
- Gaussian exponential Model (GEM- n)

3 Results

Introduction to the Monte Carlo Method

Demo - calculate π

- Define a domain of the target.

$$p(x, y) = \begin{cases} 1 & , x^2 + y^2 \leq 1 \\ 0 & , \text{otherwise} \end{cases} \quad (1)$$

- Generate random numbers (x_i, y_i) from uniform distribute $[-1, 1]$.

$$p_i = 1 \text{ if } x^2 + y^2 \leq 1; p_i = 0 \text{ otherwise} \quad (2)$$

$$\pi \approx \frac{1}{N} \sum_{i=1}^N p_i + O(1/\sqrt{N}) \quad (3)$$

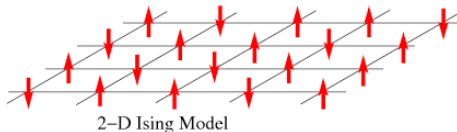
Introduction to the Monte Carlo Method

Demo - calculate π

Introduction to the Monte Carlo Method

Demo - calculate 2-D classical Ising model

- Build the configuration of a 2-D square lattice and set spins on each site. [Fig. 7]



$$H = -J \sum_{i \neq j} \sigma_i^z \sigma_j^z \quad (4)$$

$$\Psi = |\sigma_1, \sigma_j, \dots, \sigma_N\rangle \quad (5)$$

- Calculate the probability of the configuration at time t :

$$P(E, t) = e^{-\beta E(C)}, \text{ where } \beta = \frac{1}{k_B T} \quad (6)$$

Introduction to the Monte Carlo Method

Demo - calculate 2-D classical Ising model

- Importance Sampling: Metropolis algorithm

Choose a spin randomly and determined that if it should be flipped to a new configuration C'

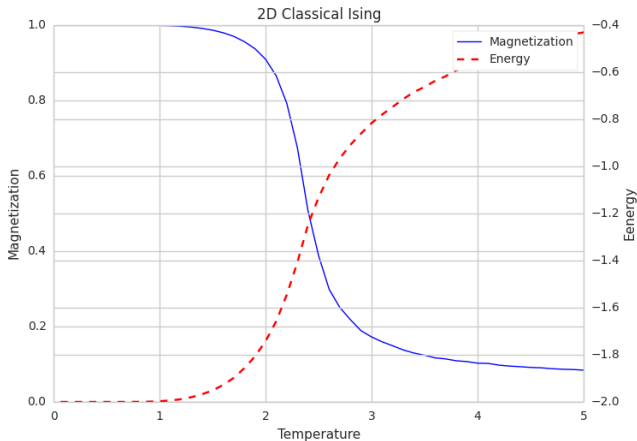
$$\Delta E = E(C') - E(C)$$

$\Delta E < 0$: accept flip

$$\Delta E > 0 = \begin{cases} \text{accept } C', \text{ if } e^{-\beta \Delta E} \geq \text{random number} \\ \text{reject } C', \text{ otherwise} \end{cases}$$

Introduction to the Monte Carlo Method

Demo - calculate 2-D classical Ising model



Introduction to the Monte Carlo Method

Calculate L-J particles in NVT ensemble

- Initialize a molecular configuration:
In this case, we can set the atoms in the cubic sites.
- Determined the Trial move:
- Importance Sampling: Metropolis algorithm
- Repeat until the energy converge.

Introduction to the models for describing the phase behaviour

Results