MSc PROJECT PRESENTATION (PHASE - 1)

Developing a Monte Carlo Model to study the magnetic ordering in the A - site ordered perovskite oxides.

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OUTLINE

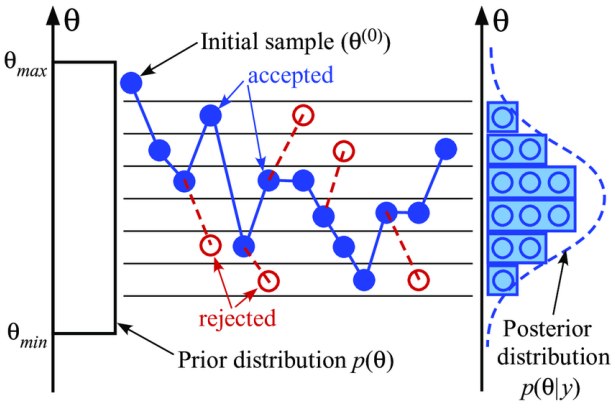
1. Monte Carlo method - overview
2. Properties of Markov chains
3. Metropolis Algorithm
4. Auto-correlation function
5. 2D Ising model - simulation
6. Future work

MONTE CARLO METHODS

[Anosh Joseph, Markov Chain Monte Carlo Methods in QFT, Springer (2020)]

- Principle : Uses random sampling to solve problems that might be deterministic in principle. And law of large numbers.

$$\langle \mathcal{O} \rangle = \int \frac{e^{-\beta\epsilon}}{\mathcal{Z}} \mathcal{O} d\epsilon \equiv \frac{1}{N} \sum_{r=1}^{N} \mathcal{O}_r$$



MCMC illustration

Image credits: Appl. Sci. 2020, 10,272

Markov Chain Monte carlo sampler :

Uses a "random walk" to help us draw samples from target distribution Using Metropolis Algorithm.

Useful when form of the distribution is known.(Canonical ensemble - $p(\epsilon_i) \propto e^{-\beta\epsilon_i}$)

PROPERTIES OF MARKOV CHAIN

[Anosh Joseph, Markov Chain Monte Carlo Methods in QFT, Springer (2020)]

Memoryless property : Its future state depends only on the present state.

$$\implies T(x_{i+1} \leftarrow x_i)$$

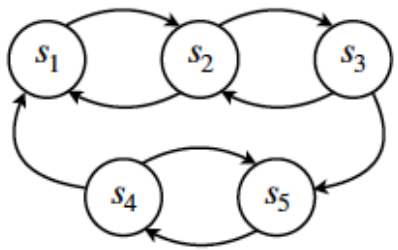
Ergodicity : Markov chain explores the entire state space and converges to a stationary distribution.

Uniqueness theorem : "Any irreducible and aperiodic markov chain has exactly one stationary distribution." $\equiv$ ERGODICITY

Detailed balance condition :

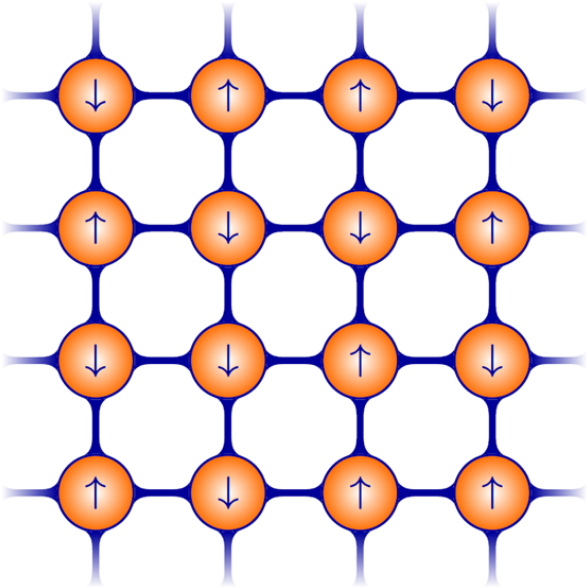
$$\boxed{T(x \leftarrow x')\rho(x) = T(x' \leftarrow x)\rho(x')}$$

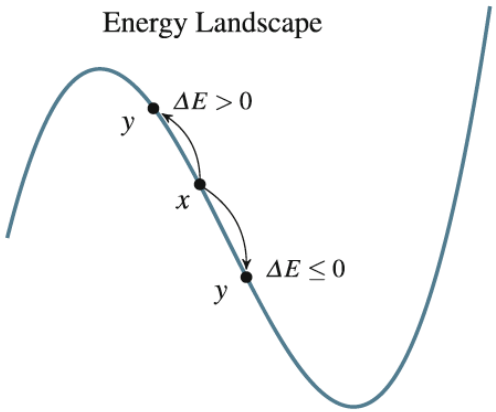
$$\frac{W_{xx'}A_{x\to x'}}{W_{x'x}A_{x'\to x}} = \frac{\rho(x')}{\rho(x)}$$

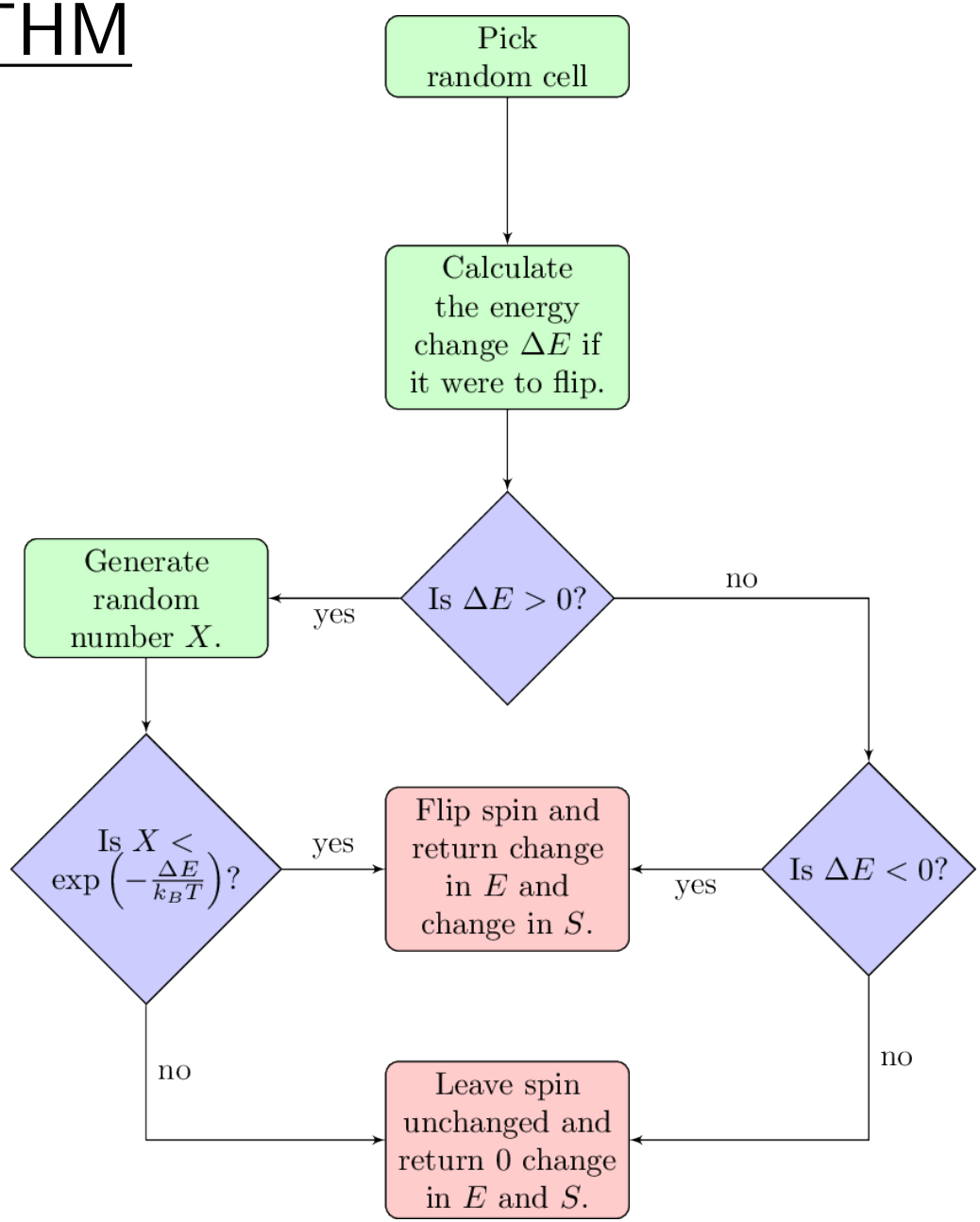


Irreducible and Aperiodic

METROPOLIS ALGORITHM

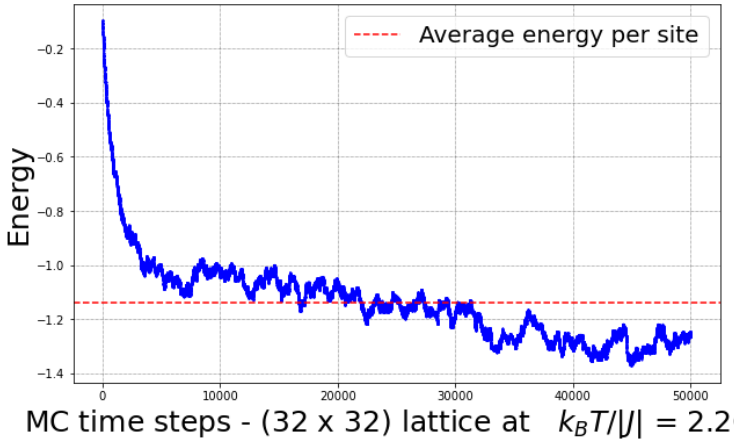


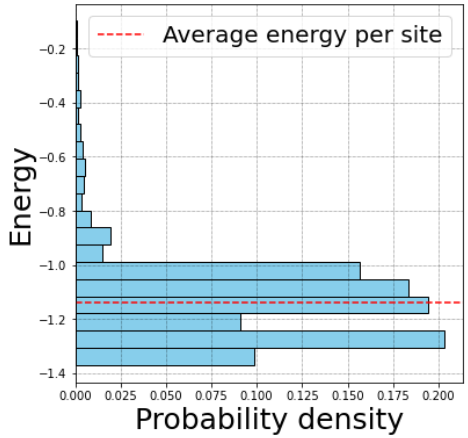




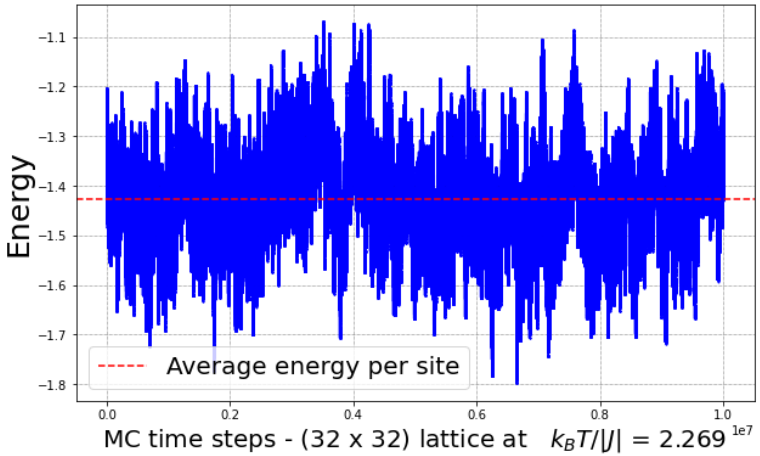
Burn in time (thermalisation) : $\Longrightarrow$ ignore first few states in the chain.

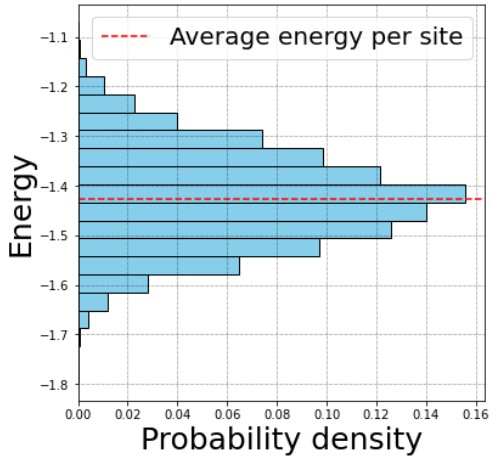
The first steps of the algorithm is biased by the random initial state.





Effect of initial random state.





Avoiding few initial states in calculation gives a stationary distribution.

AUTO CORRELATION FUNCTION

Dependence on previous state is known as auto-correlation. Its value lies between 0 and 1. 0 for no correlation and 1 for most correlation.

$$\Gamma_k = \frac{\langle \mathcal{O}_t \mathcal{O}_{t+k} \rangle - \langle \mathcal{O} \rangle^2}{\langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2} \approx e^{(-t/\tau)}$$

$$\int_0^\infty e^{-t/\tau} = \tau_{int} = \frac{1}{2} + \sum_{k=1}^{\infty} \Gamma_k$$

- τ_{int} is associated with error in the estimated quantity as follows,

$$\delta\mathcal{O} = \frac{\sigma}{\sqrt{N}} \sqrt{2\tau_{int}}$$

- $2\tau_{int}$ time steps are skipped in between to get uncorrelated samples which have reduced error.

1) Monte Carlo errors with less errors" [Comput. Phys. Comm. 156 (2004) 143–153]

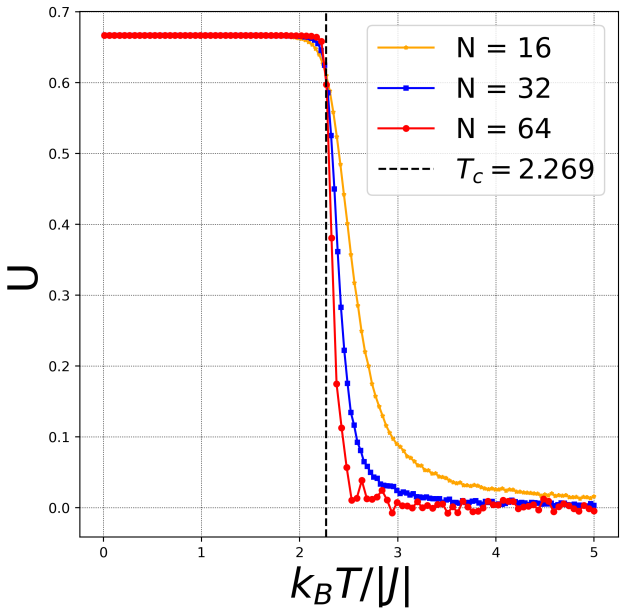
Simulation of 2D - Ising Model

$$\mathcal{H} = -J \sum_{<ij>} S_i S_j$$

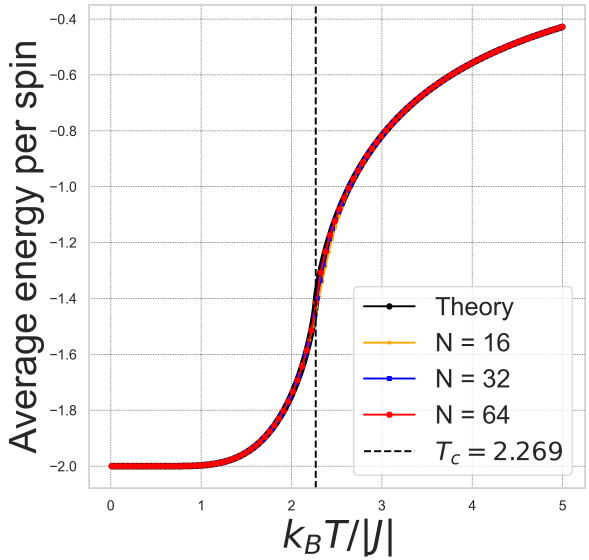
10^6 time steps for thermalisation and quantities were averaged over 10^5 time steps.

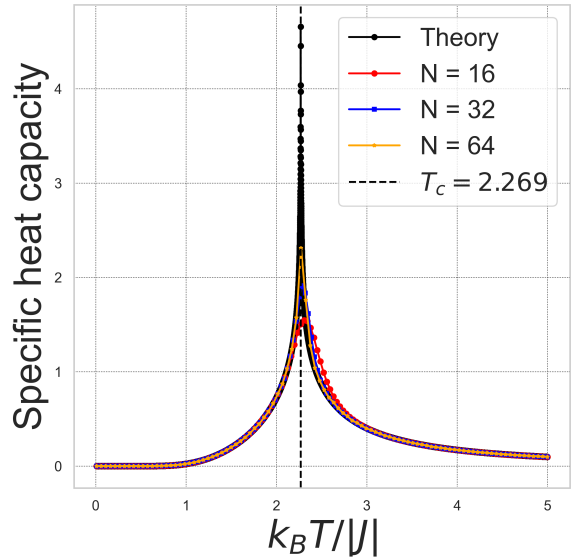
Binder's cumulant is an observation tool which is used for estimating the critical point.

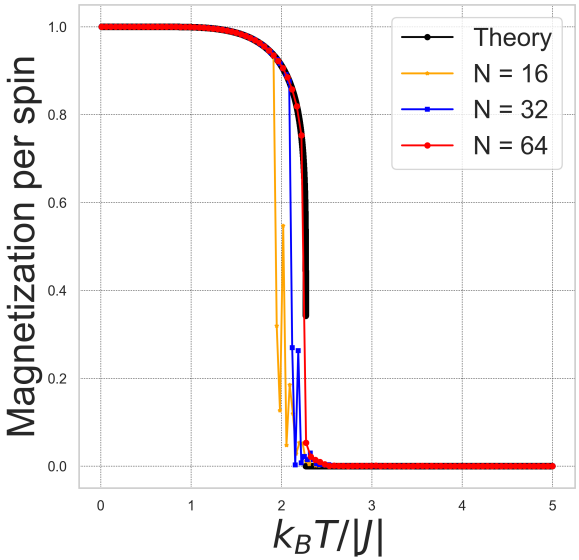
$$U = 1 - \frac{< M^4 >}{3 < M^2 >^2} = \begin{cases} 2/3 & ; T < T_c \\ U_B & ; T = T_c \\ 0 & ; T > T_c \end{cases}$$

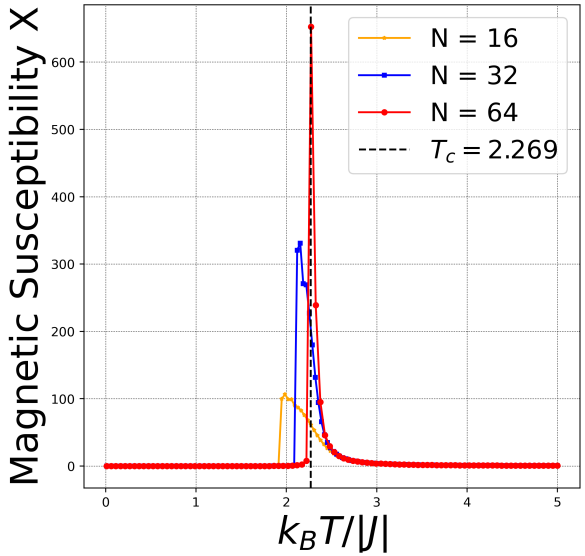


2D ising model $T_c \approx 2.269$







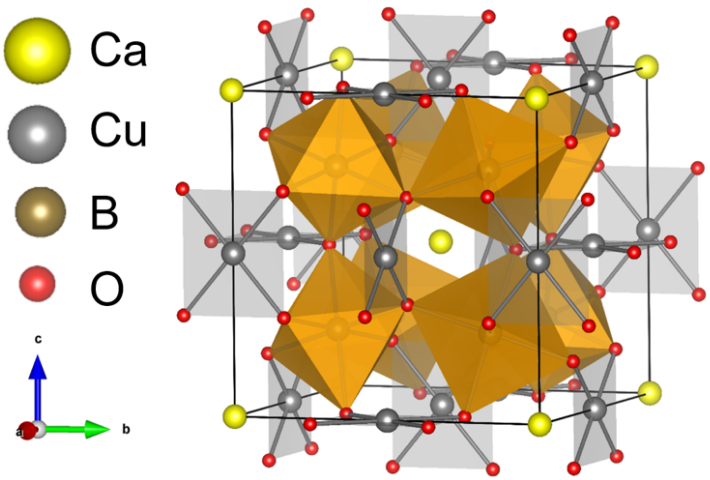


2D Ising model - MCMC Simulation ($k_B\,T_c/|J| \approx 2.269$)

FUTURE WORK

[Jatin Kumar Bidika, Amit Chauhan, and B. R. K. Nanda, PHYSICAL REVIEW B 106, 115152 (2022)]

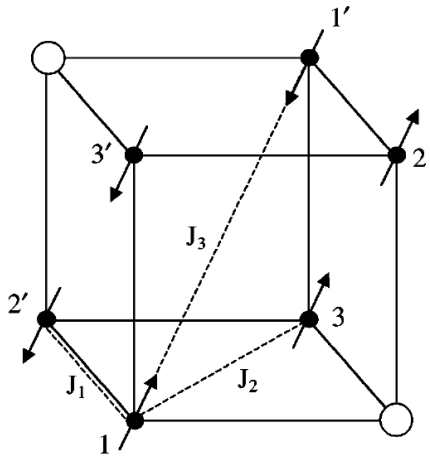
A - site ordered perovskite system ($CaCu_3Ti_4O_{12}$)



2 formula unit of system, B = Ti

Exchange Interactions identified in this system :

- J_1 - NN ferromagnetic exchange (Cu-Cu).
- J_2 - NNN ferromagnetic exchange (Cu-Cu).
- J_3 is the anti-ferromagnetic superexchange (Cu-O-Ti-O-Cu) path.

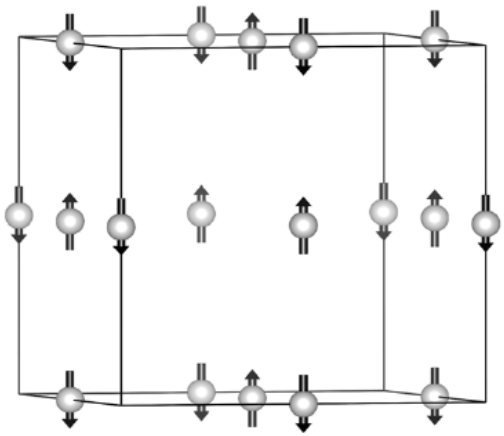


This system is simplified into a spin 1/2 lattice of Cu. So this becomes an effective Ising like system with spin vacancies at Ca sites.

[PHYSICAL REVIEW B, VOLUME 65, 052406]

$$\mathcal{H} = -J_1 \sum_{1^{st}\,NN} S_i S_j - J_2 \sum_{2^{nd}\,NN} S_i S_k - J_3 \sum_{3^{rd}\,NN} S_i S_l$$

Any randomly chosen site with spin will have 4 NN, 8 second NN and 8 third NN. The Neel transition temperature was found to be $\approx$ 25 K.



G-AFM was identified as stable configuration. It was in agreement with both experiment and DFT calculations done Jatin et al.

To perform MCMC simulation for the $CaCu_3Ti_4O_{12}$ system, and verfiy,

- Transition temperature.
- Ground state configuration

THANK YOU !

Detailed Balance condition

Random chain of independent processes,

$$P(x_1, x_2, ..., x_N) = P(x_1)P(x_2)...P(x_N)$$

Markov chain (dependent processes),

$$P(x_1, x_2, ..., x_N) = P(x_1)T(x_2 \leftarrow x_1)...T(x_N \leftarrow x_{N-1})$$

(Transition probabilities are normalised). Assume $\rho(x, t)$ is the probability of occurance of x at time t. For an ergodic chain,$\rho(x, t)$ becomes independent of t for large t. The master equation is,

$$\rho(x, t+1) - \rho(x, t) = -\sum_{x'} T(x \leftarrow x')\rho(x, t) + \sum_{x'} T(x' \leftarrow x)\rho(x', t)$$

For stationary distribution, LHS is zero. so,

$$\sum_{x'} T(x \leftarrow x')\rho(x) = \sum_{x'} T(x' \leftarrow x)\rho(x')$$

$$\implies \boxed{T(x \leftarrow x')\rho(x) = T(x' \leftarrow x)\rho(x')} \text{ (} \textit{Detailed Balance Condition} \text{)}$$

reformulating the detailed balance solution to make it suitable for practical purposes,

$$T(x' \leftarrow x) = w_{x'x}A_{x'x}; \quad (A_{x'x} \textit{ is acceptance probability })$$

$w_{xx'}$ is the trial step probability, Assuming $w_{xx'} = x_{x'x}$. It also obeys normalization. Putting it in detailed balance equation gives.

$$\frac{A_{x\to x'}}{A_{x'\to x}} = \frac{\rho(x')}{\rho(x)}$$

Metropolis selection :

- If $\rho(x') < \rho(x)$; $A_{x' \to x}$ is chosen to be 1 $\implies$ $A_{x \to x'} = \frac{\rho(x')}{\rho(x)}$ ($\therefore$ rejected with probability 1-$A_{x \to x'}$)
- If $\rho(x') > \rho(x)$; $\implies$ $A_{x \to x'} = 1$ ($\therefore$ always accepted)

MCMC SIMULATION OF 2D ISING MODEL :

$$\mathcal{H} = -J \sum_{<ij>} S_i S_j$$

In the Canonical ensemble framework the probability distribution to be sampled by using MC is the Boltzmann weight factor ($\exp(-\beta\mathcal{H})$)

The fore mentioned quantities were simulated and they were compared with the analytical solution of 2D Ising model adopted from K Huang book.

Quantities computed

- **Energy per site**

$$< E >= \frac{-J}{2N} \sum_{<ij>} S_i S_j \tag{1}$$

It is divided by factor 2 to compensate for overcounting.

- **Magnetisation per site**

$$< M >= \frac{1}{N} \sum_{i} S_i \tag{2}$$

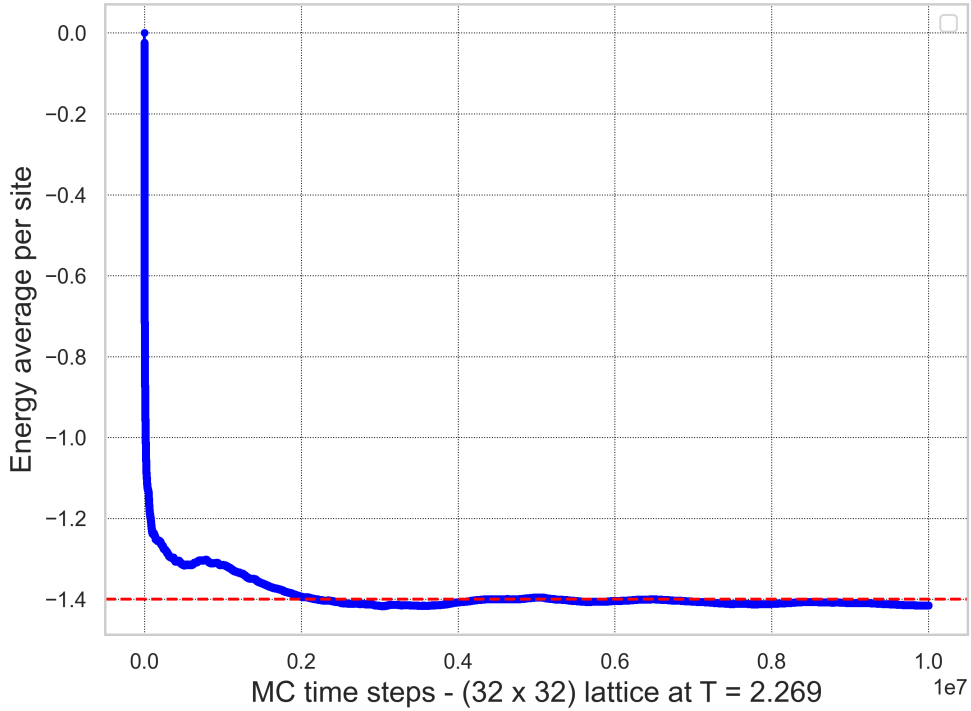
- **Specific heat capacity**

$$C = \frac{1}{T^2}(< E^2 > - < E >^2) \tag{3}$$

where $< E^2 >$ indicates average over E^2.

- **Susceptibility**

$$\chi = \frac{1}{T}(< M^2 > - < M >^2) \tag{4}$$


0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
−1.4
Energy average per site
0.0
0.2
0.4
0.6
0.8
1.0
1e7
MC time steps - (32 x 32) lattice at T = 2.269