Monte Carlo Simulation of the Ising Model

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Monte Carlo Method

- Statistical approach for physical processes.
- Statistical approach to compute integrals with samples.
- Statistical approach to analyze properties of large systems with using limited states of the system

Estimation of Expected Value

For Maxwell-Boltzmann dist. expected value of Q;

$$\langle Q \rangle = \frac{\sum_{\mu} Q_{\mu} e^{-\beta E_{\mu}}}{\sum_{\mu} e^{-\beta E_{\mu}}} \qquad \beta = 1/kT \tag{1}$$

With respect to Monte Carlo method, expected value of Q;

$$Q_M = \frac{\sum_{i=1}^{M} Q_{\mu_i} {P_{\mu_i}}^{-1} e^{-\beta E_{\mu_i}}}{\sum_{j=1}^{M} {P_{\mu_j}}^{-1} e^{-\beta E_{\mu_j}}} \tag{2}$$

$$P_{\mu} = Z^{-1} e^{-\beta E \mu} \tag{3}$$

Then, estimator of expected value is;

$$Q_M = \frac{1}{M} \sum_{i=1}^{M} Q_{\mu_i} \tag{4}$$

Getting Samples with Desired Probability Distribution

Aim: Sample states so that each one appear with its correct probability distribution (In the form of Maxwell-Boltzmann distribution for Ising Model as in eqn. (3))

- Markov Process:

$$\sum_{\nu} P(\mu \to \nu) = 1 \tag{5}$$

- Markov Chain:
  Repeated Markov Processes.
  A long run of Markov Chain = Correct Distribution

- Equilibrium condition:

$$\sum_{\nu} P_{\mu} P(\mu \to \nu) = \sum_{\nu} P_{\nu} P(\nu \to \mu) \tag{6}$$

$$P_{\mu} = \sum_{\nu} P_{\nu} P(\nu \to \mu) \tag{7}$$

- Detailed balance:

$$P_{\mu} P(\mu \to \nu) = P_{\nu} P(\nu \to \mu) \tag{8}$$

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{P_{\nu}}{P_{\mu}} = e^{-\beta(E_{\nu} - E_{\mu})} \tag{9}$$

Want to satisfy equations (5) and (9).

Acceptance ratio and Selection Probabilities:

$$P(\mu \to \nu) = g(\mu \to \nu) A(\mu \to \nu) \tag{10}$$

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{g(\mu \to \nu) A(\mu \to \nu)}{g(\nu \to \mu) A(\nu \to \mu)} = \frac{P_\nu}{P_\mu} = e^{-\beta(E_\nu - E_\mu)} \tag{11}$$

The Ising Model

- Model of magnetization of a material.
- Spins are $+1$ or -1.
- Hamiltonian is,

$$\mathrm{H} = -J \sum_{<i,j>} s_i s_j - H \sum_i s_i \tag{12}$$

- Canonical partition function is,

$$Z = \sum_{\{s_i\}} e^{-\beta \mathrm{H}} \tag{13}$$

To analyze system properties:

1. Wait a period of time called equilibration time, τ_{eq}
2. Analyze with independent samples.
   Autocorrelation function falls of exponential,

$$\chi(t) \sim e^{-t/\tau} \tag{14}$$

   To find correlation time,

$$log(\frac{\chi(\tau)}{\chi(0)}) = \frac{-t}{\tau} \tag{15}$$

3. Define errors in calculations.

3 basic methods to calculate statistical errors:

1. Blocking Method: Data is divided into several blocks.

$$\sigma = \sqrt{\frac{\frac{1}{n}\sum_{i=0}^{n}(q_i - \langle q \rangle)^2}{n-1}} = \sqrt{\frac{1}{n-1}(\langle q^2 \rangle - \langle q \rangle^2)} \tag{16}$$

2. Bootstrap Method: Data is resampled.

$$\sigma = \sqrt{\langle q^2 \rangle - \langle q \rangle^2} \tag{17}$$

3. Jackknife Method: Using n-1 data.

$$\sigma = \sqrt{\sum_{i=1}^{n}(q_i - q)^2} \tag{18}$$

Structure of Metropolis Algorithm

A single-spin-flip algorithm.
Selection probability is same for all N states,

$$g(\mu \to \nu) = \frac{1}{N} \tag{19}$$

Then, to satisfy detailed balance condition,

$$\frac{A(\mu \to \nu)}{A(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)} \tag{20}$$

Setting larger of two acceptance ratios to 1,

$$A(\mu \to \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)}, & \text{if } E_\nu > E_\mu \\ 1, & \text{otherwise} \end{cases}$$

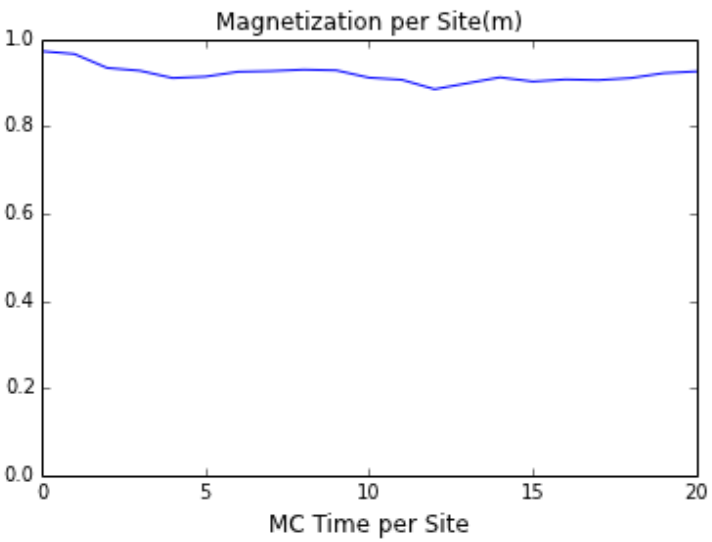
Implementation of Metropolis Algortihm

Metropolis Algorithm,

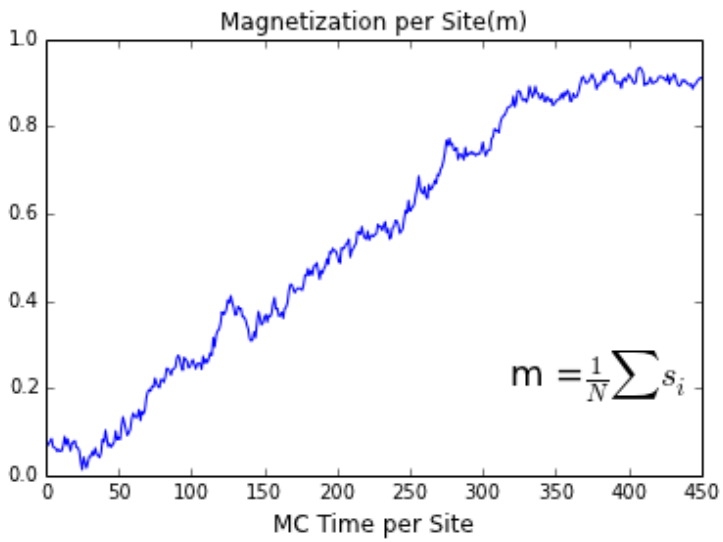
1. Arrange initial spins
2. Select a spin randomly.
3. Calculate energy difference, $\Delta E = E_\nu - E_\mu$ of states when this spin is flipped.
4. If $\Delta E \leq 0$, then flip the spin. If $\Delta E > 0$, then flip the spin according to acceptance probability.
5. Repeat the process

Equilibration Time

To analyze of properties of the system, we should get equilibrium. Look at magnetization:



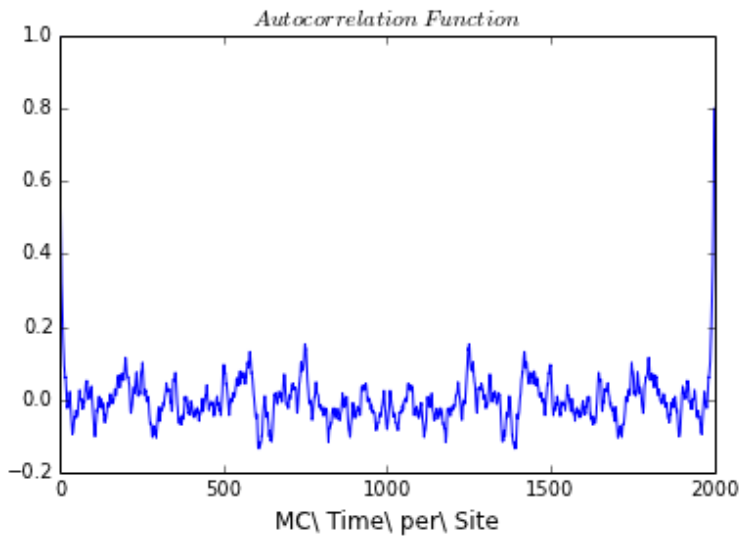
(a) Magnetization per Site vs MC Time per Site when T = 2.0 with all up initial spins corresponds to T=0



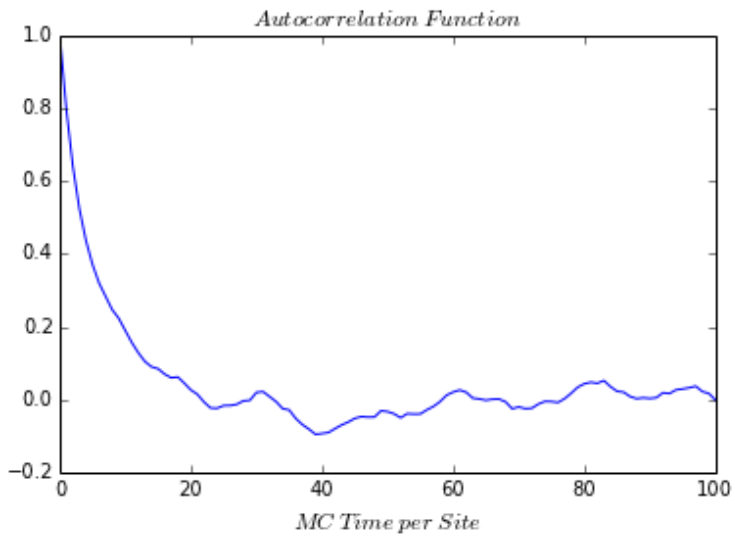
(b) Magnetization per Site vs MC Time per Site when T = 2.0 withn random initial spins corresponds to T=∞

Autocorrelation Function and Correlation Time

Autocorrelation function for magnetization is,



(a) Autocorrelation function vs MC Time per Site when T = 2.0



(b) Autocorrelation function vs MC Time per Site when T = 2.0

Fitting autocorrelation function for early times,

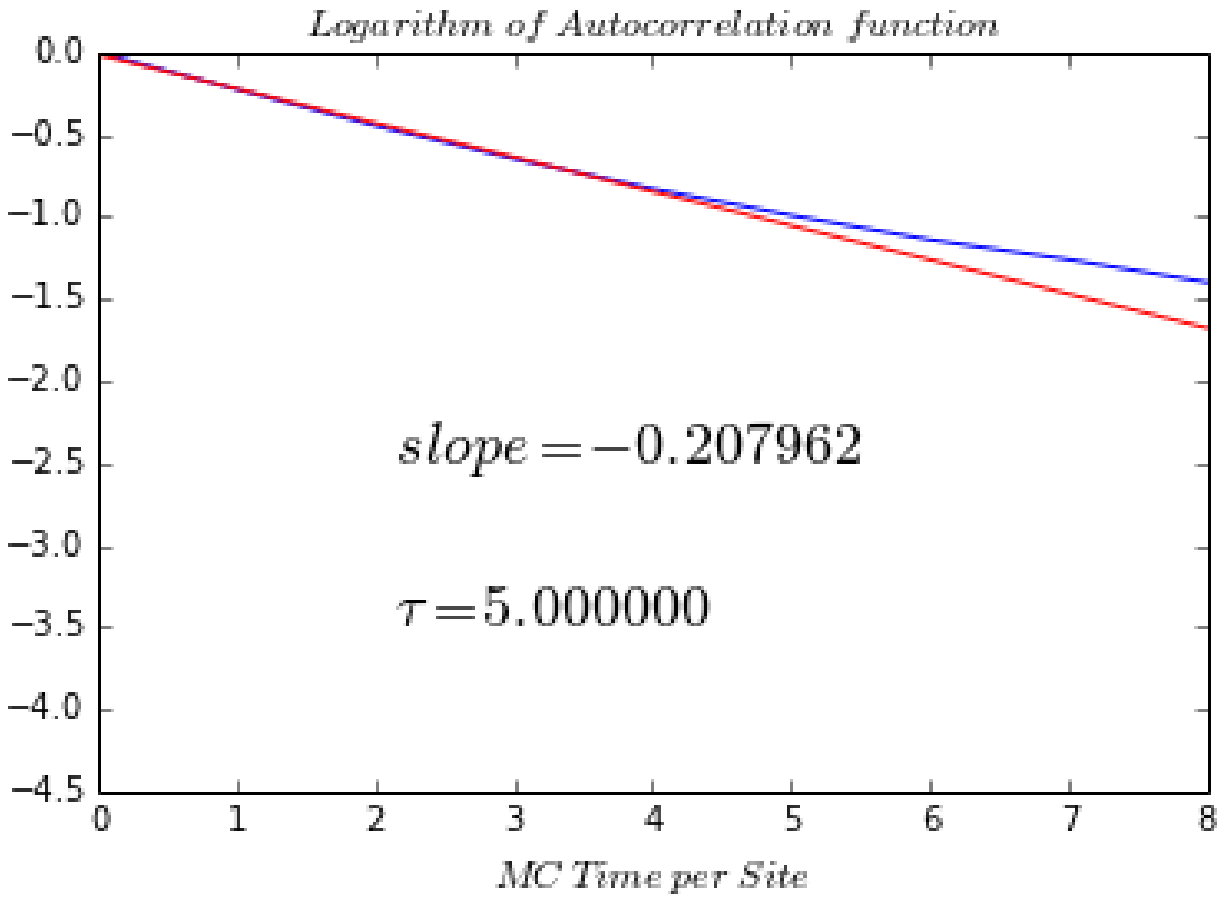
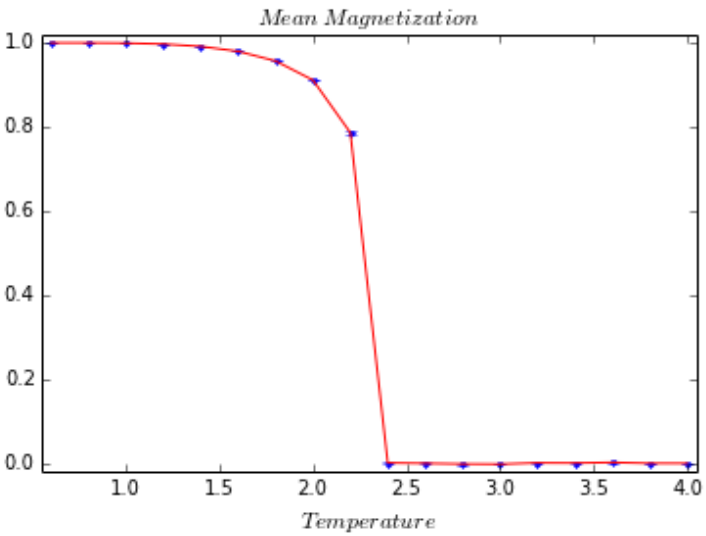
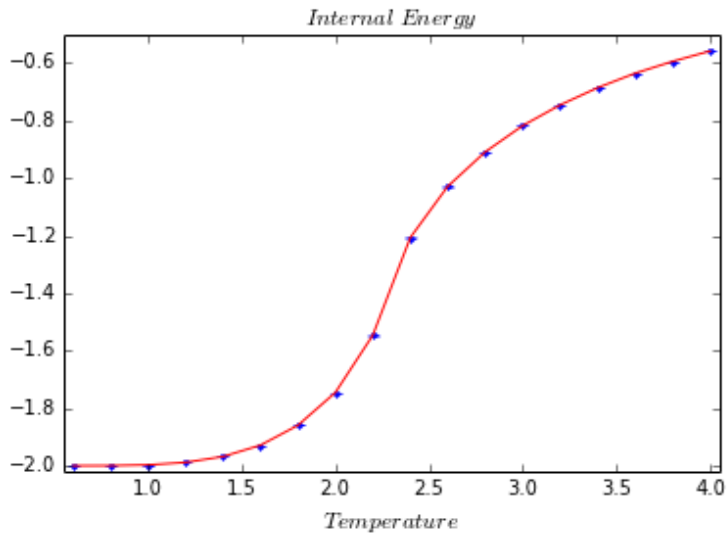


Figure : $log(\frac{\chi(t)}{\chi(0)})$ vs MC Time per Site when T = 2.0

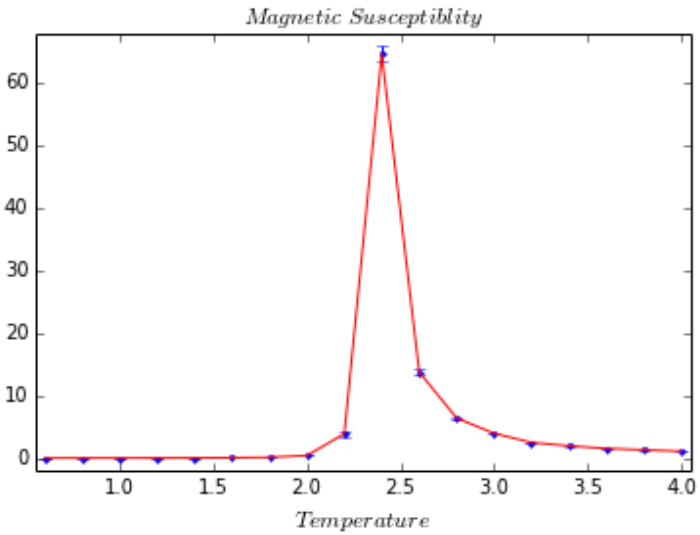
System's Properties



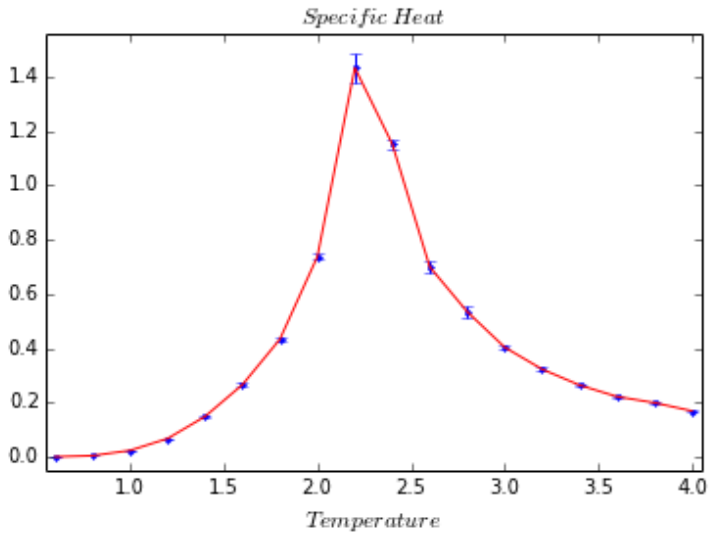
(a) Mean magnetization per site vs Temperature



(b) Internal energy per site vs Temperature



(a) Magnetic suscept. vs Temperature



(b) Specific heat vs Temperature

Look at correlation times:

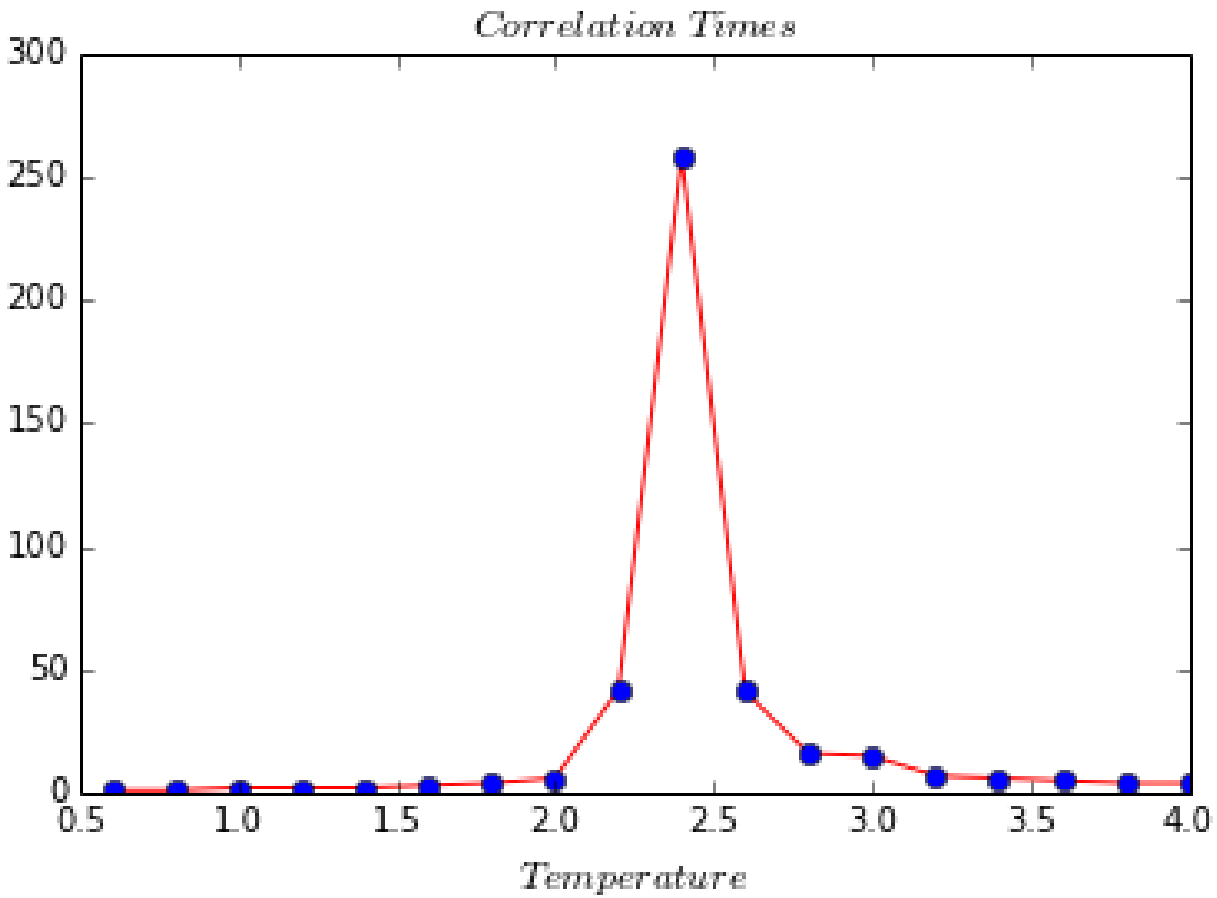


Figure : Correlation time vs Temperature

Occurs at Critical temperature T_c.
Property of Ising Model
For 2D Ising model, $T_c \approx 2.269$
Events that occur in the critical region are called critical phenomena.
Causes critical fluctuations

Critical Exponents

When we approach to phase transition correlation length increases. Reduced temperature, t, is

$$t = \frac{T - T_c}{T_c} \tag{21}$$

For Ising model, divergence of correlation length near phase transition goes like

$$\xi \propto |t|^{-\nu} \tag{22}$$

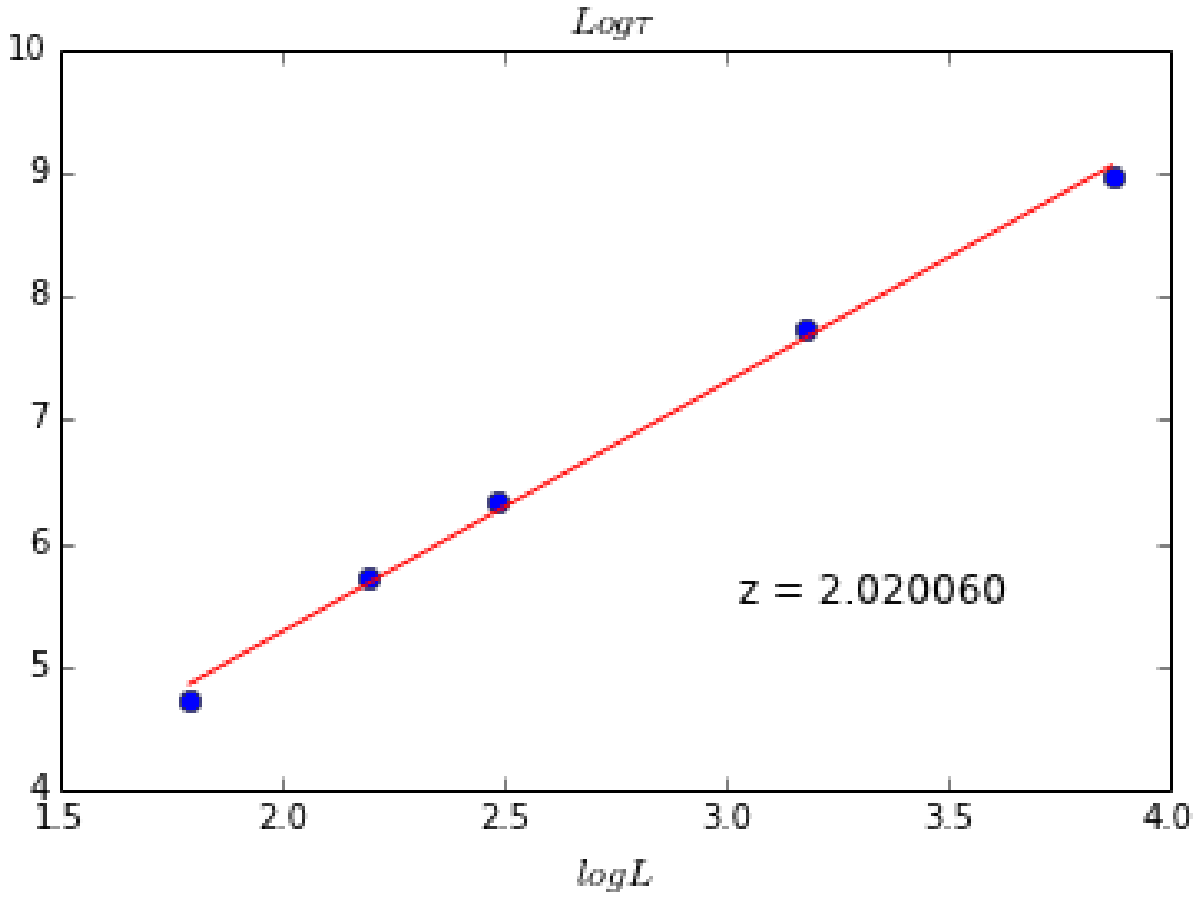
ν is critical exponent. Correlation Time per site

$$\tau \propto |t|^{-z\nu} \propto \xi^z \tag{23}$$

z is dynamic exponent.

Finite Size Scaling

$$\tau \propto L^z \tag{24}$$



Wolff Algorithm

Cluster-flipping algorithm
Look for clusters of similarly oriented spins and then flip them in their entirely all in one go, rather than trying to turn them over spin by spin.

Wolff Algorithm,

1. Select a spin randomly.
2. Look at the neighboring spins. If they are in same direction, add the cluster with probability P_{add}
3. For a spin that is added to the cluster, look at the neighboring spins of this spin and again add the spins with same direction which are not in the cluster with probability P_{add}
4. Repeat the process and complete the cluster
5. Flip the cluster

To make a fair description of τ

$$\tau = \tau_{steps} \frac{\langle n \rangle}{L^d} \tag{25}$$

$$\tau \propto L^z \tag{26}$$

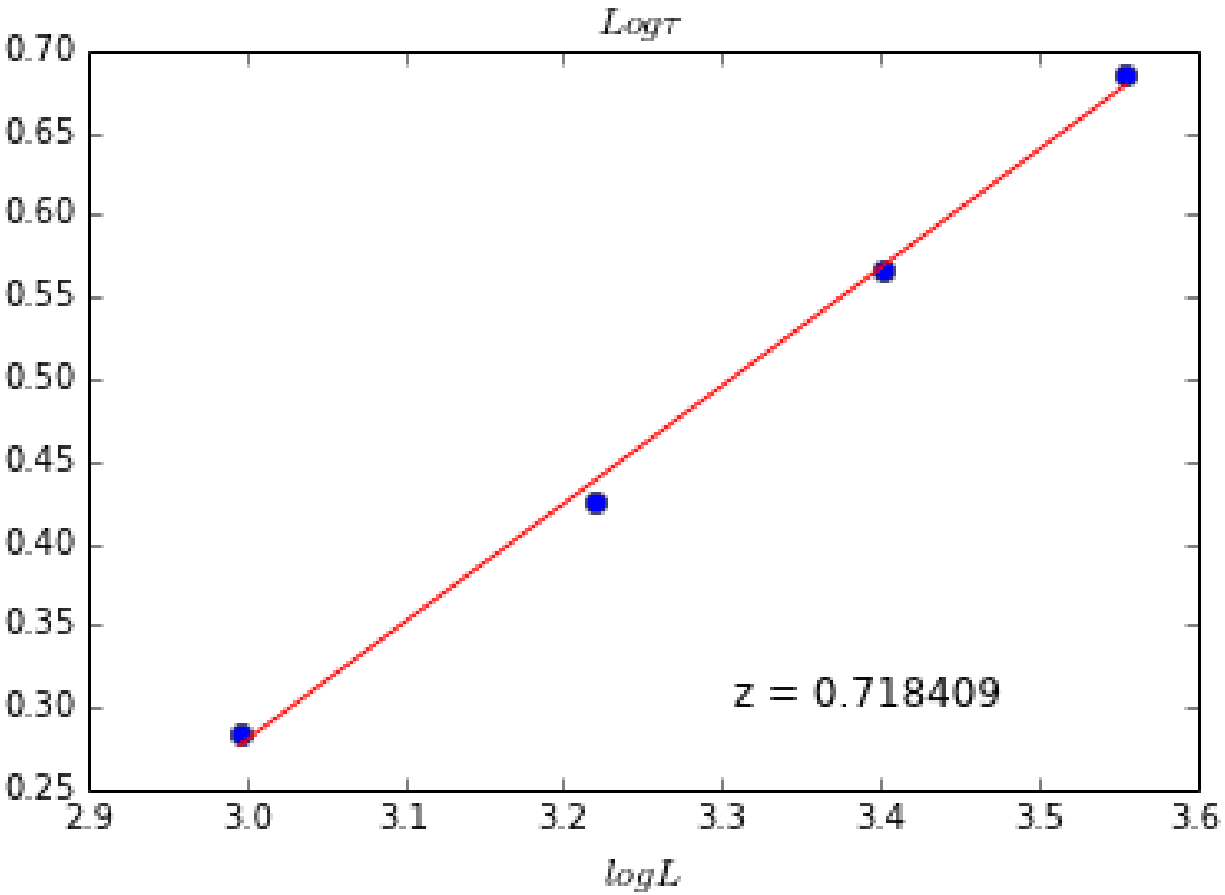


Figure : $Log\tau$ vs $LogL$