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Effective ergodicity in single-spin-flip dynamics

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A quantitative measure of convergence to effective ergodicity, the Thirumalai-Mountain (TM) metric, is applied to Metropolis and Glauber single-spin-flip dynamics. In computing this measure, finite lattice ensemble averages are obtained using the exact solution for a one dimensional Ising model, whereas the time averages are computed with Monte Carlo simulations. The time evolution of the effective ergodic convergence of Ising magnetization is monitored. By this approach, diffusion regimes of the effective ergodic convergence of magnetization are identified for different lattice sizes, nonzero temperature, and nonzero external field values. Results show that caution should be taken when using the TM metric at system parameters that give rise to strong correlations.

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I. INTRODUCTION

Cooperative phenomena are present in many different fields [1]. A unifying approach in studying cooperation among individual units emerges as a mathematical model that most resembles the nature of the problem. The first and the most successful of these models which were exactly solvable was the one-dimensional Ising model, a closed chain of n cooperating units, mimicking spins in ferromagnetic materials [2–4]. Time dependent statistics of the Ising model has been studied in depth before [5,6], where single-flip dynamics on n spins is introduced by changing a single spin's value with an associated transition probability. The natural consequence of generating such dynamics in a given statistical ensemble is the question of how and when the system behaves ergodically, i.e., ensemble averages being equivalent to the time averages. This question is not only interesting because it fulfills Boltzmann's equilibrium statistical mechanics [7–9], but for its crucial importance in practical applications, such as in simple liquids [10,11], assessing the quality of the Monte Carlo simulations [12], earthquake fault networks [13,14], and econophysics [15]. Most of these studies address the problem of identifying ergodic or nonergodic regimes. In this study, we investigate the time evolution of the rate of effective ergodic convergence under different system parameters to identify its so called diffusion regimes.

The Ising model and its analytic solution for the finite size total magnetization corresponding to the ensemble average are introduced in Sec. II. In Sec. III we provide details of our strategy of computing time averages using Metropolis and Glauber single-spin dynamics defined on the Ising model. In Sec. IV we briefly review the basic definitions of ergodicity from an applied statistical mechanics point of view. The mathematical literature based on measure theory is largely ignored. However, a quantitative measure for the identification of an effective ergodic dynamic is needed. In Sec. V the fluctuation metric [10,16] is adapted for the Ising model's total magnetization. By this approach, the rate of effective ergodic convergence of magnetization is monitored in single-spin-flip dynamics. We report the diffusion behavior of the ergodic convergence and identify different regimes depending on different lattice sizes, temperature, and external field values in Sec. VI.

II. THE ISING MODEL

Consider a one dimensional lattice that contains N sites. Each site's value can be labeled as $\{s_i\}_{i=1}^N$. In the two state version of the lattice, which is the Ising model [2–4], sites can take up two values, such as $\{1,-1\}$. These values correspond to spin up and spin down states, for example as a model of magnetic material or the state of a neuron [17].

The total energy Hamiltonian of the system can be written as follows:

$$\mathcal{H}\big(\{s_i\}_{i=1}^N, J, H\big) = J\left(\left(\sum_{i=1}^{N-1} s_i s_{i+1}\right) + (s_1 s_N)\right) + H\sum_{1}^{N} s_i. \tag{1}$$

This expression contains two interactions, one due to nearest neighbors (NNs) and one due to an external field. Note that an additional term in the NN interactions $s_1 s_N$ term appears due to periodic or cyclic boundary conditions to provide translational invariance. Coefficients J and H correspond to scaling of these interactions respectively. A reduced form is used in Eq. (1) using the unit thermal background, using the Boltzmann factor $\beta = \frac{1}{k_B T}$:

$$K = \beta J, \quad h = \beta H. \tag{2}$$

The partition function for this system can be written by using the transfer matrix technique [4],

$$Z_N = Tr(V^N), \tag{3}$$

where V is the transfer matrix defined as follows:

$$V = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}. \tag{4}$$

The resulting free energy for the finite system appears in terms of eigenvalues of the transfer matrix, λ_1 and λ_2 [4]:

$$Z_N = \lambda_1^N + \lambda_2^N, \tag{5}$$

$$\lambda_{1,2} = e^K[\cosh h \pm \sqrt{\sin^2 h + e^{-4K}}]. \tag{6}$$

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The canonical free energy for the finite system is defined as follows [4]:

$$f(N,T,h) = -k_B T \frac{1}{N} \ln Z_N, \tag{7}$$

$$\frac{1}{N} \ln\, Z_N = \ln\, \lambda_1 + \frac{1}{N} \ln[1 + (\lambda_2/\lambda_1)^N]. \tag{8}$$

We are interested in *finite size* total magnetization to compute the ensemble average of it, $M_E(N,\beta,H)$, analytically. Differentiating canonical free energy with respect to H will yield a long expression for M_E,

$$\begin{aligned} M_E(N,\beta,H) &= \left(N M_1 M_2^{N-1} + N M_3 M_4^{N-1}\right)/M_5,\\ M_1 &= \frac{\beta\, \cosh(H\beta)\, \sinh(H\beta)}{\sqrt{e^{-4\beta J} + \sinh^2(H\beta)}} + \beta\, \sinh(H\beta),\\ M_2 &= \sqrt{e^{-4\beta J} + \sinh^2(H\beta)} + \cosh(h\beta),\\ M_3 &= -M_1 + 2\beta\, \sinh(H\beta),\\ M_4 &= -M_2 + 2\cosh(H\beta),\\ M_5 &= (\sqrt{e^{-4\beta J} + \sinh^2(H\beta)} + \cosh(H\beta))^N\\ &\quad + (\cosh(H\beta) - \sqrt{e^{-4\beta J} + \sinh^2(H\beta)})^N. \end{aligned} \tag{9}$$

Note that in Eq. (9), the Boltzmann factor is explicitly written. Further explorations of the analytical solutions are beyond the scope of this study.

III. METROPOLIS AND GLAUBER SINGLE-SPIN-FLIP DYNAMICS

One of the ways to generate dynamics for a lattice system similar to the Ising model in a computer simulation is by changing the value of a randomly chosen site to its opposite value. This procedure is called *single-spin-flip dynamics* in the context of Monte Carlo simulations [6]. However, the quality of this kind of dynamics depends highly on the quality of the random number generator (RNG) [18,19] we employ in selecting the site to be flipped. However, we gather that Marsenne-Twister as an RNG [20] is sufficiently good for this purpose.

In generating such a dynamics, there is an associated transition probability in the single spin flip. This probability would determine if the flip introduced by the Monte Carlo procedure is an acceptable physical move. Two forms of transition probability can be used that correspond to Boltzmann density. The following expressions generate Glauber and Metropolis dynamics, respectively:

$$\begin{aligned} p_{\text{Glauber}}\left(\{s_i\}_{i=1}^N\right) &= \exp(-\beta\Delta\mathcal{H})/\left(1+\exp(-\beta\Delta\mathcal{H})\right)\\ &= 1/(1+\exp(\beta\Delta\mathcal{H})), \end{aligned} \tag{10}$$

$$p_{\text{Metropolis}}\left(\{s_i\}_{i=1}^N\right) = \min(1, \exp(-\beta\Delta\mathcal{H})), \tag{11}$$

where $\Delta\mathcal{H}$ is the total energy difference between single-spin-flipped and nonflipped configurations. The resulting transition probability is compared against a randomly generated number r, where $r \in [0,1]$. The move is accepted if the transition probability is smaller than r. This procedure, generally known as the Metropolis-Hastings Monte Carlo algorithm, samples the canonical ensemble [6].

IV. ERGODICITY

Boltzmann made the hypothesis that the solution of any dynamical system, and its trajectories, will evolve in time over phase-space regions where macroscopic properties are close to the thermodynamic equilibrium [9]. Consequently, ensemble averages and time averages will yield the same measure in thermodynamic equilibrium. A form of this hypothesis states that average values of an observable g over its ensemble of accessible state points, namely ensemble averaged value, can be recovered by time averaged values of the observable's time evolution, $g(t)$, from t_0 to t_N,

$$\langle g \rangle = \lim_{t_N \to \infty} \int_{t_0}^{t_N} g(t) dt, \tag{12}$$

where $\langle \rangle$ indicates ensemble averaged value. Note that, the definition of *ergodicity* is not uniform in the literature [10,21,22]. Some works require that the system should visit all accessible states in the phase space to reach ergodic behavior. This is seldom true. And considering the fact that coarse graining of phase space occurs, most of the accessible state values are clustered. Frequently, *effective ergodicity* can be reached if the system uniformly samples the coarse-grained regions relatively quickly [10].

Conditions of *ergodicity* in the transition states, a stochastic matrix of transition probabilities, generated by *spin-flip dynamics* is studied in the context of Markov chains [22,23]. This type of *ergodicity* implies that any state can be reached from any other. The Monte Carlo procedure explained above may be ergodic by construction in this sense for long enough times.

V. CONCEPT OF ERGODIC CONVERGENCE

A quantitative measure of effective ergodic convergence relies on the fact that identical components of the system, particles or discrete sites, carry identical average characteristics at thermal equilibrium [10]. Hence, effective ergodic convergence, $\Omega_G(t)$, can be quantified over time for an observable, a property, g. Essentially it can be computed as a difference the between ensemble averaged value of g and the sum of the instantaneous values of g for each of the components. This is termed the Thirumalai-Mountain (TM) G-fluctuating metric [10,16], expressed as follows at a given time t_k:

$$\Omega_G(t_k) = \frac{1}{N} \sum_{j=1}^{N} [g_j(t_k) - \langle g(t_k) \rangle]^2, \tag{13}$$

where $g_j(t_k)$ is the time averaged per component and $\langle g(t_k) \rangle$ is the instantaneous ensemble average defined as

$$g_j(t_k) = \frac{1}{k} \sum_{i=0}^{k} g_j(t_i), \tag{14}$$

$$\langle g(t_k) \rangle = \frac{1}{N} \sum_{j=1}^{N} g_j(t_k). \tag{15}$$

Hence the rate of ergodic convergence is measured with

$$\Omega'_G = \frac{\Omega_G(t)}{\Omega_G(0)} \to \frac{1}{t D_G}, \tag{16}$$

where D_G is the property's diffusion coefficient and Ω_G the effective ergodic convergence. If $1/\Omega'_G$ is linear in time, any point in phase space is said to be equally likely. This approach is used in simple liquids [10,11] and earthquake fault networks [13,14].

We would like to investigate the behavior of $1/\Omega'_G$ for the Ising model. The adaption of the Ω_G for total magnetization at time t_k as a function of temperature and external field values reads

$$\Omega_M(t_k,N,\beta,h) = [M_T(t_k) - M_E]^2, \tag{17}$$

$$M_T = \frac{1}{k}\sum_{i=0}^{k} M(t_i), \tag{18}$$

where $M_T(N,\beta,h)$ and $M_E(N,\beta,h)$ correspond to time and ensemble averaged total magnetization. Note that the value of $M_E(N,\beta,h)$ is fixed and is computed using the analytical solutions given in Sec. II, whereas $M_T(N,\beta,h)$ is computed in the course of Metropolis or Glauber dynamics. Here we slightly differ in comparison to the TM approach and use a constant ensemble average, because in our case the value of the ensemble average is available in exact form as given in Eq. (9).

VI. DIFFUSION REGIMES

We have identified the time evolution of the effective ergodic convergence measure, $\Omega_M(t_k,N,\beta,h)$, for the total magnetization of a one dimensional Ising model. Depending on which transition probability is used for the acceptance criterion, we generate Metropolis and Glauber single-spin-flip dynamics for the following model parameters: number of spin sites $N = \{32,64,128,256,512\}$, Boltzmann factor $\beta = \{0.5,1.0\}$, and nonzero external field values $H = \{0.50,1.0\}$ with setting short-range interaction strength to $J = 1.0$ for all cases [24]. We generate a dynamics of up to half a million Monte Carlo steps for all combination of parameters, hence the maximum k. At the rejected moves, rejected single-spin-flip configurations, the value of $\Omega_M(t_k,N,\beta,h)$ is set to the previously accepted value. We did not use external field values and temperatures close to zero, because the total magnetization's exact solution fails for zero temperature. In the case of zero external field, total magnetization is zero and Monte Carlo relaxation time is long.

We have generated a set of time evolutions of the effective ergodic convergence measure combined in three different schemes: varying external fields, increasing number of spin sites, and different temperature values. For better statistics, 512 spin sites are used for the variation of external fields and temperatures. By employing such a combination scheme, we could judge the relations among the variation of different parameters in the behavior of the ergodic convergence measure over time. The Monte Carlo steps play a role of *pseudodynamical* time.

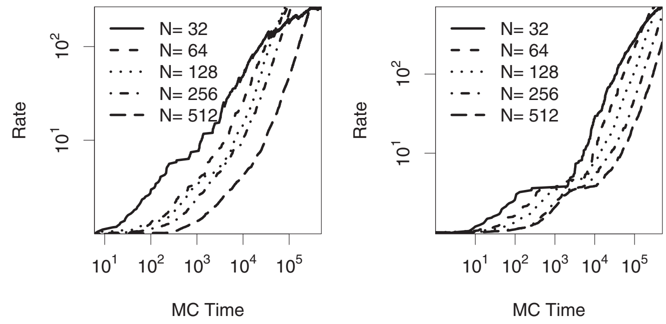
To be able to judge the diffusion behavior of the time evolutions of the effective ergodic convergence measure, we used the following expression with D_M, the diffusion coefficient:

$$1/\Omega'_M = \frac{\Omega_M(t_0,N,\beta,h)}{\Omega_M(t_k,N,\beta,h)} \to t D_M. \tag{19}$$

We call this value the so called *inverse effective ergodic convergence rate*, or simply the *rate*. The rate in our plots shows an increasing value over time. A higher value implies that the system is closer to the ergodic regime.

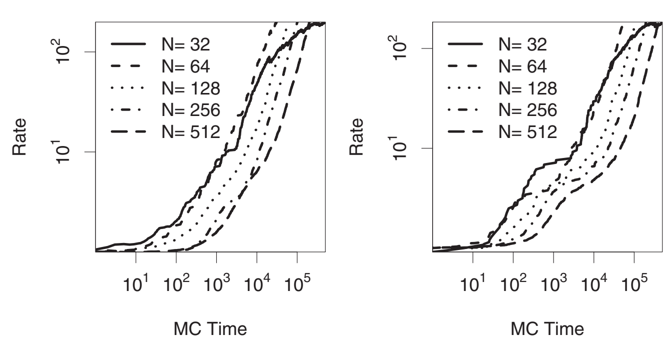
Figures 1(a), 1(b), 2(a), and 2(b) show the effect of the lattice size, different number of spin sites, and two different external field values at fixed unit thermal background, for Glauber and Metropolis dynamics, respectively. It is seen in all cases that smaller size leads to *faster* ergodic convergence. This behavior is more pronounced with the Glauber dynamics. It is well known that Glauber dynamics provides faster convergence to equilibrium [6]. When the external field is higher, at 1.0, we observe two different diffusion regimes. Those regimes can be clearly judged from inflection points given on the rate curves. Those inflection points, plateau regions, are significant in the Glauber dynamics. Again, the plateau regions are shifted for smaller size configurations to the left of the figure, due to the faster convergence we mentioned.

For varying external field values, there is only a single diffusion regime for low external field values. However, upon increasing the field values we again observe an inflection point



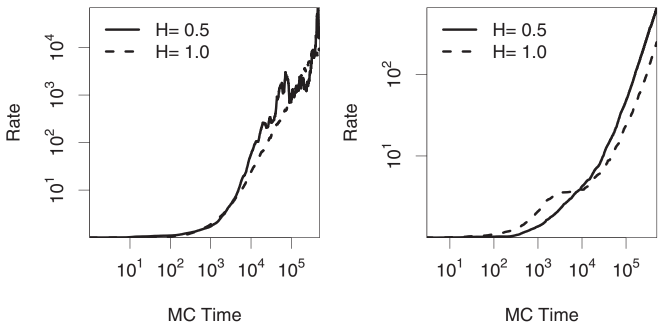
(a) (b)

FIG. 1. Inverse effective ergodic convergence in Glauber dynamics with different system sizes with fixed temperature $\beta = 1.0$ and external fields $H = \{0.5,1.0\}$ at (a) and (b), respectively.



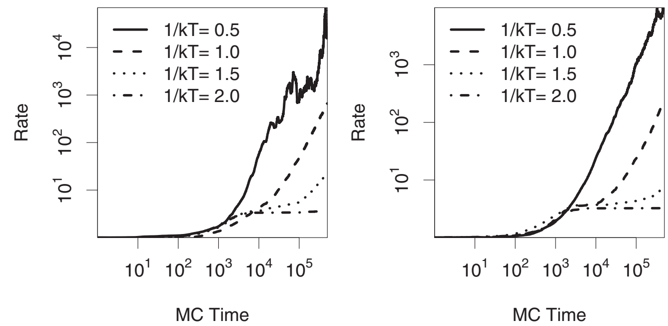
(a) (b)

FIG. 2. Inverse effective ergodic convergence in Metropolis dynamics with different system sizes with fixed temperature $\beta = 1.0$ and external fields $H = \{0.5,1.0\}$ at (a) and (b), respectively.



(a) (b)

FIG. 3. Effective ergodic convergence in Glauber dynamics with different external field values with fixed size $N = 512$ and temperature $\beta = \{0.5, 1.0\}$ at (a) and (b), respectively.



(a) (b)

FIG. 4. Effective ergodic convergence in Glauber dynamics with different temperatures with fixed size $N = 512$ and external fields $H = \{0.5, 1.0\}$ at (a) and (b), respectively.

in the rate curves. This signifies two different diffusion regimes for the rate. This is demonstrated in Figs. 3(a) and 3(b).

The temperature dependence of the rate curve is shown in Figs. 4(a) and 4(b). We see that the combination of higher temperature and external field values induces a change in the diffusion behavior. We observe that plateau regions become larger upon increasing the temperature.

VII. SUMMARY

The behavior of the *rate* of convergence to ergodicity is characterized for the Ising model using the modified TM metric for the total magnetization. We aimed at determining the rate's behavior over time. We conclude that the combination of stronger temperature or external field values generates a regime change in the ergodic convergence. Hence, caution should be taken when using the TM metric at system parameters that give rise to strong correlations.

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[1] G. H. Wannier, Rev. Mod. Phys. **17**, 50 (1945).
[2] Ernst Ising, Z. Phys. A **31**, 253 (1925).
[3] Stephen G. Brush, Rev. Mod. Phys. **39**, 883 (1967).
[4] R. J. Baxter, *Exactly Solvable Models in Statistical Mechanics* (Academic Press, London, 1982).
[5] Roy J. Glauber, J. Math. Phys. **4**, 294 (1963).
[6] Kurt Binder and Dieter W. Heermann, *Monte Carlo Simulation in Statistical Physics: An Introduction* (Springer, New York, 2010).
[7] R. C. Tolman, *The Principles of Statistical Mechanics* (Oxford University Press, New York, 1938).
[8] I. E. Farquhar, *Ergodic Theory in Statistical Mechanics* (Interscience Publishers, New York, 1964).
[9] Jay Robert Dorfman, *An Introduction to Chaos in Nonequilibrium Statistical Mechanics*, Vol. 14 (Cambridge University Press, Cambridge, U.K., 1999).
[10] Raymond D. Mountain and D. Thirumalai, J. Phys. Chem. **93**, 6975 (1989).
[11] Vanessa K. de Souza and David J. Wales, J. Chem. Phys. **123**, 134504 (2005).
[12] J. P. Neirotti, David L. Freeman, and J. D. Doll, Phys. Rev. E **62**, 7445 (2000).
[13] K. F. Tiampo, J. B. Rundle, W. Klein, J. S. Sá Martins, and C. D. Ferguson, Phys. Rev. Lett. **91**, 238501 (2003).
[14] K. F. Tiampo, J. B. Rundle, W. Klein, J. Holliday, J. S. Sá Martins, and C. D. Ferguson, Phys. Rev. E **75**, 066107 (2007).
[15] Ole Peters, Quant. Finance **11**, 1593 (2011).
[16] D. Thirumalai, R. D. Mountain, and T. R. Kirkpatrick, Phys. Rev. A **39**, 3563 (1989).
[17] John J. Hopfield, Proc. Natl. Acad. Sci. USA **79**, 2554 (1982).
[18] Aaldert Compagner, Am. J. Phys. **59**, 700 (1991).
[19] Wolfhard Janke, in *Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms*, NIC Series Vol. 10, edited by J. Grotendorst, D. Marx, and A. Muramatsu (John von Neumann Institute for Computing, Jülich, 2002), p. 447.
[20] M. Matsumoto and T. Nishimura, ACM Trans. Model. Comput. Simul. **8**, 3 (1998).
[21] S. K. Ma, *Statistical Mechanics* (World Scientific, Singapore, 1985).
[22] J. F. C. Kingman, Biometrika **48**, 391 (1961).
[23] A. G. Pakes, Oper. Res. **17**, 1058 (1969).
[24] M. Süzen, isingLenzMC: Monte Carlo for classical Ising Model, Version 0.2, http://cran.r-project.org/web/packages/isingLenzMC/index.html