Monte Carlo simulation of energy relaxation in the two-dimensional Ising model

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The energy relaxation in the two-dimensional Ising model, with temperature greater than T_c and in a spin system having a 5120×5120 lattice, is studied using supercomputer-conducted Monte Carlo simulation. The critical exponents of the linear and nonlinear relaxation times of the internal energy are respectively estimated to be $\Delta_E^{(l)}=2.064\pm0.026$ and $\Delta_E^{(\mathrm{nl})}=1.132\pm0.080$, being consistent with the Racz scaling law $\Delta_E^{(l)}-\Delta_E^{(\mathrm{nl})}=1-\alpha$, where α is the critical exponent of the specific heat. Based on the author's previous result in which the critical exponent of the linear relaxation for magnetization was determined as $\Delta_M^{(l)}=2.076\pm0.005$, it is strongly suggested that $\Delta_E^{(l)}=\Delta_M^{(l)}$.

Following the pioneering work by Ogita *et al.*[1] on the kinetic Ising model using Monte Carlo (MC) simulation, many studies have utilized computer modeling techniques to investigate the dynamics of a second-order phase transition. The vast improvements in both computer system hardware and MC simulation algorithms have significantly contributed to obtaining more accurate exponents near the critical point, as have several theoretical estimates, e.g., the high-temperature expansion method,[2] real-space renormalization-group analysis,[3] and the finite-size-scaling method.[4] In particular, various estimates were obtained of the exponents of the relaxation time of magnetization, with the associated linear and nonlinear critical exponents having been previously reported to, respectively, be $\Delta_M^{(l)}=2.076\pm0.005$ and $\Delta_M^{(\mathrm{nl})}=1.932\pm0.018$ (Ref. 5). This led to the present study which uses MC simulation under nearly similar conditions to better estimate the critical exponents of the linear and nonlinear relaxation times of internal energy, $\Delta_E^{(l)}$ and $\Delta_E^{(\mathrm{nl})}$, respectively. These estimates are additionally shown to correlate with the Racz scaling law.

In a two-dimensional (2D) Ising system the relaxation of the internal energy near the critical point is considered from a critical dynamics perspective. When far from equilibrium, the nonlinear relaxation time $\tau_E^{(\mathrm{nl})}$ of the internal energy is defined[6] as

$$\tau_E^{(\mathrm{nl})}=\int_0^\infty \frac{E(t)-E(\infty)}{E(0)-E(\infty)}dt \ , \tag{1}$$

where $E(t)$ is the internal energy. Divergence of $\tau_E^{(\mathrm{nl})}$ is expected as $\tau_E^{(\mathrm{nl})}\propto\varepsilon^{-\Delta_E^{(\mathrm{nl})}}$, where $\varepsilon=(T-T_c)/T_c$, T is the temperature of a spin system, and T_c is the critical temperature. Although it is not difficult to numerically calculate $\tau_E^{(\mathrm{nl})}$, a much longer simulation time is necessary to obtain $E(\infty)(\neq0)$ in equilibrium than to obtain the magnetization $M(\infty)(\rightarrow0)$. As a result, here we represent $E(\infty)$ as time averages $\langle E\rangle$ in equilibrium, where $\langle E\rangle$ is defined by

$$\langle E\rangle=\frac{1}{t_2-t_1}\int_{t_1}^{t_2}E(t)dt \ . \tag{2}$$

Equation (2) was adopted following a comparison of the resultant $\langle E\rangle$ value with the exact Onsager's solution value.

The linear relaxation time $\tau_E^{(l)}$ of the internal energy is similarly defined[7] as

$$\tau_E^{(l)}=\int_0^\infty \frac{\langle(E-\langle E\rangle)[E(t)-\langle E\rangle]\rangle}{\langle(E-\langle E\rangle)^2\rangle}dt \ , \tag{3}$$

where $\tau_E^{(l)}$ is expected to diverge as $\tau_E^{(l)}\propto\varepsilon^{-\Delta_E^{(l)}}$. If a completely ordered state is originally present, then a third relaxation time τ_E, termed here as the initial relaxation time, can be defined for an intermediate stage occurring in the approach to equilibrium by

$$E(t)=\langle E\rangle-(1+\langle E\rangle)\exp(-t/\tau_E) \ .$$

Hence by applying a scaling argument,[8,9] the initial relaxation time τ_E is also expected to diverge as $\tau_E\propto\varepsilon^{-\Delta_E^{(l)}}$.

With respect to the Racz scaling law,[8]

$$\Delta_Q^{(l)}=\Delta_Q^{(\mathrm{nl})}+\beta_Q \ , \tag{4}$$

where $\Delta_Q^{(l)}$ and $\Delta_Q^{(\mathrm{nl})}$ are, respectively, the critical exponents of the linear and the nonlinear relaxation times of quality Q. If Q is magnetization, then β_Q is β, i.e., the critical exponent of the order parameter. This magnetization scaling law was shown to correlate with the corresponding critical exponents of $\Delta_M^{(l)}$ and $\Delta_M^{(\mathrm{nl})}$ obtained by our previous study.[5] Here, however, Q is energy and β_Q is $1-\alpha$, where α is the critical exponent of the specific heat.

The present study utilizes the kinetic Ising model which considers nearest-neighbor interactions on a 2D square lattice in the absence of an external field, and which also incorporates a periodic boundary condition. The Metropolis method was employed to enable updating each spin stochastically. In order to numerically solve the MC simulation algorithm, a FACOM VP-2600 supercomputer was applied to perform the super-spin coding technique (lattice size 5120×5120) by Williams and Kalos[10] in which the temperature is quantized and discrete. The reduced temperature T_N is an interger presented in two dimensions as $T_N=2N\exp(-4/T)$, where N is a quantum number of bits and T the tempera-

ture of a spin system. Several simulation programs were coded in FORTRAN77 for $N=4-8$ with all simulation temperatures being greater than T_c. A maximum number of 2.23×10^8 spin-flip attempts was obtained at $N=8$. The algorithm R250 by Kirkpatrick and Stoll[11] was used as a random number generator. The MC simulation results were verified to correlate exceptionally well with the exact results obtained using Onsager's solution, e.g., the energy at $T_N=45$ was $-0.670\,696$ versus the exact value of $-0.670\,694$, and at $T_N=46$, $-0.646\,665$ versus $-0.646\,669$.

Figure 1 shows the resultant relaxation process of energy $E(t)$ with respect to MC time increments for a 5120×5120 lattice at temperatures $T_N=45$, 52, and 68; where $E(t)$ approaches equilibrium as $E(t)\propto\langle E\rangle-(1+\langle E\rangle)\exp(-t/\tau_E)$. The initial relaxation time τ_E was calculated using this relation, as was the nonlinear relaxation time $\tau_E^{(\mathrm{nl})}$ [Eq. (1)]. Table I summarizes results at various temperatures, whereas Fig. 2 shows a log-log plot of τ_E and $\tau_E^{(\mathrm{nl})}$ versus ε. For the linear relaxation, the following relation for τ_E versus ε was obtained after several trials to correct $\tau_E\propto\varepsilon^{-\Delta_E^{(l)}}$:

$$\tau_E=\text{const}\times\varepsilon^{-\Delta_E^{(l)}}|\ln\varepsilon|^{\omega}\ . \tag{5}$$

Least-squares analysis gave const$=0.1295$, $\Delta_E^{(l)}=2.064\pm0.026$, and $\omega=-0.3653$ in the temperature region $0.014\lesssim\varepsilon\lesssim0.27$. The error in $\Delta_E^{(l)}$ indicates a standard error, with the best-fit curve being shown in Fig. 2. The results at $\varepsilon\gtrsim0.28$ are not reliable. The slight logarithmic correction in Eq. (5) should be noted.

On the other hand, the relation between the nonlinear relaxation time $\tau_E^{(\mathrm{nl})}$ and ε is rather simple, with the best fit being determined by the least-squares method to be

$$\tau_E^{(\mathrm{nl})}=\text{const}\times\varepsilon^{-\Delta_E^{(\mathrm{nl})}}\ , \tag{6}$$

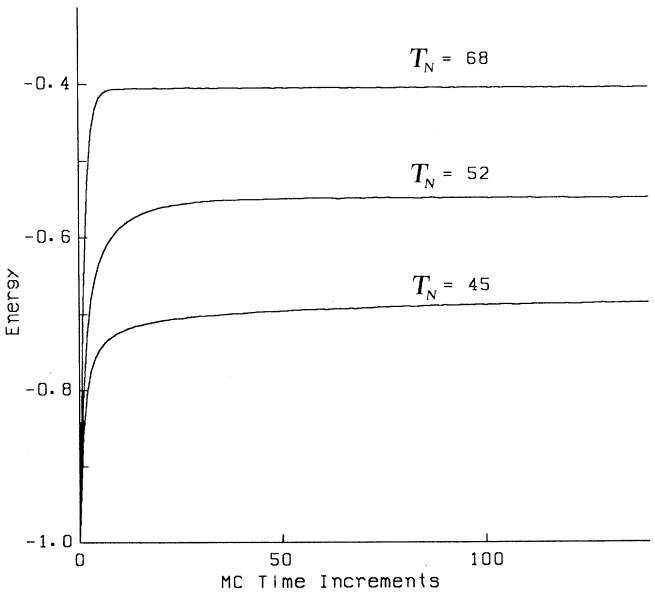

FIG. 1. Energy vs MC simulation time intervals in a two-dimensional, 5120×5120 lattice, Ising model at various T_N. The initial state is completely ordered.

TABLE I. Simulation results of τ_E and $\tau_E^{(\mathrm{nl})}$ for a 5120×5120 lattice. The system temperature T is given by $T_N=256\exp(-4/T)$ for $N=8$.

T_N	Linear	Nonlinear
45	505.098±3.793	31.598±0.377
46	142.316±4.924	14.315±0.115
47	68.061±2.366	9.270±0.093
48	36.938±1.244	6.698±0.109
49	24.215±0.831	5.244±0.088
50	17.401±0.946	4.227±0.077
52	10.373±0.251	2.988±0.019
54	6.436±0.220	2.358±0.008
56	4.419±0.032	1.941±0.030
58	3.324±0.072	1.636±0.065
60	2.561±0.042	1.365±0.067
62	2.124±0.047	1.195±0.038
64	1.826±0.065	1.073±0.018
66	1.608±0.053	0.955±0.039
68	1.514±0.082	0.866±0.029

where const$=0.2422$ and $\Delta_E^{(\mathrm{nl})}=1.132\pm0.080$ in the temperature region $0.014\lesssim\varepsilon\lesssim0.32$.

In a finite-size system, simulation results are affected by the shift of T_c and ΔT_c, where ΔT_c is expressed[12] as

$$\Delta T_c/T_c\simeq-0.36/\sqrt{n}\ , \tag{7}$$

with n representing the number of spins of the system. In the present system it is estimated that $\Delta T_c\simeq-0.000\,16$,

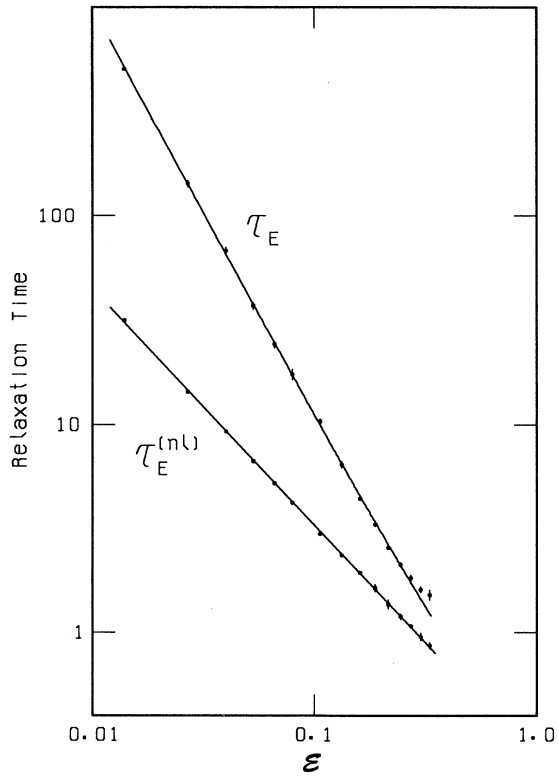

FIG. 2. Initial relaxation (linear) and nonlinear relaxation times vs ε for a 5120×5120 lattice. τ_E contains the logarithmic correction from Eq. (5), whereas $\tau_E^{(\mathrm{nl})}$ utilizes Eq. (6).

and since the closest temperature to the critical temperature ($T_c=2.269\,18$) in the spin system of the present data is $T=2.271\,45$, the subsequent results will not be significantly affected by this shift. In addition, when these results are compared to those using a $10\,240\times10\,240$ lattice,[5] nearly the same critical exponents were obtained, although the resultant errors were different.

The values of $\Delta_E^{(l)}=2.064\pm0.026$ and $\Delta_E^{(\mathrm{nl})}=1.132\pm0.080$ are consistent in comparison to estimates of $\Delta_E^{(l)}\simeq2$ obtained by Yahata[13] using the high-temperature expansion method. Achiam[14] obtained a larger value of $\Delta_E^{(l)}=2.203\pm0.03$ with real-space renormalization-group analysis by assuming $\nu=1.0$, where ν is the critical exponent of the correlation length. Further support (within errors) was provided by Stoll, Binder, and Schneider[15] using a standard MC simulation to obtain $\Delta_E^{(l)}=2.00\pm0.10$ in a small lattice system (200×200). Recently, using the finite-size-scaling method, Tang and Landau[16] estimated $\Delta_E^{(l)}=2.13\pm0.07$. Few estimates have been obtained for $\Delta_E^{(\mathrm{nl})}$, however, Bolton and Johnson[17] used MC simulation to calculate $\Delta_E^{(\mathrm{nl})}=0.40\pm0.04$, although their data were fairly distributed. On the other hand, Kretschmer, Binder, and Stauffer[18] applied the same method and estimated $\Delta_E^{(\mathrm{nl})}\sim0.9$, with this believed to be a more reliable value, being in good agreement with the present one.

Using the Racz scaling law, the difference between $\Delta_E^{(l)}$ and $\Delta_E^{(\mathrm{nl})}$ can be predicted as

$$\Delta_E^{(l)}-\Delta_E^{(\mathrm{nl})}=1-\alpha\ , \tag{8}$$

and, in fact, the present results correlate well with Eq (8). In the one-dimensional Ising model, Csepes and Racz[19] showed this relation to exactly hold. It is realized, nonetheless, that since the above-described previous estimates lack consistency, especially with respect to $\Delta_E^{(\mathrm{nl})}$, this scaling prediction cannot be fully established in two dimensions. However, the difference $\Delta_E^{(l)}-\Delta_E^{(\mathrm{nl})}=0.932\pm0.084$ is slightly less than unity. The reason of the slight disagreement may be why $\tau_E^{(\mathrm{nl})}$ cannot be characterized by a single exponent.[20]

When the critical exponents of $\Delta_M^{(l)}$ and $\Delta_E^{(l)}$ were compared, their closeness led many researchers[4,13,14] to suggest that $\Delta_M^{(l)}=\Delta_E^{(l)}$. Schneider[21] derived this relation using various inequalities to obtain the exponents of critical slowing down in the 2D Ising model. Furthermore, previous results[5] using the same numerical model, but in a spin system having a $10\,240\times10\,240$ lattice, gave $\Delta_M^{(l)}=2.076\pm0.005$, i.e., coinciding with $\Delta_E^{(l)}$ within errors. Stoll, Binder, and Schneider[15] also obtained $\Delta_M^{(l)}=1.85\pm0.10$ and $\Delta_E^{(l)}=2.00\pm0.10$ by MC simulation using similar conditions, and although these two exponents are slightly different, they similarly coincide within errors. Therefore, the present MC simulation results strongly support the hypothesis that $\Delta_M^{(l)}=\Delta_E^{(l)}$.

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