An extended chain Ising model and its Glauber dynamics*

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It was first proposed that an extended chain Ising (ECI) model contains the Ising chain model, single spin double-well potentials and a pure phonon heat bath of a specific energy exchange with the spins. The extension method is easy to apply to high dimensional cases. Then the single spin-flip probability (rate) of the ECI model is deduced based on the Boltzmann principle and general statistical principles of independent events and the model is simplified to an extended chain Glauber–Ising (ECGI) model. Moreover, the relaxation dynamics of the ECGI model were simulated by the Monte Carlo method and a comparison with the predictions of the special chain Glauber–Ising (SCGI) model was presented. It was found that the results of the two models are consistent with each other when the Ising chain length is large enough and temperature is relative low, which is the most valuable case of the model applications. These show that the ECI model will provide a firm physical base for the widely used single spin-flip rate proposed by Glauber and a possible route to obtain the single spin-flip rate of other form and even the multi-spin-flip rate.

Keywords: Ising model, Glauber dynamics, single spin-flip probability

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1. Introduction

The dynamics of the Ising model was first well studied by Glauber[1] and the key assumption contains a single spin-flip probability (rate) of definite form, which is now commonly known as the kinetic Ising model, also called as Glauber–Ising (GI) model.[2−7] Nowadays, not only the GI model and its extended forms, such as the models of inhomogeneous coupling constants,[8−18] inhomogeneous single spin-flip rate,[12,19] two temperatures,[20,21] general form of single spin-flip rate,[22−25] time-dependent single spin-flip rate,[26−29] or high spins,[30] but also some related models, for example, the Glauber–Potts model,[31] and molecular string model,[32−35] etc. have been widely used in many systems in various fields, such as the critical phenomena,[36−42] relaxation kinetics of glass transition,[32−35,43−48] granular compaction,[49,50] kinetics of adsorption and chemical reactions,[21−22,51−56] helix-coil transition in biopolymers and kinetics of denaturation in DNA, etc.[57−59] It can be said that the GI model and its related models have become an important basis in the researches of the relaxation phenomena in condensed matters.

In the specific applications of the above models, special designations of the single spin-flip rate are all involved; in other words, the GI model and its related model selves cannot determine the rate based on the model assumptions.[1−59] So it is a question worth exploring how we could use some more basic models and physical principles to obtain the corresponding rate. In this paper, an extended chain Ising model is first proposed and then the single spin-flip rate of the model is deduced based on the Boltzmann principle and general statistical principles of independent events. Moreover, the relaxation dynamics of the model at the obtained rate is simulated by the Monte Carlo method,[35] and a comparison with the results of

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the special chain GI model[1,32−35] is presented, too. We would like to point out that the extension method is easy to apply to high-dimensional cases.

2. Extended chain Ising model

According to the inspiration of the molecular string model,[32−35] the Hamiltonian of an extended chain Ising (ECI) model in this article is

$$\left.\frac{H_{\rm ECI}}{kT}\right|_{g_0,\nu_0} = -\frac{J}{2kT}\sum_{m=1}^{\infty}\sum_{i=1}^{n}(\sigma_{i-1}^{mn}+\sigma_{i+1}^{mn})\sigma_i^{mn} + \frac{U}{kT}\sum_{m=1}^{\infty}\sum_{i=1}^{n}\cos(\sigma_i^{mn}\pi), \quad (1)$$

where σ_i^{mn} expresses the states of the i-th spin in the Ising chain labeled as m and containing n spins and $\sigma_i^{mn}=-1,0,1, i=1,\ldots,n$, $\sigma_0^{mn}=\sigma_{n+1}^{mn}=0$; k is the Boltzmann constant and $H_{\rm ECI}/(kT)|_{g_0,\nu_0}$ means the system is in a heat bath of temperature T. In order to facilitate the calculation below, we assume that the heat bath only consists of phonons with a constant density of energy states g_0 and the energy exchange number per unit time for each spin with the heat bath, i.e. the phonon absorption or emission rate of each spin is ν_0.

The first term on the right-hand side in Eq. (1) is the classical Ising model, which includes infinite individual Ising chains. J, independent of T, is the interaction constant between the adjacent spins, and we let $J>0$ here.

The second term on the right-hand side in Eq. (1) is an extension to the original Ising model, which means that each Ising spin is also in a double-well potential with barrier height U ($U>0$) independent of T. Furthermore, the form $\cos(\sigma_i^{mn}\pi)$ plights that the state $\sigma_i^{mn}=0$ must be passed through when an Ising spin changes from $\sigma_i^{mn}=\pm1$ to $-\sigma_i^{mn}=\mp1$.

3. Single spin-flip rate of the ECI model

In this section, we will deduce the single spin-flip rate of the ECI model just based upon the Boltzmann principle, the Bose–Einstein statistics of Bosons and the general statistical principles of independent events. We only consider the case $\mathrm{e}^{(U-2J)/kT}\gg1$ to work out the formal solution of the rate.

For the single spin-flip process,[1,32−35] namely when the transition of an Ising spin in an Ising chain among the different states of σ_i^{mn}, the other spins in this chain remain unchanged, so a single spin energy can be introduced as

$$E_{\sigma_i^{mn}} = -J\left(\sigma_{i-1}^{mn}+\sigma_{i+1}^{mn}\right)\sigma_i^{mn} + U\cos\left(\sigma_i^{mn}\pi\right). \quad (2)$$

We assume there are $N^E_{\sigma_i^{mn}=-1}$, $N^E_{\sigma_i^{mn}=0}$, and $N^E_{\sigma_i^{mn}=1}$ spins in the states $\sigma_i^{mn}=-1$, $\sigma_i^{mn}=0$, and $\sigma_i^{mn}=1$, respectively, as the Ising spins and heat bath are in thermal equilibrium. According to the Boltzmann principle, we have

$$N^E_{\sigma_i^{mn}=1} : N^E_{\sigma_i^{mn}=-1} : N^E_{\sigma_i^{mn}=0} = \mathrm{e}^{-E_{\sigma_i^{mn}=1}/kT} : \mathrm{e}^{-E_{\sigma_i^{mn}=-1}/kT} : \mathrm{e}^{-U/kT}. \quad (3)$$

When studying the low-frequency (i.e., the external field frequency $f\ll(U-2J)/h$, where h is the Planck constant) and linear response or relaxation dynamics of the Hamiltonian (Eq. (2)),[60,61] the variations of the spin numbers $\Delta N^E_{\sigma_i^{mn}=-1}$, $\Delta N^E_{\sigma_i^{mn}=0}$, and $\Delta N^E_{\sigma_i^{mn}=1}$ in each state due to external perturbation fields satisfy

$$\begin{aligned}&\Delta N^E_{\sigma_i^{mn}=-1}\propto N^E_{\sigma_i^{mn}=-1},\quad \Delta N^E_{\sigma_i^{mn}=0}\propto N^E_{\sigma_i^{mn}=0},\\ &\Delta N^E_{\sigma_i^{mn}=1}\propto N^E_{\sigma_i^{mn}=1},\quad \Delta N^E_{\sigma_i^{mn}=-1}\ll N^E_{\sigma_i^{mn}=-1},\\ &\Delta N^E_{\sigma_i^{mn}=0}\ll N^E_{\sigma_i^{mn}=0},\quad \Delta N^E_{\sigma_i^{mn}=1}\ll N^E_{\sigma_i^{mn}=1}. \quad (4)\end{aligned}$$

From Eqs. (3) and (4), it is easy to obtain $\Delta N^E_{\sigma_i^{mn}=0}\ll\Delta N^E_{\sigma_i^{mn}=-1}\sim\Delta N^E_{\sigma_i^{mn}=1}$ under the temperature condition $\mathrm{e}^{(U-2J)/k_BT}\gg1$, as mentioned in the first paragraph of this section. The results show that we need only consider the spin-flips from the initial states $\sigma_i^{mn}=\pm1$ through intermediate state $\sigma_i^{mn}=0$ to the final states $-\sigma_i^{mn}=\mp1$, and ignore the transitions from $\sigma_i^{mn}=0$ to $\sigma_i^{mn}=\pm1$, when computing the low-frequency and linear response of relaxation.

We label the flip rate for each Ising spin changing from states $\sigma_i^{mn}=\pm1$ to state $\sigma_i^{mn}=0$ as $q_{\sigma_i^{mn}=\pm1\to\sigma_i^{mn}=0}$ and from state $\sigma_i^{mn}=0$ to states $\sigma_i^{m1}=\pm1$ as $q_{\sigma_i^{mn}=0\to\sigma_i^{mn}=\pm1}$. When the Ising spins and heat bath are in thermal equilibrium, the average spin number of each state does not change with time t. This requires in unit time, the number of the Ising spins jumping from states $\sigma_i^{mn}=\pm1$ to state $\sigma_i^{mn}=0$ is equal to that from state $\sigma_i^{mn}=0$ to states $\sigma_i^{mn}=\pm1$ and that is

$$q_{\sigma_i^{mn}=\pm1\to\sigma_i^{m1}=0}N^E_{\sigma_i^{mn}=\pm1} = q_{\sigma_i^{mn}=0\to\sigma_i^{mn}=\pm1}N^E_{\sigma_i^{mn}=0}. \quad (5)$$

By using the Bose–Einstein statistics, the phonon number $N_{\rm p}$ in the heat bath with an energy $E_{\rm p}$ is[61,62]

$$N_{\rm p}\propto\frac{g_0}{\mathrm{e}^{E_{\rm p}/kT}-1}\approx g_0\,\mathrm{e}^{-E_{\rm p}/kT}. \quad (6)$$

For the Ising spins at the initial states $\sigma_i^{mn} = \pm 1$, they can absorb the energy of phonons $E_{\rm p} = U$ in heat bath and jump to the excited state $\sigma_i^{mn} = 0$. From Eqs. (2) and (6), it is easy to obtain that the transition rate of each Ising spin from states $\sigma_i^{mn} = \pm 1$ to state $\sigma_i^{mn} = 0$ is

$$\begin{aligned} & q_{\sigma_i^{mn}=\pm 1\to\sigma_i^{mn}=0} \\ \approx\ & \nu_0\ \mathrm{e}^{E_{\sigma_i^{mn}}/kT}\Big|_{\sigma_i^{mn}=\pm 1} \\ =\ & \frac{1}{\tau_0}\ \mathrm{e}^{-(\sigma_{i-1}^{mn}+\sigma_{i+1}^{mn})\sigma_i^{mn}J/kT}\Big|_{\sigma_i^{mn}=\pm 1}, \end{aligned} \tag{7}$$

where $\tau_0 = \nu_0^{-1}\,\mathrm{e}^{U/kT}$.

For Ising spins already transferred to state $\sigma_i^{mn} = 0$, they can not only go back to the original states $\sigma_i^{mn} = \pm 1$ but can also jump to the new states $-\sigma_i^{mn} = \mp 1$ by releasing energy (transmitting phonons) to the heat bath.

From Eqs. (5) and (7) as well as the general statistical principle of independent events,[61,62] the single spin-flip rate for each Ising spin from the initial states $\sigma_i^{mn} = \pm 1$ through the excited states $\sigma_i^{mn} = 0$ to the final state $-\sigma_i^{mn} = \mp 1$ is

$$\begin{aligned} & \nu_{\sigma_i^{mn}=\pm 1\to -\sigma_i^{mn}=\mp 1} \\ =\ & \frac{q_{\sigma_i^{mn}=\pm 1\to\sigma_i^{mn}=0} q_{\sigma_i^{mn}=0\to -\sigma_i^{mn}=\mp 1}}{q_{\sigma_i^{mn}=0\to\sigma_i^{m1}=\pm 1} + q_{\sigma_i^{mn}=0\to -\sigma_i^{mn}=\mp 1}} \\ \cong\ & \frac{1}{2\tau_0}\ \mathrm{e}^{-(\sigma_{i-1}^{mn}+\sigma_{i+1}^{mn})\sigma_i^{mn}J/kT}\Big|_{\sigma_i^{mn}=\pm 1} \\ =\ & \frac{1}{2\tau_0}\cosh^2 J/kT(1-(\sigma_{i-1}^{mn}+\sigma_{i+1}^{mn})\sigma_i^{mn}\tanh J/kT \\ & + \sigma_{i-1}^{mn}\sigma_{i+1}^{mn}\tanh^2 J/kT)\big|_{\sigma_i^{mn}=\pm 1}. \end{aligned} \tag{8}$$

The above results indicate that the Hamiltonian of 3 σ_i^{mn} $(-1, 0, 1)$ states (Eq. (1)) can be simplified to the following kinetic Hamiltonian of 2 states with a specific single spin-flip rate under the condition of $\mathrm{e}^{(U-2J)/k_BT} \gg 1$,

$$\begin{aligned} H_{\rm I} &= -\frac{J}{2}\sum_{m=1}^{\infty}\sum_{i=1}^{n}\left(s_{i-1}^{mn}+s_{i+1}^{mn}\right)s_i^{mn}, \\ \nu_{s_i^{mn}\to -s_i^{mn}}^{\rm ECGI} &= \frac{1}{2\tau_0}\,\mathrm{e}^{-(s_{i-1}^{mn}+s_{i+1}^{mn})s_i^{mn}J/kT}, \end{aligned} \tag{9}$$

where $s_i^{mn} = -1, 1, i = 1, \ldots, n$, $s_0^{mn} = s_{n+1}^{mn} = 0$ and in order to facilitate the description below, we call it extended chain Glauber–Ising (ECGI) model.

We can easily find that $\nu_{s_i^{mn}\to -s_i^{mn}}^{\rm ECGI}$ of the ECGI model differs from the generally used Metropolis spin-flip rate,[62]

$$\begin{aligned} & \nu_{s_i^{mn}\to -s_i^{mn}}^{\rm MCI} \\ =\ & \begin{cases} \tau_0^{-1}, & \text{for } s_i^{mn}\left(s_{i-1}^{mn}+s_{i+1}^{mn}\right)\le 0, \\ \tau_0^{-1}\,\mathrm{e}^{-2J/kT}, & \text{for } s_i^{mn}\left(s_{i-1}^{mn}+s_{i+1}^{mn}\right) > 0, \end{cases} \end{aligned}$$

and the special single spin-flip rate given by Glauber

$$\nu_{s_i^{mn}\to -s_i^{mn}}^{\rm SGI} = \frac{\alpha}{2}\left[1-\frac{\gamma}{2}s_i^{mn}\left(s_{i-1}^{mn}+s_{i+1}^{mn}\right)\right]$$

of the original GI model.[1,32–35] Actually, $\nu_{s_i^{mn}\to -s_i^{mn}}^{\rm ECGI}$ is a special case of the general spin-flip rate

$$\begin{aligned} & \nu_{s_i^{mn}\to -s_i^{mn}}^{\rm GCGI} \\ =\ & \frac{\alpha}{2}\left[1-\frac{\gamma(1+\delta)}{2}s_i^{mn}\left(s_{i-1}^{mn}+s_{i+1}^{mn}\right)+\delta s_{i-1}^{mn}s_{i+1}^{mn}\right] \end{aligned}$$

meeting the detailed balance condition also given by Glauber.[1]

4. Computer simulations and discussions

So far, we cannot obtain the exact solution of the relaxation dynamics of the ECGI model (Eq. (9)) and we detailed the nature of the model relaxation dynamics through computer simulations. The specific simulation method is the same as that in Ref. [35] and the relaxation characteristic quantity in the simulation is defined as

$$R(t) = \frac{1}{Mn}\sum_{m=1}^{M}\sum_{i=1}^{n}s_i^{mn}(t), \tag{10}$$

where M is the number of Ising chains in the simulated system and we let $M = 5\times 10^4$ in this article. When $t = 0$, we set all the Ising spin states in the system $s_i^{mn}(t) = 1$, $i = 1, \ldots, n$, $m = 1, \ldots, M$, and the corresponding relaxation function is

$$\varphi(t) \equiv R(t)/R(0). \tag{11}$$

In addition, the Monte Carlo time step is $t_{\rm MS} \equiv \tau_0\,\mathrm{e}^{-2J/kT}$ in our simulations. In a $t_{\rm MS}$, the jump probability of any Ising spin transferring from initial states $s_i^{mn} = \pm 1$ to the final states $-s_i^{mn} = \mp 1$ is $p_{s_i^{mn}\to -s_i^{mn}}^{\rm ECGI} = \mathrm{e}^{-2J/kT}\,\mathrm{e}^{-(s_{i-1}^{mn}+s_{i+1}^{mn})s_i^{mn}J/kT}/2$.

For a set of temperature T and Ising chain length n, the simulated relaxation function $\varphi(t)$ versus the reduced time $t/\tau_0\,\mathrm{e}^{-2J/kT}$ is shown in Figs. 1 and 2. It is found that, for all T and n, the variation of simulated $\varphi(t)$ with t can be described in exponential quite well,

$$\varphi(t) = \mathrm{e}^{-t/\tau}, \tag{12}$$

where τ is the relaxation time.

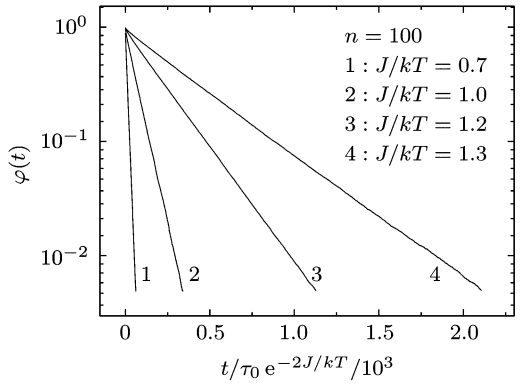


Fig. 1. Simulated relaxation function $\varphi(t)$ versus time t of the ECGI model for $n = 100$ and for a set of J/kT values.

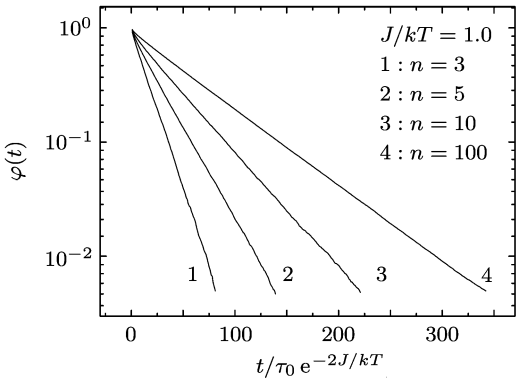


Fig. 2. Simulated relaxation function $\varphi(t)$ versus time t of the ECGI model for a set of n values with $J/kT = 1.0$.

By fitting Eq. (12) to the simulated $\varphi(t)$ for a series of T and n values, we can obtain the results that τ changes with T and n, as shown in Figs. 3 and 4, respectively.

As can be seen from Fig. 3, τ increases monotonically with decreasing T for definite n values. Furthermore, the variation of τ in the entire simulated temperature range can be described by two Arrhenius relationships approximately when n is large enough, formally indicating that the relaxation of the ECGI model crosses over from a high-temperature activation process with larger activation energy to a low-temperature one with smaller activation energy, though intrinsically originating from the competition between the interaction and thermal fluctuations of the Ising spins. It is worth noting that Lunkenheimer *et al* first found the phenomenon when measuring the high temperature relaxations of orientational glasses,[63] so the corresponding crossover temperature is defined as T_{L} (Fig. 3).

Figure 4 shows that τ increases monotonically with increasing n at definite T and specifically, it goes up rapidly when n is small but the increasing tendency becomes slow when n is large enough.

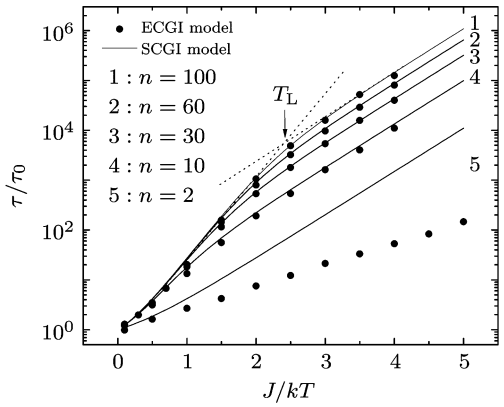


Fig. 3. Relaxation time τ of the ECGI model (black dot) and SCGI model (solid line) versus J/kT for a set of n values.

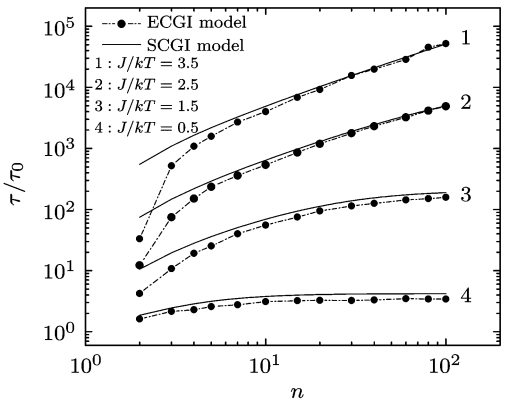


Fig. 4. Relaxation time τ of the ECGI model (point dotted line) and SCGI model (solid line) versus n for a set of J/kT values.

As a comparison, we also give the theoretical results of the special chain GI (SCGI) model[1,32–35] in Figs. 3 and 4,

$$H_{\mathrm{I}} = -\frac{J}{2}\sum_{m=1}^{\infty}\sum_{i=1}^{n}\left(s_{i-1}^{mn} + s_{i+1}^{mn}\right)s_i^{mn},$$

$$\nu_{s_i^{mn}\to -s_i^{mn}}^{\mathrm{SCGI}} = \frac{1}{\tau_0}\frac{1}{1+\mathrm{e}^{2(s_{i-1}^{mn}+s_{i+1}^{mn})s_i^{mn}J/kT}}. \quad (13)$$

It can be found that, when n is small or T is high, the relaxation time τ of the ECGI model has a clear deviation from the SCGI model (Eq. (13)), but when n is large enough ($n > 20$) and T is relatively low ($J/kT > 2$) that is the most valuable case in the model applications,[2–58] the results of the two models are consistent with each other. These show that, although the physical origin of the single spin-flip rate in the SCGI model is not clearly more or less,[1,32–35] the model has reasonable and effective aspects because its relaxation dynamics can be solved exactly, so it has the value that could not be replaced in dealing with

the Glauber dynamics of some specific systems. On the other hand, the ECGI model will provide a firm physical base for the single spin-flip rate proposed by Glauber, which is widely used in many systems and a possible route to obtain the single spin-flip rate of other forms and even the multi-spin transition rate.[2−15,18−26,28,30−59,64]

The authors would like to point out that, for the simplicity of the deducing procedure and the results to be concise in this paper, it is assumed that the heat bath in the ECI model only contains phonons and the phonon density of energy states $g(E)$ is constant, which is not the usual case in real systems. Therefore, the influence of taking into account the change of $g(E)$ with energy E on the single spin-flip rate of the ECGI model (Eqs. (8) and (9)) will be a question worth studying further in-depth. In addition, although the phonon thermal bath is most common, it will also be an interesting problem to consider the influence of a non-phonon thermal bath or a mixed heat bath on the Glauber dynamics of the Ising model.

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