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Measurement of the correlation length on Ising model

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Abstract

We present a method for measuring the correlation length of the Ising model. Starting from a ground state, we consider a quantity $K(t,T) \equiv L(\langle M^2(t)\rangle/\langle M(t)\rangle^2 - 1)^{1/d}$, where $M(t)$, L and d denote the magnetization, the system size, and substrate dimension of the model, respectively. $K(t,T)$ follows a power-law behavior $K(t,T_c) \sim t^{1/z}$ at the critical temperature T_c and the saturation value of $K(\infty,T)$ shows that $K_{\mathrm{sat}}(T) \sim |T_c - T|^{-\nu}$. The critical exponents $\nu = 1.00(1)$ and $z = 2.15(1)$ are estimated in a two dimensional square lattice. By calculating solely $K(t,T)$, we could obtain the correlation-length exponent directly. Also, the correlation length and critical exponents of the three dimensional Ising model on a cubic lattice are discussed. We believe that this is an effective method, which can be feasibly applied to various spin models.

Keywords Correlation length · Ising model · Critical temperature · Correlation length exponent

1 Introduction

The Ising model is the simplest lattice model originally developed as a mathematical model of ferromagnetism in statistical mechanics [1]. Subsequently, the model was found to exhibit potential for application in modelling the critical point of fluids and binary alloy phase separation [2]. Further, the variants of the model have been used in high-energy physics to explore the behavior of simple lattice gauge theories [3]. The Ising model is crucial for studying phase transition phenomena [4–12]. The model includes discrete variables representing magnetic dipole moments of atomic spins that can be in one of the two states (i.e., up or down). Their interaction with their neighboring spins is described with the Hamiltonian

$$H(\sigma) = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_j \sigma_j, \tag{1}$$

where $\sigma_i = \pm 1$. J denotes nearest-neighbor coupling constant, h the external field, and $< i,j >$ the nearest-neighbor pair interaction. J is set as a constant for simplification.

In one dimension, the exact solution was obtained by Ising. The canonical partition function

$$Z(T) = \sum_{\sigma_1,\ldots,\sigma_L} e^{-H(\sigma)/k_B T}, \tag{2}$$

where k_B and T represent the Boltzmann constant and absolute temperature, respectively, were accurately calculated and all thermodynamic quantities were obtained accordingly. The solution shows no phase transition at a finite temperature. In two dimensions, the exact solution was found by Onsager [4] on a square lattice; the model is known to yield a phase transition at a finite temperature. Therefore, the two-dimensional Ising model in a square lattice is the simplest statistical model that shows a phase transition. The exact critical temperature of the two-dimensional Ising model is $T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269185$ in unit of J/k_B and the correlation length exponent is known to be $\nu = 1$ [4, 13, 14].

In general, measuring the correlation length directly in a spin model is difficult. In this study, we consider the fluctuation of magnetization for the ferromagnetic Ising model on a square lattice and introduce a new quantity to measure the correlation length. An Ising model is used to verify whether the proposed method yields consistent critical exponents with known exact values. We found that the variance of the relative fluctuation of magnetization is associated with the correlation length, therefore we could calculate the correlation length and the related critical exponents by measuring the relative fluctuation of the magnetization.

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2 Order parameter

In the Ising model, the magnetization M is defined as $M(t) = \frac{1}{N}\sum_i \sigma_i(t)$, where N is the total number of substrate sites. Near the critical temperature, the following thermodynamic quantities are known to exhibit power-law behaviors: magnetization M, susceptibility χ, correlation length ξ, and specific heat C [13, 14]. The relations are as follows:

$$\begin{aligned} \langle M\rangle &\sim |T-T_c|^{\beta}, \\ \chi &\sim |T-T_c|^{-\gamma}, \\ \xi &\sim |T-T_c|^{-\nu}, \\ C &\sim |T-T_c|^{-\alpha}. \end{aligned} \tag{3}$$

Using $|T-T_c| \sim \xi^{-1/\nu}$, χ and $\langle M\rangle$ can be expressed as a function of ξ following $\langle M\rangle \sim \xi^{-\beta/\nu}$ and $\chi \sim \xi^{\gamma/\nu}$. With the hyper scaling relations $\alpha + 2\beta + \gamma = 2$ and $\alpha = 2 - d\nu$, we obtain the following :

$$\frac{\chi}{\langle M\rangle^2} \sim \frac{L^d\left(\langle M^2\rangle - \langle M\rangle^2\right)}{\langle M\rangle^2} \sim \xi^{\frac{\gamma+2\beta}{\nu}} \sim \xi^d. \tag{4}$$

Thus, we introduce a quantity $K(t, T)$ defined as

$$K(t,T) = L\left(\frac{\langle M^2\rangle - \langle M\rangle^2}{\langle M\rangle^2}\right)^{1/d} \sim \left(\frac{\chi}{\langle M\rangle^2}\right)^{1/d} \sim \xi, \tag{5}$$

where L is the system size. Then $K(t)$ should be proportional to the correlation length $\xi(t)$ near the critical temperature. Even though the susceptibility itself is a good quantity to describe the phase transition [15], it is quite interesting that the relative fluctuation of the magnetization is related to the correlation length.

Note that we have introduced a similar quantity for the surface roughness problem, where M is replaced by the square of the surface width [16]. Various models describing surface growth exhibit self-organized critical behavior [17–21]. In a previous study on non-equilibrium surface growth, the fluctuation of surface height was demonstrated to be associated with the correlation length [16] where no temperature-like control parameter exists.

Here we assume that the relative variance of magnetization is proportional to $1/N$, where N is the number of independent samples. When the correlation length ξ is smaller than the system size L, magnetization is considered to be effectively averaged over $(L/\xi)^d$ independent samples; i.e., 1portional to ξ and scales as $K(t) \sim t^{1/z}$ initially and saturates to L later for a finite system.

3 Monte Carlo method

To develop $K(t)$ as a function of time, the system is assigned to start from the ground state of all spins pointing up. As time increases, thermal fluctuation flips neighboring spins, following the Metropolis-Hasting algorithm [9, 10, 22]. We choose a site k randomly in the lattice and calculate the energy difference ΔE_k between the energies before and after the spin is flipped. The energy of the system is given as

$$E = -\sum_{<i,j>} \sigma_i \sigma_j \tag{6}$$

in the unit of J without an external field. If $\Delta E_k < 0$, we accept the new configuration, and if $\Delta E_k > 0$, we accept it with a probability $\exp(-\Delta E_k/k_B T)$. At low temperatures, the system remains in the lower-energy state because the probability of flipping toward a higher energy is low. As the temperature increases, the probability of flipping toward higher energy state gradually increases and the fluctuation of $K(t)$ increases with time. At the critical temperature, we expect that $K(t)$ to exhibit the power-law $K(t) \sim t^{1/z}$, provided that the system is sufficiently large. On the contrary, for a finite system, $K(t)$ saturates to L as the correlation length does. Time t is defined as the number of Monte Carlo steps where t is increased by 1 with L^2 spin flip trials in two dimensions.

Assuming that $K(t, T, L)$ is a homogeneous function, the scaling theory enables to write

$$K(t, T_c, L) = t^{1/z} F(L/b, t/b^z) = L\mathcal{F}(t/L^z) \tag{7}$$

at the critical point, where b is the scaling factor and z is the dynamic exponent. However, for a sufficiently large system of $L \gg \xi$,

$$K(t,T,L) = t^{1/z} G(t/b^z, \Delta b^{1/\nu}) = \Delta^{-\nu}\mathcal{G}(\Delta t^{1/\tau}), \tag{8}$$

where ν and $\tau(= z\nu)$ are the spatial and temporal correlation length exponents, respectively, and $\Delta = T_c - T$. The scaling function $\mathcal{G}(x)$ is proportional to x^ν for $x \ll 1$ and becomes constant for $x \gg 1$ with $T < T_c$. Note that, because the system develops from the ground state, the correlation length increases with time as $\xi \sim \tau^{1/z}$. As $t \to \infty$, $K(t, \Delta) \to K_{\rm sat}(\Delta) \sim \Delta^{-\nu}$, therefore, we can calculate the correlation length exponent ν by plotting $K_{\rm sat}$ versus $T_c - T$ on a log-log plot.

4 Results and discussions

4.1 Two dimensional Ising model on square lattice

Starting from the ferromagnetic ground state of all spins up, Monte Carlo simulation are performed on $L = 1000$ square lattice with periodic boundary conditions. We calculate $K(t)$ for various temperatures ranging $K_B T/J = 2.15 \sim 2.35$ up to 10^6 Monte Carlo time steps to determine the critical temperature. As shown in Fig. 1, at low temperatures, $K(t, T)$ is small and remains saturated, implying that the system stays in a low-energy state. As the temperature increases, $K(t)$ initially increases following a power-law and eventually becomes saturated. At (or at least near) the critical temperature $T_c = 2.2692\ J/k_B$, $K(t)$ exhibits a power-law behavior $K(t) \sim t^{1/z}$. As the temperature further increases beyond the critical temperature, $K(t)$ deviates in the opposite direction. Therefore, using the data of $K(t)$, $k_B T_c/J = 2.2692$ is estimated, which is close to the expected critical temperature. The least-square fit over the data for $T = 2.2692\ J/k_B$ gives a power of $1/z = 0.465(2)$ with $z = 2.15(1)$. This is consistent with the previous result $z = 2.1665(12)$ [23].

The saturation values $K_{\rm sat}(T)$ is also calculated and it is plotted against $T_c - T$ as shown in Fig. 2. The power-law behavior $K_{\rm sat}(T) \sim (T_c - T)^{-\nu}$ using $T_c = 2.2692\ J/k_B$ yields the correlation-length exponent $\nu = 1.00(1)$, which is in excellent agreement with the known exact value $\nu = 1$. This ensures that the proposed method is a powerful tool for calculating the correlation lengths and is applicable for exploring phase transitions in equilibrium spin systems.

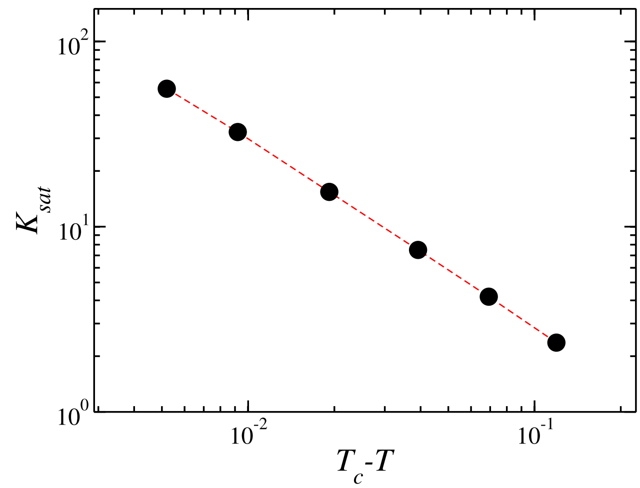

Fig. 2 Plot of $K_{\rm sat}(T)$ as a function of $T_c - T$ on a log-log scale using $T_c = 2.2692\ J/k_B$. The data show the power law $K_{\rm sat}(T) \sim |T_c - T|^{-\nu}$ with $\nu = 1.00(1)$

We examined off-critical and finite-size scaling to validate the estimated critical exponents. Following Eq. (8), the off-critical data of $K(t, T)$ extracted from Fig. 1 are shown in Fig. 3. The scaled data of $(T_c - T)^\nu K(t, T)$ for various values of T in the subcritical region against the scaled value $(T_c - T)t^{1/z\nu}$ collapse onto a single curve, supporting our estimates of $\nu = 1$ and $z = 2.15$. The data for $T > T_c$ also collapse onto a single curve, which is different from the curve obtained from the data for $T < T_c$. The scaling function $\mathcal{G}(t^{1/z}|T_c - T|)$ curves upwards for $T > T_c$ and curves downwards and eventually becomes saturated for $T < T_c$.

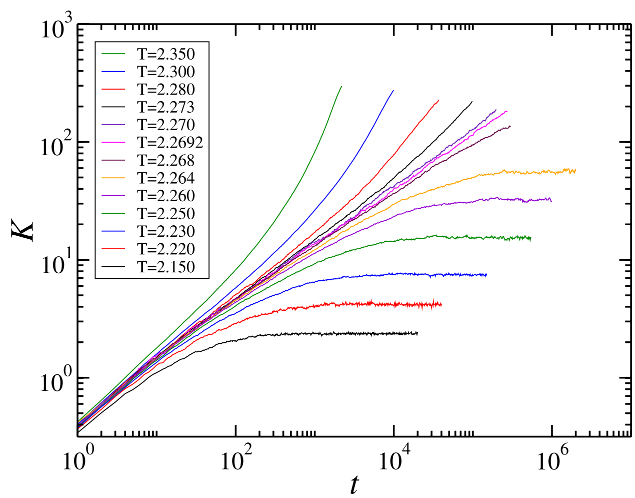

Fig. 1 Data of $K(t, T)$ for various temperature values on a system size $L = 1000$. At the known critical temperature $T = 2.2692$, the data show a power-law behavior $K(t) \sim t^{1/z}$, with $1/z = 0.465(2)$. Below T_c, $K(t, T)$ saturates to a constant of $K_{\rm sat}(T)$

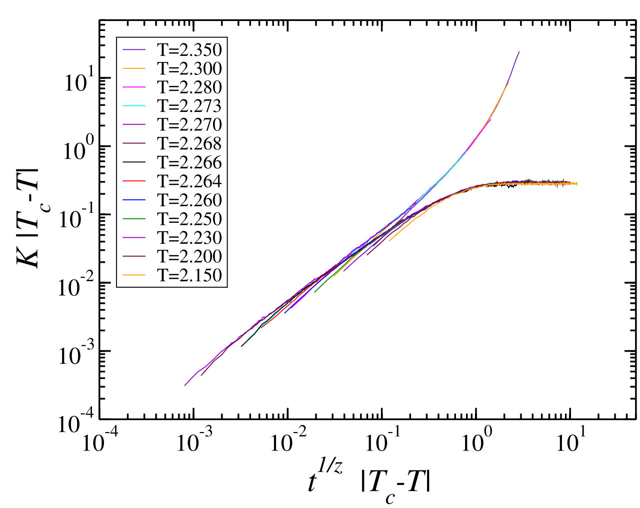

Fig. 3 Off-critical scaling plot of $K(t)$ for the data of Fig. 1, $K(t, T) \sim (T_c - T)^{-\nu}\mathcal{G}(t^{1/z\nu}|T_c - T|)$. The scaled data of $K(t, T)|T_c - T|$ plotted against the scaled variable $t^{1/z\nu}|T_c - T|$ show an excellent collapse when the estimated values of $z = 2.15$, $\nu = 1$ and $T_c = 2.2692$ are used

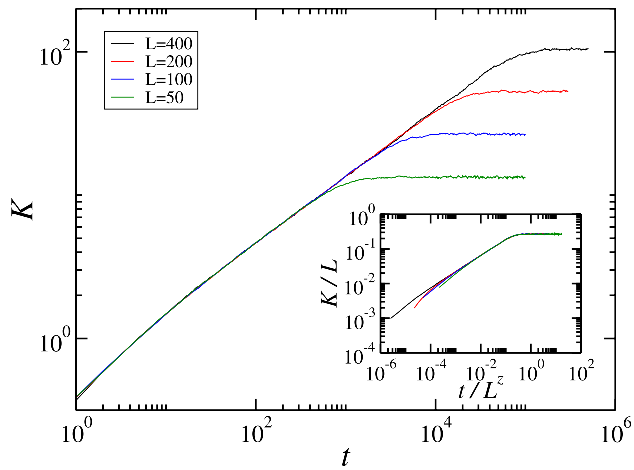

Fig. 4 Data of $K(t, T_c, L)$ as a function of t for various system sizes at the critical temperature of $T_c = 2.2692\ J/k_B$. In the inset, the scaled data of $K(t)/L$ plotted against scaled variable t/L^z collapse onto a single curve for various system sizes of L with $z = 2.15$

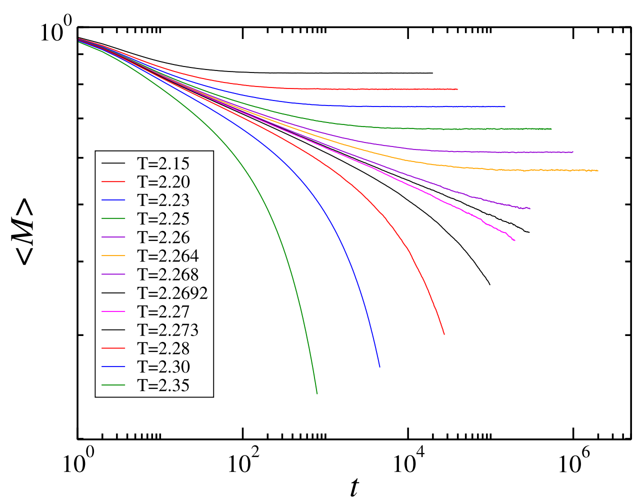

Fig. 5 The magnetization as a function of time t for the Ising model on a square lattice of system size $L = 1000$

To examine the critical scaling, we carried out simulations for various system sizes, i.e., $L = 50$, 100, 200, and 400 at the critical temperature $T_c = 2.2692\ J/k_B$. The data plotted in Fig. 4 of the main panel are the raw data of $K(t, T_c, L)$ and those in the inset are the scaled data for $z = 2.15$. They exhibit a perfect collapse on a single curve. Therefore, the scaled plots shown in Figs. 3 and 4 confirm that the data of $K(t, T)$ give the correct critical exponents and satisfy the scaling analysis.

We also monitor the magnetization $M(t)$ as a function of time t at various temperatures. As shown in Fig. 5, the critical temperature is found to be $T_c \approx 2.2692$ where $M(t)$ follows a good power law behavior. Because $\langle M \rangle \sim \xi^{-\beta/\nu} \sim t^{-\beta/z\nu}$, we expect $\langle M(t) \rangle \sim t^{-\kappa}$ with $\kappa = \beta/z\nu = 1/8z$ from the exact values $\nu = 1$ and $\beta = 1/8$ in the two dimensional Ising model. At the critical temperature $T_c = 2.2692$, using the relation $\langle M(t) \rangle \sim t^{-\kappa}$, we obtain $\kappa = 0.0581(6)$, and $z = 2.15(1)$ from the relation $z = 1/8\kappa$. This is consistent with the previous estimate of $z \approx 2.15$ from $K(t)$. By monitoring the time dependent magnetization, the critical temperature could be determined and the dynamic exponent z could be obtained indirectly.

In general, to obtain the correlation length, one should consider the spin-spin correlation function $G(r, t, T)$ which is defined by $G(r, t, T) = \langle \sigma(0)\sigma(r) \rangle - \langle \sigma(0) \rangle \langle \sigma(r) \rangle$ at time t. For $T \neq T_c$, it falls off exponentially following

$$G(r, t, T) \sim \exp\left(-\frac{r}{\xi(t, T)}\right), \tag{9}$$

where $\xi(t, T)$ is the correlation length. One can estimate $\xi(t, T)$ by fitting the obtained $G(r, t, T)$ to Eq. (9) or by the structure factor of the spin for the lowest value of the wave vector k [24]. The dynamic critical exponent z was determined from a finite-size scaling analysis of the correlation times [23] or by the second-largest eigenvalue of the single spin flip Markov matrix for the Ising model [23]. Therefore, it is very time consuming to measure the correlation length and dynamic exponent z. However, here we find that $K(t)$ is proportional to the correlation length and follows a power law at the critical temperature. From the relation $K(t) \sim t^{1/z}$, we can obtain critical temperature easily and z directly.

4.2 Three dimensional Ising model on a cubic substrate

We apply our method to the three dimensional Ising model for higher dimensions. Starting from all spins up configuration on a cubic substrate with a periodic boundary condition, $K(t)$ is monitored for a linear system size $L = 200$. Data are averaged over 2000 independent samples to reduce fluctuations.

As shown in Fig. 6, $K(t)$ follows a good power-law behavior at $T_c = 4.51155$. $K(t)$ curves upwards above T_c and curves downwards below T_c. We found $T_c = 4.51155(15)$ where the data shows a good power-law behavior. $z = 2.025(8)$ is estimated through the relation $K(t) \sim t^{1/z}$ at $T = 4.51155$. Estimates of the critical temperature and dynamic exponent are in a good agreement with the previous results $T_c = 4.5115(2)$, $z = 2.0245(15)$ of Ref. [25, 26]. Our numerical results support that $K(t)$ is proportional to the correlation length even in $3d$ Ising model. To obtain the correlation length exponent ν, the saturated value $K_{sat}(T)$ was monitored and expressed as a function of $T_c - T$ in Fig. 7. The data show a very good straight line supporting the power-law behavior $K_{sat}(T) \sim (T_c - T)^{-\nu}$ at $T_c = 4.51155\ J/K_B$ where the correlation length exponent $\nu = 0.631(4)$ is estimated.

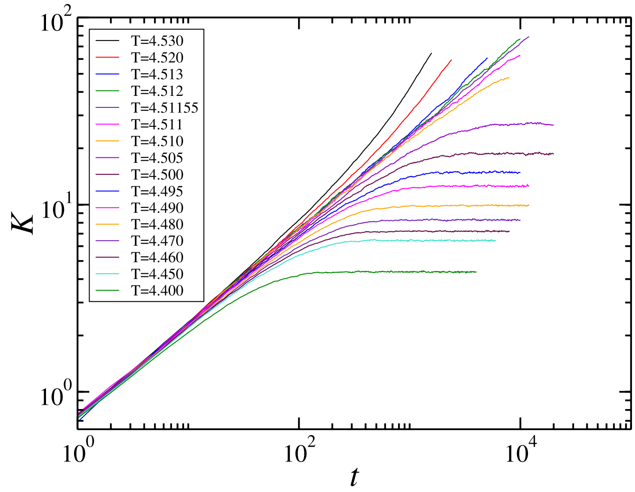

Fig. 6 Numerical data of $K(t)$ for various temperatures on the three dimensional Ising model with a system size $L = 200$. It shows a power-law behavior $K(t) \sim t^{1/z}$ with $z = 2.025(8)$ at $T = 4.51155$

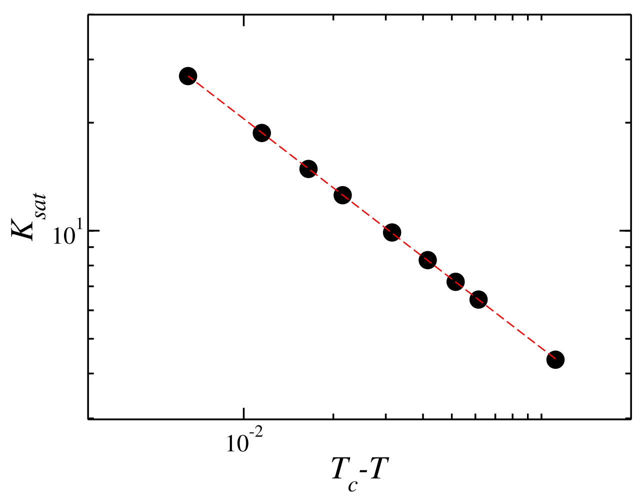

Fig. 7 $K_{sat}(T)$ as a function of $T_c - T$ in log-log scale for various T with $T_c = 4.51155J/K_B$ on three dimensional Ising model. It shows a good power-law with $\nu = 0.631(4)$

This value is slightly larger but in good agreement with the reported value 0.630 [10, 24, 27] within the error bars.

5 Conclusion

In general, it is not easy to find the correlation length directly. Here we introduce a quantity $K(t)$ and estimate ν directly using the power-law $K_{sat}(T) \sim |T - T_c|^{-\nu}$. At least it can be a method of obtaining the correlation length as a function of time for a given temperature. We found that $K(t)$ is effectively proportional to the correlation length below T_c and follows the power-law behavior $K(t) \sim t^{1/z}$ at the critical temperature. Below and above T_c, the data deviated downwards and upwards, respectively. Thus, the power-law behavior of $K(t)$ serves as a method for determining the critical temperature. The dynamic critical exponent z was calculated from the power-law behavior of $K(t)$ at the criticality. The obtained z is in good agreement with the previous result [23]. Because $K(t)$ is directly proportional to the correlation length, $K(t)$ also provides additional information about the crossover behavior. The saturation value $K_{sat}(T)$ shows a power-law of $K_{sat}(T) \sim |T - T_c|^{-\nu}$. In this relation, $\nu = 1.00(1)$ is obtained on two dimensional Ising model which is in a good agreement with the exact value $\nu = 1$. We have applied this method to the three dimensional Ising model also and obtained ν and the critical temperature that agree well with previous results [6–8, 10]. We believe that our method of using $K(t)$ is a powerful tool that can be applied to other related spin systems.

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