

Behavior of damage spreading in the two-dimensional Blume-Capel model

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The damage spreading technique has been used to study the general integer and half-integer spin- S Blume-Capel model on the square lattice within a Metropolis-type dynamics. For $S=1$ and 2 integer spins, our results suggest that there exists one multicritical point along the order-disorder transition line; for $S=3/2$ and $5/2$ half-integer spins, our results show that this multicritical behavior does not exist for this model.

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I. INTRODUCTION

The $S=1$ Blume-Capel model was originally proposed to study the first-order phase transition in magnetic systems [1,2] and has also been used in describing He^3 - He^4 mixtures [3]. The Hamiltonian can be written as

$$H = -J \sum_{\langle ij \rangle} S_i S_j + G \sum_i S_i^2. \quad (1)$$

The first summation is carried out only over nearest-neighbor pairs of spins, the second summation runs over all sites of a square lattice. $J>0$ is the ferromagnetic exchange interaction between nearest neighbor spins, G is the single spin anisotropy parameter. The spin variable S_i assumes values $-S, -S+1, \dots, S-1, S$, where S is either a positive integer or a positive half integer. The $S=1$ case has been extensively studied by a variety of methods such as mean-field [1,2], variational methods [4], constant coupling approximation [5], Monte Carlo simulations [6,7], transfer matrix [8], renormalization-group [9,10], finite-size scaling based on transfer matrix [11], etc. It is well established that for dimension $d \geq 2$, the $S=1$ Blume-Capel model exhibits a line of continuous phase transition (Ising-type), a line of first-order phase transitions and a tricritical point where those two lines meet.

For values of spin $S>1$, however, the situation is quite unclear and fewer results are available. For the $S=3/2$ case, the mean-field calculation [12], correlated effective-field treatment [13], differential operator technique [14], finite-size scaling based on transfer matrix [11], and conventional equilibrium Monte Carlo simulations [15,16] indicate a second-order phase transition with no tricritical point and a separated first-order transition line that terminates in an isolated multicritical point. In contradiction with these results, a renormalization-group calculation [10] presents a unique first-order transition line at low temperature, which terminates in the second-order transition line at a tetracritical point. Similar results are also obtained by finite-size renormalization-group calculations [17] and other conventional equilibrium Monte Carlo simulations [18].

The damage spreading (DS) technique, i.e., measuring the Hamming distance between two different initial configurations subject to a specific dynamics and to the same thermal noise as they evolve in time, has been successfully applied to many magnetic models. It turns out that this method is less sensitive to the static fluctuations, when compared to the conventional Monte Carlo method where the time evolution of a single copy is investigated. The DS technique represents presently an important tool in the study of the dynamics as well as the static behavior in magnetic systems [19–28]. In fact, for the controversies surrounding the $S=3/2$ Blume-Capel model, the DS method allows us for the first time to distinguish definitely between the two conflicting scenarios discussed in the literature.

In this paper, the DS technique is also applied to study the Blume-Capel model on the square lattice. Our results show that for the integer $S=1$ and 2 Blume-Capel models, there exists a multicritical point at low temperature, which is not present for the half-integer $S=3/2$ and $5/2$ spin models.

The layout of this paper is as follows. In Sec. II, we describe the damage spreading technique and the Metropolis-type dynamics that we will use. In Sec. III, we present the results for the integer spin $S=1$ and 2 Blume-Capel models. In Sec. IV, we perform the DS calculations for the half-integer spin $S=3/2$ and $5/2$ cases. Finally, Sec. V presents the conclusions.

II. THE DAMAGE SPREADING TECHNIQUE AND A METROPOLIS-TYPE DYNAMICS

Our numerical simulations are implemented on square lattice with N spins and linear size L ($N=L^2$ sites) submitted to periodic boundary conditions. A configuration of lattice spins at time t is

$$C(t) = \{S_i(t)\} \quad i = 1, 2, 3, \dots, N. \quad (2)$$

In order to make a configuration $C(t)$ evolve in time, we use a Metropolis-type dynamics that has been successfully applied to the $S=1/2$ and $S=1$ Ising models and the mixed spin Ising model on the square lattice [29,30].

During each time interval $\delta t = 1/N$, one spin site i is chosen randomly. The spin value $\Delta_i(t + \delta t)$ at time $t + \delta t$ is then proposed by

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$$\Delta_i(t + \delta t) = \begin{cases} -S, & 0 \leq Z_{i1}(t) < 1/(2S+1) \\ -S+1, & 1/(2S+1) \leq Z_{i1}(t) < 2/(2S+1) \\ \dots & \dots \\ S-1, & (2S-1)/(2S+1) \leq Z_{i1}(t) < 2S/(2S+1) \\ S, & 2S/(2S+1) \leq Z_{i1}(t) < 1, \end{cases} \quad (3)$$

where $Z_{i1}(t)$ is an uniform random number, $0 \leq Z_{i1}(t) \leq 1$.

One then updates the spin according to the following dynamics rule

$$C_i(t + \delta t) = \begin{cases} \Delta_i(t + \delta t), & P_i(t) \geq Z_{i2}(t) \\ C_i(t), & \text{otherwise,} \end{cases} \quad (4)$$

where

$$P_i(t) = \exp(-\Delta H_i/T), \quad (5)$$

$$\Delta H_i = H\{\Delta_i(t + \delta t)\} - H\{C_i(t)\}, \quad (6)$$

where $0 \leq Z_{i2}(t) \leq 1$ is another uniform random number, T is the temperature of the system in units of J/K_B , G is in units of J , and K_B is the Boltzmann's constant.

We consider two different initial configurations $C^A(0)$ and $C^B(0)$ at time $t=0$, and let them evolve in time according to the same above dynamic rule with the same sequence of random numbers for updating the spins. Then two configurations at time t , $C^A(t)$ and $C^B(t)$, are computed through the following Hamming distance (or damage) between them

$$D(t) = \frac{1}{N} \sum_{i=1}^N [1 - \delta(C_i^A(t), C_i^B(t))], \quad (7)$$

where $\delta(\cdot)$ is the Kronecker delta function. Physically $D(t)$ measures the fractions of the spins that differ in the two replicas at time t . In calculations, we average $D(t)$ over many samples. The average distance is

$$\langle D(t) \rangle = \frac{1}{N_s} \sum_{j=1}^{N_s} D_j(t), \quad (8)$$

where $D_j(t)$ is the damage distance for the j th independent trial, N_s is the number of independent sample, the sum is over all trials (here, we have not used the conventional method that the average was taken over only those samples where their $\langle D(t) \rangle$ are not zero).

We also study the ‘‘damage susceptibility’’

$$\sigma_{D(t)} = \sqrt{\langle D^2(t) \rangle - \langle D(t) \rangle^2}, \quad (9)$$

which measures the fluctuations of damage $D(t)$. This quantity will provide a set of information to characterize different phases of the system, and is very sensitive to the phase transition.

We will investigate a quantity that we define as the ratio of $N_{S_i=c}$ (number of spins whose spin S_i takes one specified

value $c \in (-S, -S+1, \dots, S-1, S)$ to N at the equilibrium state. In order to decrease the fluctuations, we take an average over those two replicas (configuration A and B)

$$\langle P_{S_i=c} \rangle = \frac{1}{N_s} \sum_{k=1}^{N_s} \left[\frac{N_{S_i=c}^A + N_{S_i=c}^B}{2N} \right]_k. \quad (10)$$

$\langle P_{S_i=c} \rangle$ depends on the temperature, time, initial conditions, and the noise. $\langle \cdot \rangle$ in Eq. (10) denotes an average over many samples. It is actually another type of order parameter.

In the following calculations presented here, the initial configuration is chosen to be

$$C^A(0) = -C^B(0) \neq 0, \quad \forall i, \quad (11)$$

i.e., we choose $\langle D(0) \rangle = 1$. For example, for the $S=2$ case, we may choose $C^A(0) = -C^B(0) = \{2\}$, or, $C^A(0) = -C^B(0) = \{1\}$, these two choices will not alter the features of the calculation results. The calculations could have been done starting with other initial conditions, e.g., two random initial configurations. With this condition, the equilibrium of the system takes longer to be established at low temperature, however, the results would also be very similar [29].

Those three quantities $\langle D(t) \rangle$, $\sigma_{D(t)}$, and $\langle P_{S_i=c} \rangle$, together with temperature, initial condition, and any other parameters, will lead to information about the criticality of the system.

III. RESULTS FOR THE BLUME-CAPEL MODEL WITH $S=1$ AND 2

We choose to study several values of G by our DS procedure. The simulations have been performed for system size $L=40$, $t=1000$, and the results are averaged over $N_s=200$ samples. We observed that the finite-time effect for $t=1000$ and $t=2000$ is relatively small for our chosen initial condition. In the following calculations, we will assume that the systems have reached their equilibrium states at $t=1000$ for the chosen initial condition of Eq. (11).

We first study the Blume-Capel model with spin $S=1$ and initial condition $C^A(0) = -C^B(0) = \{1\}$. The results are plotted in Fig. 1. We explain the Fig. 1 as follows. Figure 1(a) shows the results of $\langle D(t) \rangle$ as a function of T and G . We may observe a completely different behavior of $\langle D(t) \rangle$: for $G/J \leq 2.0$, there exist Ising-like continuous phase transitions for the model for those G values. We clearly observe two distinct regions, a low-temperature region ($T < T_D$), where $\langle D(t) \rangle$ does not vanish and a high-temperature region ($T \geq T_D$), where the $\langle D(t) \rangle$ vanishes; for $G/J > 2.0$, contrary to the $G/J \leq 2.0$ cases, $\langle D(t) \rangle$ are zero for all temperature regions. For $G/J \leq 2.0$ cases in Fig. 1(a), two distinct temperature regions divided by a damage spreading transition temperature T_D are believed to denote the corresponding static continuous phase transition, and has been observed in most of the Ising-like systems. From Fig. 1(a) we may estimate the approximate (continuous) dynamical transition temperature T_D to be 2.35, 2.3, 2.2, 2.1, 1.85, 1.55, and 0.6 for $G/J = -4.0, -3.0, -2.0, -1.0, 0.0, 1.0$, and 2.0, respectively. In Fig. 1(b), we plot the temperature dependence of the fluctuation

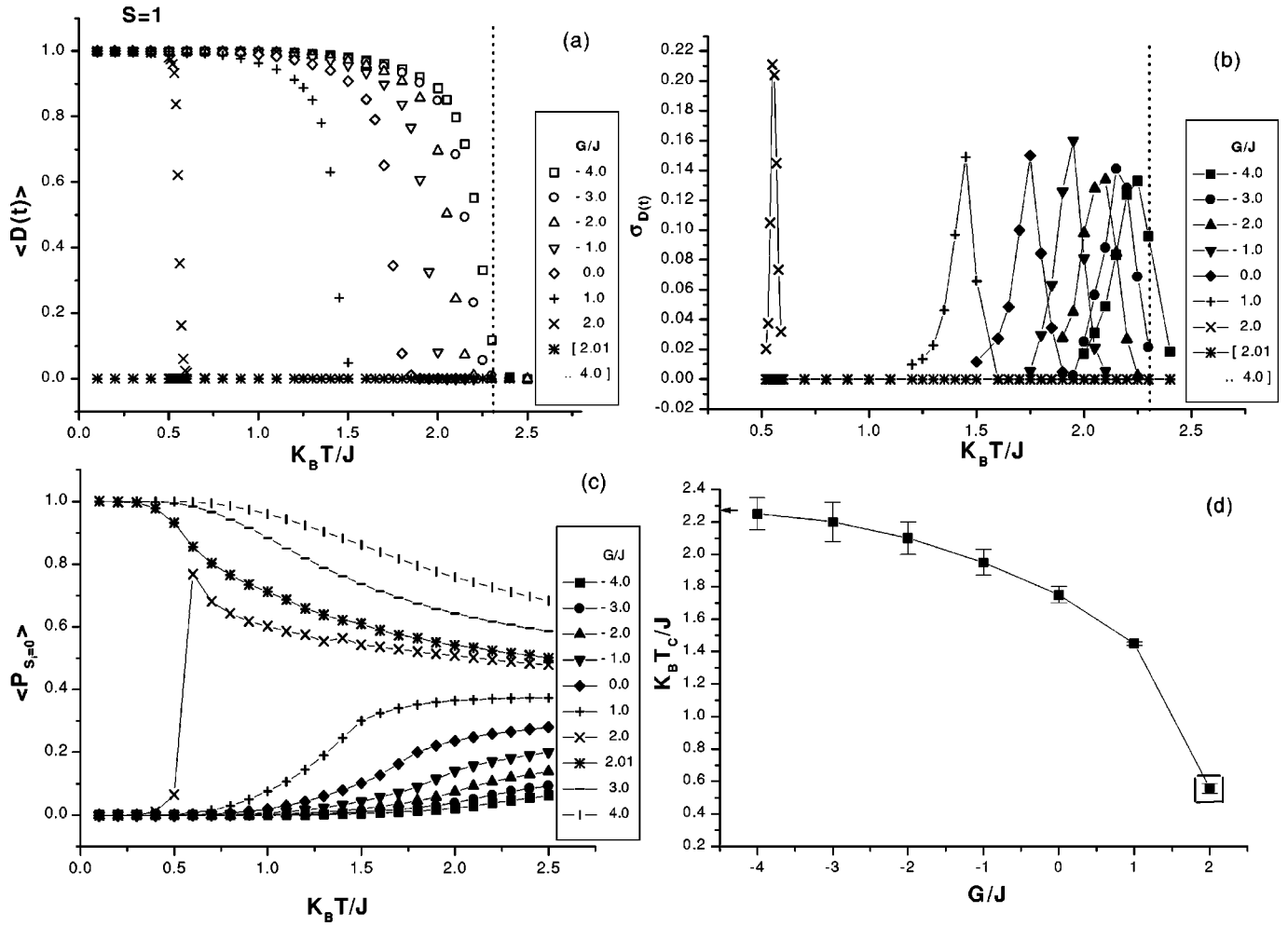


FIG. 1. The damage spreading results for $S=1$ Blume-Capel model on the square lattice at $L=40$, $t=1000$, and $N_s=200$. In the figure, a completely different behavior can be observed for $G/J \leq 2.0$ and for $G/J > 2.0$. The vertical dotted line marks the exactly known value of T_c for the standard Ising model on the square lattice. Figure 1(a) shows the average damage $\langle D(t) \rangle$ as a function of temperature T and G . Figure 1(b) shows the damage susceptibility $\sigma_{D(t)}$ as a function of temperature and G . The full line is a guide to the eye. From the maximum values of $\sigma_{D(t)}$, we may locate the phase transition temperature. Figure 1(c) shows the ratio $\langle P_{S_i=0} \rangle$ as a function of temperature T and G . The $\langle P_{S_i=0} \rangle = 0.0$ corresponds to the standard Ising model. Figure 1(d) shows the finite-temperature phase diagram for $S=1$ Blume-Capel model on the square lattice by damage spreading procedure. The solid line represents the second-order transition. The white square denotes the tricritical point at which the phase transition changes from second order to first order.

tuation $\sigma_{D(t)}$ for our chosen G values. We have observed that: for $G/J \leq 2.0$, the simulations show that there is an almost null fluctuation in the low- and high-temperature regions, except near the damage spreading transition temperature T_D where it rises abruptly; for $G/J > 2.0$, $\sigma_{D(t)} = 0$ for all temperature regions. The peaklike curves of $\sigma_{D(t)}$ in the $G/J \leq 2.0$ regions are the features of second-order transition, and from the maximum values of $\sigma_{D(t)}$ we may get the more accurate (continuous) dynamical transition temperatures than T_D . We estimate (run for several different random number sequences) T_σ to be $T_\sigma = 2.25 \pm 0.10$, 2.20 ± 0.12 , 2.10 ± 0.10 , 1.95 ± 0.08 , 1.75 ± 0.05 , 1.45 ± 0.01 , and 0.56 ± 0.03 for $G/J = -4.0, -3.0, -2.0, -1.0, 0.0, 1.0$, and 2.0 , respectively. In Fig. 1(c), the interesting features of $\langle P_{S_i=0} \rangle$ as a function of T and G/J are plotted. We regard $\langle P_{S_i=0} \rangle$ as an important factor to explain the multicritical behavior for this model. We

can also see there exist two different regions for those G values: for $G/J \leq 2.0$, the $\langle P_{S_i=0} \rangle$ increases as the temperature increases. In the limit of $G \rightarrow -\infty$, this model is reduced to the standard Ising model, and S can only take $+1$ or -1 values. For $G/J \geq 2.01$, contrary to $G/J \leq 2.0$ cases, $\langle P_{S_i=0} \rangle$ decreases as the temperature increases. In the limit of $G \rightarrow +\infty$, this model reaches a phase where S_i reaches 0 at every site.

The behavior of this $S=1$ Blume-Capel model could be explained as follows. In this model, we only consider the nearest-neighbor interaction between S_i spins. If we regard the $S_i=0$ state as a ‘‘hole,’’ then the lattice sites are occupied by either $S_i = \pm 1$ spins and the holes. Parameter G can change the relative number of $S_i = \pm 1$ spins and the holes in the system (representing chemical potential). When $G \rightarrow -\infty$, there is no hole in the system, corresponding to the

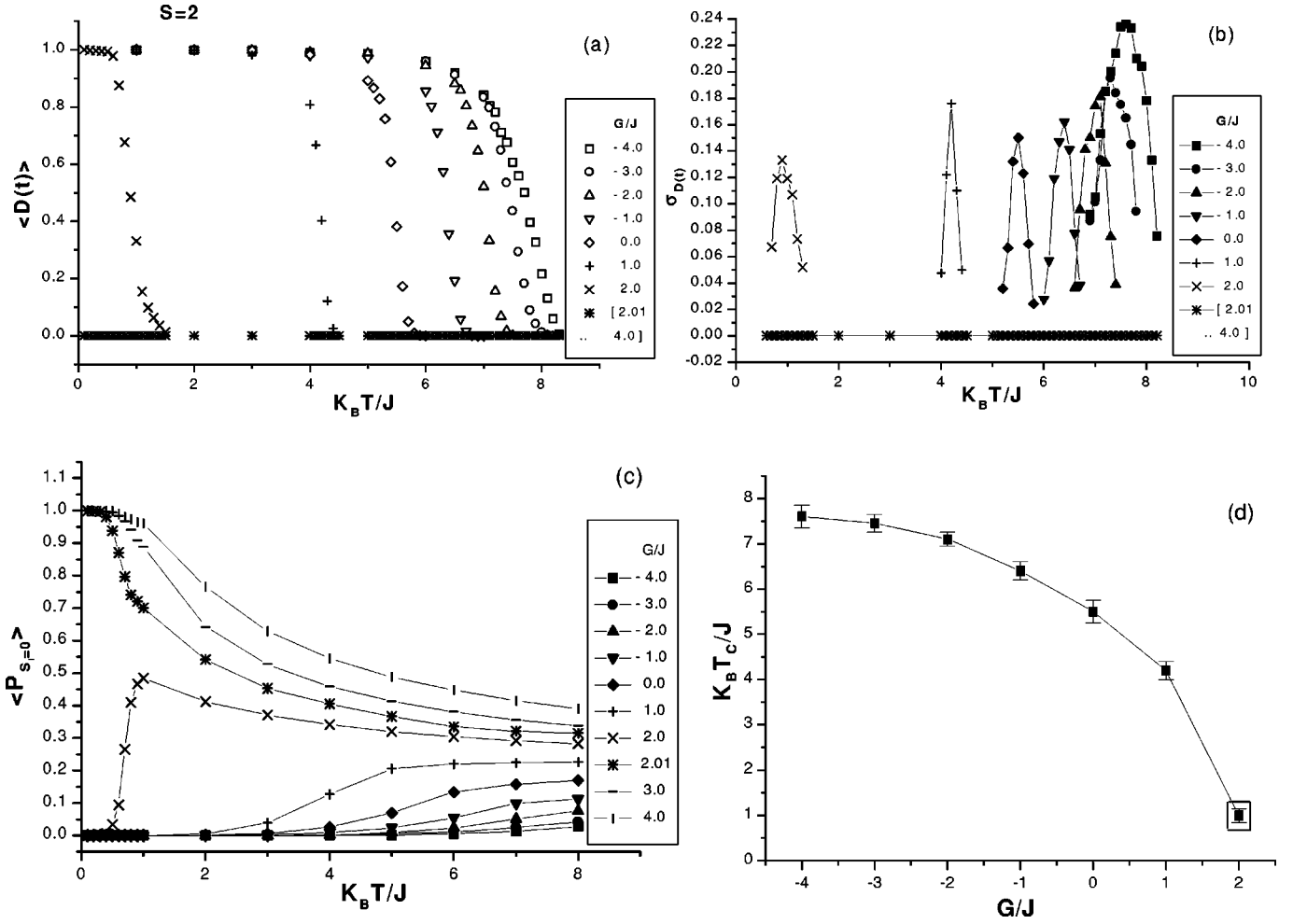


FIG. 2. The damage spreading results for $S=2$ Blume-Capel model on the square lattice at $L=40$, $t=1000$, and $N_s=200$. The notes are the same as in Fig. 1

standard Ising model. When G increases, the number of holes increases, the interaction of the total system becomes smaller, the second-order phase transition temperature also becomes smaller. When G increases to a critical value, the $S_i = \pm 1$ spins can no longer form the infinite clusters, the interaction of the system becomes weak and can no longer support the long range order of the system, then there are no continuous phase transitions, however, the clusters composed of $S_i = \pm 1$ spins and the holes can support the first-order phase transition for the system. From the angle of our Metropolis-type dynamics, because of the smaller interaction [i.e., ΔH_i in Eq. (6) approaches to zero], when G is larger than this critical G value, the probability [i.e., P_i in Eq. (5)] to accept the proposed spin value increases quickly, and then causes $\langle D(t) \rangle$ to go to zero quickly for those G values. The above critical G value is, therefore, the multicritical point, i.e., the meeting point of the second-order and the first-order transition lines. For the $S=1$ Blume-Capel model, this meeting point is $G_{tri} = 2.0$ in our DS simulations, and at this point an obvious discontinuity or “jump” of $\langle D(t) \rangle$ and $\langle P_{S_i=0} \rangle$ can be observed in Figs. 1(a) and 1(c). At last, when $G \rightarrow +\infty$, the sites are all occupied by $S_i=0$ spin state.

According to our DS results, we may schematically plot

the finite-temperature phase diagram for this model as in Fig. 1(d). We use T_σ obtained from $\sigma_{D(t)} - T$ relationship in Fig. 1(b) as the (second-order) phase transition temperature. In Fig. 1(d), the general shape of the phase diagram shows very good agreement between our calculations and other familiar results. From the data of our results, we estimate the tricritical point [white square in Fig. 1(d)] for $S=1$ Blume-Capel model to be $(T_{tri}, G_{tri}/J) = (0.56 \pm 0.03, 2.00)$. The known static values for the tricritical point for this model are $(0.609, 1.965)$ [11], $(0.608, 1.967)$ [7], $(0.610 \pm 0.005, 1.966 \pm 0.001)$ [8], $(1.088, 1.8848)$ [14], $(1.333, 1.848)$ [12], etc.

Figure 2 shows the calculation results for the integer $S=2$ Blume-Capel model with the initial condition $C^A(0) = -C^B(0) = \{1\}$. Very similar features to $S=1$ case are obtained by our DS simulations. From the maximum values of $\sigma_{D(t)}$ in Fig. 2(b) we may get the (continuous) dynamical transition temperatures to be $T_\sigma = 7.60 \pm 0.25$, 7.45 ± 0.20 , 7.10 ± 0.15 , 6.40 ± 0.20 , 5.50 ± 0.25 , 4.20 ± 0.20 , and 1.00 ± 0.15 for $G/J = -4.0, -3.0, -2.0, -1.0, 0.0, 1.0, \text{ and } 2.0$, respectively, and then we get the phase diagram for $S=2$ Blume-Capel model in Fig. 2(d) with the tricritical point [white square in Fig. 2(d)] for $S=2$ Blume-Capel model to be $(T_{tri}, G_{tri}/J) = (1.00 \pm 0.15, 2.00)$. The general shape of

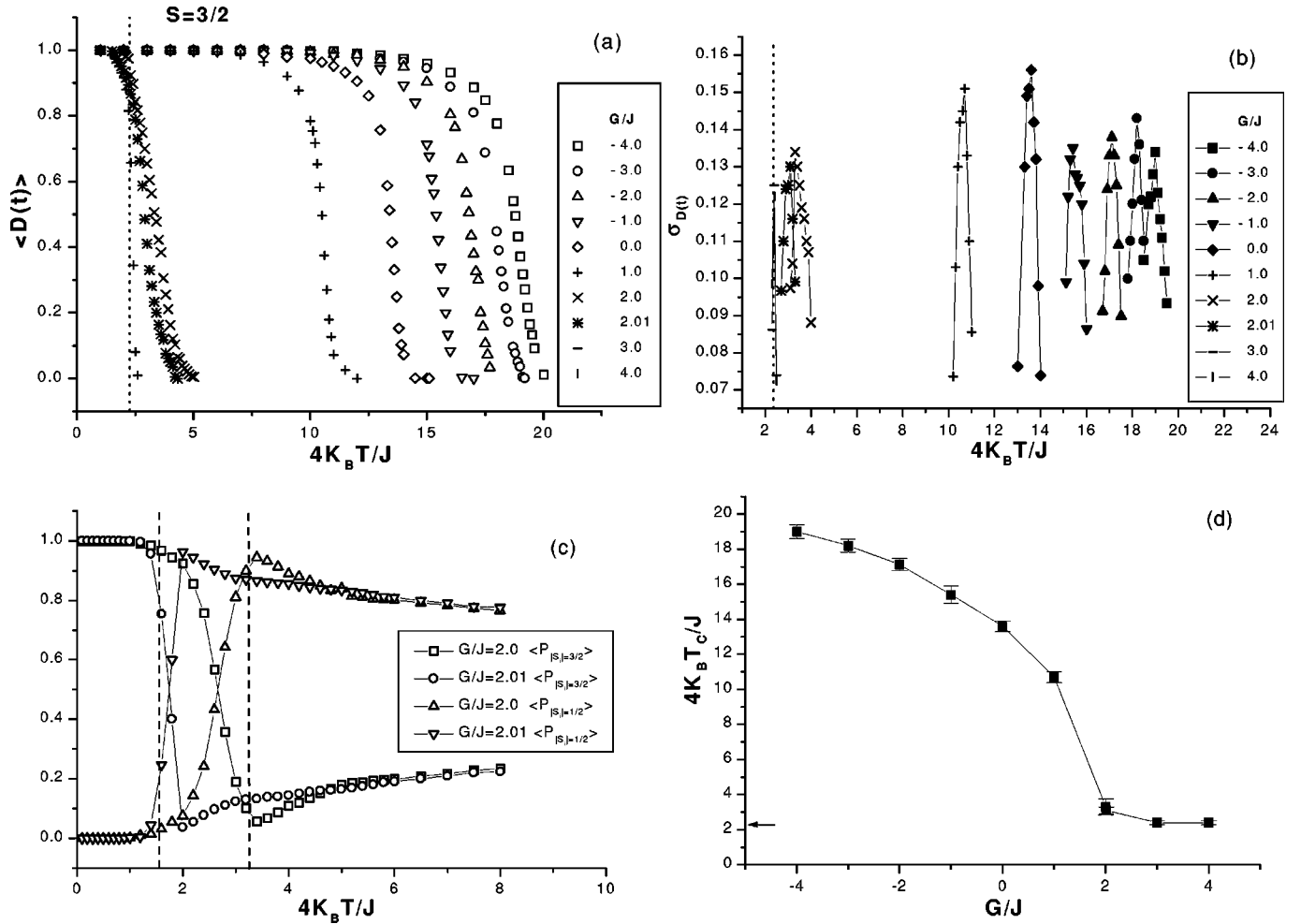


FIG. 3. The damage spreading results for $S=3/2$ Blume-Capel model on the square lattice at $L=40$, $t=1000$, and $N_s=200$. Figure 3(a) shows the average damage $\langle D(t) \rangle$ as a function of temperature T and G . Figure 3(b) shows the damage susceptibility $\sigma_{D(t)}$ as a function of temperature and G . The full line is a guide to the eye. Figure 3(c) shows $\langle P_{|S_i|=3/2} \rangle$ and $\langle P_{|S_i|=1/2} \rangle$ as a function of temperature at $G/J = 2.0$ and 2.01 . Figure 3(d) shows the phase diagram for $S=3/2$ Blume-Capel model on the square lattice by damage spreading procedure. The solid line represents the second-order transition. The lower arrow points to the transition temperature ($4K_B T_c/J = 2.269$) of the standard Ising model on the square lattice. See text for details.

this phase diagram is also in agreement with the known results, such as the mean-field theory [12] and the effective-field theory [14]. The known static values for the tricritical point for this model are $(1.645, 1.994)$ [14], $(1.333, 1.848)$ [12], etc.

So far, we have had the knowledge of integer $S=1$ and $S=2$ Blume-Capel models with the existence of multicritical behavior. In the following section, we use the same DS procedure to investigate the half-integer $S=3/2$ and $S=5/2$ Blume-Capel models. We found that the behavior of those models are different from above integer spin models.

IV. RESULTS FOR THE BLUME-CAPEL MODEL WITH $G=3/2$ AND $5/2$

For the half-integer spin Blume-Capel model, we choose to put the factor of $1/4$ (product of the two S_i spin values of $1/2$) into the J and G parameters in Eq. (1). For example, for $S=3/2$ model, the parameters in Eq. (1) become $J/4$ and

$G/4$, and the spin S_i can take one of the values among $(-3, -1, 1, 3)$. One advantage of this procedure is that it is easy for us to calculate $D(t)$ in Eq. (7), since the spin S_i still takes the integer values now. We first apply our DS procedure to the controversial case of $S=3/2$ Blume-Capel model concerning the existence or nonexistence of a multicritical point along the transition line, which we have mentioned in Sec. I.

The results are plotted in Fig. 3 with the initial condition $C^A(0) = -C^B(0) = \{3\}$. For this model we have observed a different behavior from previous integer models. Figure 3(a) shows the results of $\langle D(t) \rangle$ as a function of T and G . There exist only Ising-like continuous phase transitions for the model. When $G \rightarrow +\infty$, the model goes to the standard Ising model with the critical temperature $4K_B T_c/J = 2.269$ (the dotted line in the figure), which is consistent with the temperature $4t_c = 4K_B T_c/J = 4\{1/[2 \ln(\sqrt{2} + 1)]\} = 2/\ln(\sqrt{2} + 1) = 2.269$ as shown in Ref. [11]. In Fig. 3(b), we plot the temperature dependence of the fluctuation $\sigma_{D(t)}$ for our cho-

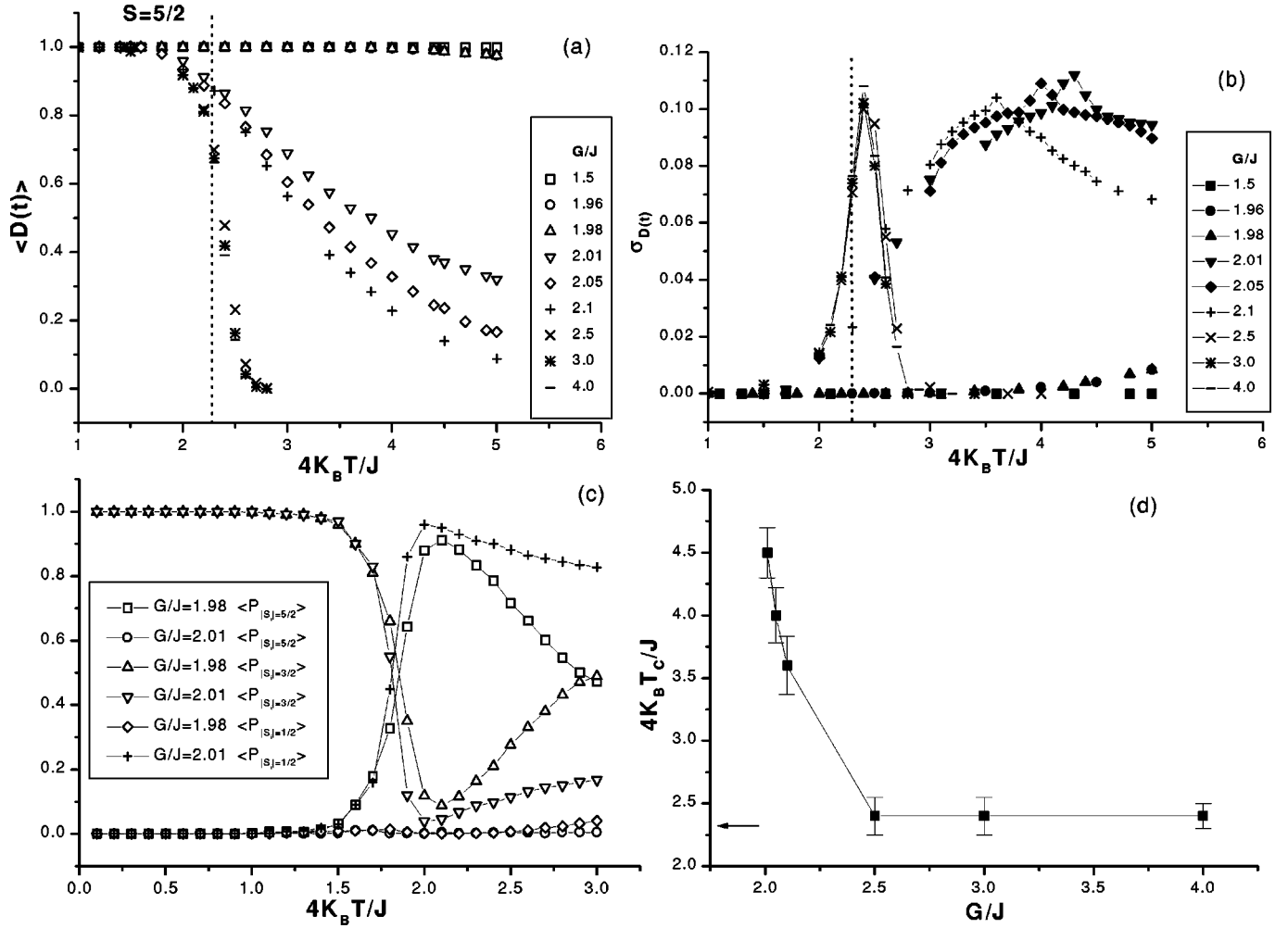


FIG. 4. The damage spreading results for $S=5/2$ Blume-Capel model on the square lattice at $L=40$, $t=1000$, and $N_s=200$. The notes are the same as in Fig. 3.

sen G values [the dotted line has the same meaning as in Fig. 3(a)], and we estimate the continuous transition temperature to be $4K_B T_c/J = 19.00 \pm 0.40$, 18.20 ± 0.36 , 17.12 ± 0.34 , 15.40 ± 0.50 , 13.60 ± 0.30 , 10.70 ± 0.30 , 3.30 ± 0.45 , 3.10 ± 0.20 , 2.40 ± 0.10 , and 2.40 ± 0.10 for $G/J = -4.0, -3.0, -2.0, -1.0, 0.0, 1.0, 2.0, 2.01, 3$, and 4 , respectively. Our results indicate the absence of a multicritical point along the phase transition line.

In order to detect the existence or nonexistence of an isolated first-order phase transition line as shown in Refs. [12,11,16] for this model, we plot $\langle P_{|S_i|=3/2} \rangle$ and $\langle P_{|S_i|=1/2} \rangle$ at $G/J=2.0$ and 2.01 in Fig. 3(c). In the literature [11,16], the range of this isolated first-order transition line is presented between $(4K_B T/J, G/J) = (3.2, 1.96)$ and $(1.6, 2.0)$, we plot two dashed lines in Fig. 3(c) to cover this temperature range. In Fig. 3(c), we can observe an obvious exchange of the spin values, indicating the first-order transition of two different ordered ferromagnetic phases, one is magnetization $m_1 \rightarrow 3/2$ and the other is $m_2 \rightarrow 1/2$. Figure 3(d) is the plot of the phase diagram for this model. We still use T_σ obtained from $\sigma_{D(t)} - T$ relationship in Fig. 3(b) as the (second-order) phase transition temperature. In Fig. 3(d), the general shape of the phase diagram shows very good agreement between our cal-

culations and other known results [12,11,16]. In this model, because of the absence of zero value for the spins, the long range order will not vanish, therefore, we can only observe the second-order transition along the transition line when G is changed.

Figure 4 shows the calculation results for the half-integer $S=5/2$ Blume-Capel model with the initial condition $C^A(0) = -C^B(0) = \{3\}$. Features very similar to $S=3/2$ case are obtained by our DS simulations. Because the transition temperatures are very high for negative G for this model, we only present the results for several positive G values. From the maximum values of $\sigma_{D(t)}$ in Fig. 4(b) we estimate continuous dynamical transition temperatures to be $4K_B T_c/J = 4.50 \pm 0.20$, 4.00 ± 0.22 , 3.60 ± 0.23 , 2.40 ± 0.15 , 2.40 ± 0.15 , and 2.40 ± 0.10 for $G/J = 2.01, 2.05, 2.10, 2.5, 3$, and 4 , respectively. In Fig. 4(c), we plot $\langle P_{|S_i|=5/2} \rangle$, $\langle P_{|S_i|=3/2} \rangle$, and $\langle P_{|S_i|=1/2} \rangle$ as a function of temperature T at $G/J = 1.98$ and 2.01 . We can also observe an obvious exchange of the spin values, indicating the first-order transitions of three different ordered ferromagnetic phases, one is the magnetization $m_1 \rightarrow 5/2$, $m_2 \rightarrow 3/2$ and the other is $m_3 \rightarrow 1/2$, and therefore, having confirmed the mean-field theory results about

the existence of two isolated first-order transition lines for this model [12]. At last, we plot the phase diagram for $S = 5/2$ Blume-Capel model in Fig. 4(d), where the model also goes to the standard Ising model with $4K_B T_c / J = 2.269$ when $G \rightarrow +\infty$.

V. CONCLUSIONS

In this work, we investigate, by means of the damage spreading technique, the dynamical behavior of integer $S = 1, 2$ and half-integer $S = 3/2, 5/2$ Blume-Capel models on a square lattice within a Metropolis-type dynamics. We find that the behavior of the systems are qualitatively different for the integer- and the half-integer-spin versions of this model. For the $S = 1$ and $S = 2$ Blume-Capel models, there exists a multicritical point along the transition line, which strongly depends on the values of the G parameter; For the $S = 3/2$ and $S = 5/2$ cases, our results indicate the absence of a mul-

ticritical point along the transition line when G is changed. In the context of the controversies surrounding the $S = 3/2$ Blume-Capel model, our DS results allow us to distinguish definitely between two proposed contradictory scenarios. In addition, our DS simulations present evidence of isolated first-order transition line(s) for the half-integer Blume-Capel model. A physical explanation to this quite distinct critical behavior is given.

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