Vacancy mechanism for Ising critical dynamics

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(Received 15 October 1974)

A kinetic Ising model with a vacancy mechanism of relaxation is introduced. This model is believed to give a realistic picture of the critical dynamics of binary alloys while existing models do not represent the actual microscopic mechanism of ordering. The initial decay time of the relaxation of the order is calculated exactly and the existence of critical slowing down is proved. A Monte Carlo calculation indicates that although the order parameter and the energy are not conserved quantities, the critical index of the order parameter relaxation Δ_n is different from that of the one-spin-flip kinetic Ising model. In the temperature region $0.074 < (T - T_c)/T_c < 1$, the Monte Carlo estimate yields $\Delta_n = \gamma \pm 7\%$, with γ being the critical index of the susceptibility. In the same temperature region the nonlinear relaxation time cannot be described by a single exponent.

I. INTRODUCTION

One of the most attractive features of second-order phase transitions is the property of universality[1]; critical behavior does not depend on such details of the Hamiltonian as the interaction strength but only on fairly general properties of the system such as the symmetry of the order parameter, the dimensionality, and the range of interaction.

Concerning static critical properties, Wilson's renormalization-group treatment[2] has greatly improved our understanding about the universality classes. The method has been extended to dynamic phenomena,[3] but the classification of dynamic critical behavior is far from complete. From works on the most extensively studied continuum analogs of different kinetic Ising models,[4,5] it has been deduced that every static universality class is divided into dynamic universality classes according to the conservation laws in the system and the symmetry of coupling of the order parameter to the slowly varying quantities. The multicomponent Bose-gas model[6] and the lattice model with an infinite number of displacement components[7] show more diversity of critical behavior.

The experimental situation is rather sparse: firstly, because the expected differences between the dynamic classes are so small that they can hardly be distinguished by present techniques and secondly, because there are only a few systems exhibiting an Ising-like interaction.

The best examples of Ising systems are the binary alloys. Their dynamics are governed mainly by the motion of the vacancies[8] which is a quite different mechanism of relaxation than the spin-flip dynamics of the kinetic Ising model. Since it is not clear to what extent critical dynamics is affected by the relaxation mechanism, we were led to introduce a new kinetic Ising model with a vacancy mechanism of relaxation.

It turned out that the critical dynamics is quite sensitive to this change of the relaxation mechanism. From the point of view of conservation laws the model belongs to the class where neither the order parameter nor the energy is conserved, but still the critical index of the order-parameter relaxation time differs from that of the corresponding kinetic Ising model.[3] It should be pointed out that the results concerning the critical exponents were obtained by the Monte Carlo method and should be interpreted with the usual caution due to the limitations of every computer experiment.[9-11]

In Sec. II we explain the physical ground for introducing the model, while in Sec. III the initial decay time is calculated and the existence of critical slowing down is proved. Finally Sec. IV contains the discussion of the nonlinear and linear relaxation time of the order in the temperature region $0.074 < (T - T_c)/T_c < 1$ calculated from a computer experiment.

II. MODEL

Concerning the static properties of binary alloys, the Ising model is a reasonable starting point.[12,13] It is not so obvious, however, how to describe its dynamic behavior. In the kinetic Ising model introduced by Glauber[14] only one spin is permitted to flip at once and, since in an alloy an atom of type A never turns into atom type B, this mechanism clearly does not correspond to any real process in a binary alloy. Kawasaki's model[15] might be more suitable; this is an Ising model where the dynamics is introduced through interchange of spins on neighboring sites. This is a physically possible process; it corresponds to the atomic exchange mechanism in binary alloys. However, there are a number of other physically possible processes (ring, interstitial, interstitialcy, crowdian, vacancy, divacancy, etc.) which can contribute to diffusion in alloys

and when the diffusing atoms are approximately the same size the dominant process is the vacancy mechanism.[8] It is believed that most of the commonly studied order-disorder processes in alloys are controlled by this vacancy mechanism. The aim of the present paper is to construct a kinetic Ising model with a vacancy mechanism of relaxation.

The vacancy mechanism itself is very simple; the vacancy moves through the crystal exchanging position with one of the neighboring atoms. A question arising is what is the rate of these exchanges. To answer this question, let us consider the potential (Fig. 1) in which the atom moves when jumping into the adjacent vacancy.

One can note at once that the activation energy for the process, which is called the migration energy E_m, depends only very weakly on the configuration around the vacancy and the jumping atom. That means that the frequency of jumps is actually independent of the configuration. Of course, the small differences in E_m play an important role since they underlie the thermodynamic force driving the system to equilibrium.

The situation will be approximated by separating the role of the small differences in migration energy and the average migration energy

(i) We assume that the frequency of jumps ν_0 is determined by the average migration energy $\bar{E}_m$ so it does not depend on the configuration. For simplicity we also assume the frequency to be temperature independent although it has a well-defined smooth dependence on temperature[16] which has to be taken into account in experiments.[17]

(ii) The deviations from $\bar{E}_m$ depend on the configuration $\{\sigma\}_r$ where $\{\sigma\}$ is a set of variables $\sigma_i = \pm 1$ depending on whether an atom of type A or B is on the site i and r denotes the site where the vacancy is situated: $\sigma_r = 0$. These deviations determine the probabilities $w_a(\{\sigma\}_r)$ that the vacancy moves to the neighboring sites $r+a$ in unit time $\tau_0 = 1/\nu_0$. The probabilities are subject to the condition that they must bring the system to the equilibrium of the Ising system with vacancies. To avoid quite complicated questions about the static properties of the dilute Ising model, we introduce our last assumption.

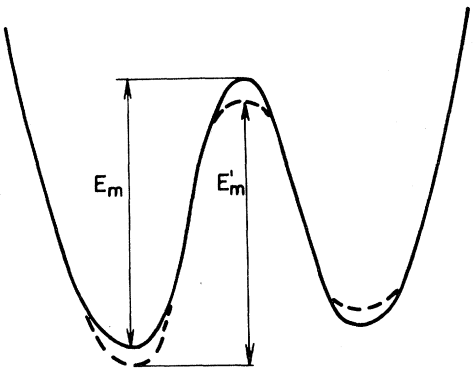

FIG. 1. Potential profile for an atom neighboring the vacancy. The dashed line shows how the potential depends on the configuration. The migration energy E_m is usually of order 1–2 eV while the change in the migration energy $\Delta E_m = |E_m - E_m'|$ due to changes in configuration is of order of the interaction energy of the atoms in their equilibrium position ($\lesssim 0.1$ eV).

(iii) There is only one vacancy in the system and the unit of time is rescaled by a factor N, where N is the number of atoms in the system

$$\tau = (1/N)\tau_0 \ . \tag{1}$$

Apart from a scale change of time, physically this situation corresponds to the limit when the density of vacancies is so small that their interaction can be neglected (actually at this point we neglect the divacancy mechanism of relaxation).

Having the condition (iii), the static properties of the model in the thermodynamic limit will be that of the standard Ising model.

To find a concrete form for $w_a(\{\sigma\}_r)$, let us consider the master equation for the time dependent distribution function of configurations $p(\{\sigma\}_r : t)$

$$\tau \frac{d}{dt} p(\{\sigma\}_r ; t) = -\sum_a w_a(\{\sigma\}_r) p(\{\sigma\}_r ; t) + \sum_a w_{-a}(\{\sigma\}_{r+a}) p(\{\sigma\}_{r+a} ; t) \ , \tag{2}$$

where the sums are over the vectors pointing from the position of the vacancy (r) to the nearest-neighbor sites, τ determined by (1) sets the time scale, and the configuration $\{\sigma\}_{r+a}$ differs from $\{\sigma\}_r$ by exchanging the vacancy and the atom at site $r+a$. The first sum on the right-hand side of (2) describes the hopping out of state $\{\sigma\}_r$, while the second sum is the "hopping in" term.

There are two obvious conditions restricting the choice of $w_a(\{\sigma\}_r)$:

(a) The equilibrium distribution function $p_{eq}(\{\sigma\}_r)$ does not change in time, i.e., it is a steady-state solution of the master equation

$$\tau \frac{d}{dt} p_{eq}(\{\sigma\}_r) = -\sum_a w_a(\{\sigma\}_r) p_{eq}(\{\sigma\}_r) + \sum_a w_{-a}(\{\sigma\}_{r+a}) p_{eq}(\{\sigma\}_{r+a}) = 0 \ , \tag{3}$$

where $p_{eq}(\{\sigma\}_r)$ is the canonical distribution

$$p_{eq}(\{\sigma\}_r) = (1/Z) e^{-\beta E(\{\sigma\}_r)} \ . \tag{4}$$

Here β, Z and $E(\{\sigma\}_r)$ are the usual notations for the

inverse temperature, the partition function, and the energy of configuration $\{\sigma\}_r$. The number of linear homogeneous equations given by this condition is equal to the number of configurations K.

(b) The conservation of probability

$$\sum_{r,\{\sigma\}_r} p(\{\sigma\}_r;t)=1 \quad , \tag{5}$$

yields one more equation for $w_a(\{\sigma\}_r)$ if we differentiate (5) by t and use (2)

$$\sum_{r,\{\sigma\}_r}\Big(-\sum_a w_a(\{\sigma\}_r)p(\{\sigma\}_r;t) + \sum_a w_{-a}(\{\sigma\}_{r+a})p(\{\sigma\}_{r+a};t)\Big)=0 \quad . \tag{6}$$

Since the number of transition probabilities $w_a(\{\sigma\}_r)$ is of order kK, where k is the number of nearest neighbors (there are k probabilities for every configuration except when the vacancy is on the boundary), they are not determined uniquely by the two conditions (3) and (6).

If there was no more restriction on the choice of $w_a(\{\sigma\}_r)$, one could easily find a suitable form. It is a matter of substitution to verify that for example the transition probabilities

$$w'_a(\{\sigma\}_r)\sim \exp\{-\tfrac{1}{2}\beta[E(\{\sigma\}_{r+a})-E(\{\sigma\}_r)]\} \quad , \tag{7}$$

used by Kikuchi[18] in his path probability treatment of the dynamics of interacting two level systems, satisfy both conditions (3) and (6).

In our model we have, however, a third condition:

(c) The vacancy moves every unit time determined by τ so the sum of probabilities that the vacancy leaves a certain site must be one

$$\sum_a w_a(\{\sigma\}_r)=1 \quad . \tag{8}$$

This normalization gives K linear equation but now the conservation of probabilities (6) is automatically satisfied. There is still arbitrariness in $w_a(\{\sigma\}_r)$ because (3) and (8) yield $2K$ equations for the kK transition probabilities and $k \geq 3$ in every lattice where the relaxation can take place by the vacancy mechanism.

The normalization condition (8) gives rise to problems in finding a form for $w_a(\{\sigma\}_r)$ which would satisfy both (3) and (8). The difficulty stems from the following: (3) is satisfied if one requires the detailed balance condition and in (3) not only the two sums cancel each other but the terms from the sums in pairs also cancel

$$w_a(\{\sigma\}_r)p_{eq}(\{\sigma\}_r)=w_{-a}(\{\sigma\}_{r+a})p_{eq}(\{\sigma\}_{r+a}) \quad . \tag{9}$$

Then in these equations only the transition probabilities $w_a(\{\sigma\}_r)$ and $w_{-a}(\{\sigma\}_{r+a})$ are coupled and this makes it possible to find a solution (7) which depends only on the configurations $\{\sigma\}_r$ and $\{\sigma\}_{r+a}$. With the additional equation, (8), all the $w_a(\{\sigma\}_r)$ become coupled and a simple solution depending only on a few configuration does not seem to be at hand.

One can, however, reverse the question and ask what will be the equilibrium distribution function if the normalized form of (7),

$$w_a(\{\sigma\}_r)=\frac{w'_a(\{\sigma\}_r)}{\sum_a w'_a(\{\sigma\}_r)}=\frac{\exp[-\frac{1}{2}\beta E(\{\sigma\}_{r+a})]}{\sum_a \exp[-\frac{1}{2}\beta E(\{\sigma\}_{r+a})]} \tag{10}$$

is used as the transition probability.

Putting (10) into (9) one can see that the detailed balance condition is satisfied by choosing

$$\tilde{p}_{eq}(\{\sigma\}_r)=\frac{1}{Z}\sum_a \exp\{-\tfrac{1}{2}\beta[E(\{\sigma\}_r)+E(\{\sigma\}_{r+a})]\} \, . \tag{11}$$

Since in the thermodynamic limit this distribution function leads to the same equilibrium properties as the canonical distribution, the transition probabilities (10) can be used as an approximate solution of (3) and (8).

Summarizing this section, as a model for binary alloys, we have a nearest-neighbor Ising antiferromagnet with a vacancy in it. The dynamics of the system is governed by the master equation (2) with transition probabilities given by (10).

III. CRITICAL SLOWING DOWN

Critical slowing down means that as we approach the critical point the decay time of certain nonequilibrium states becomes longer and longer. Since these states usually involve the order parameter or energy perturbations, the critical slowing down manifests itself in the divergence of the relaxation times of the corresponding physical quantities, or if these quantities are conserved, in the singularity of certain transport coefficients.

In binary alloys the order can be characterized by the difference in the number of atoms on their "own" and "other" sublattice, i.e., using spin terminology the order parameter is defined as the staggered magnetization

$$n=\frac{1}{N}\sum_i \eta_i\sigma_i \tag{12}$$

where $\eta_i=+1$ on one sublattice and -1 on the other. The dynamics introduced by the master equation (2) does not conserve both the order parameter and the energy and the existence of critical slowing down can be investigated by examining quantities like the relaxation time of the order parameter. In this paper only properties in the high-temperature phase are considered, although extension to temperatures below the critical temperature should be straightforward.

Having a solution $p(\{\sigma\}_r;t)$ of the master equation satisfying certain initial condition $p(\{\sigma\}_r;0)$, the time development of the order parameter is completely determined

$$n(t)=\sum_{\{\sigma\}_r} np(\{\sigma\}_r;t) \quad , \tag{13}$$

and the relaxation time in the high-temperature phase ($\langle n\rangle=0$) can be defined as

$$\tau_n=\int_0^\infty \frac{n(t)}{n(0)}\,dt \quad . \tag{14}$$

This definition is meaningful only if there is a prescription how the initial state in which $n(0)\neq 0$ is prepared. If for $t<0$ an infinitesimal field δh conjugate to the order parameter is switched on then at $t=0$ the system is in equilibrium under this field so the initial distribution $p(\{\sigma\}_r;0)$ to order δh can be written

$$p(\{\sigma\}_r;0)=\tilde{p}_{eq}(\{\sigma\}_r)(1+\beta n\delta h) \quad , \tag{15}$$

where $\tilde{p}_{eq}(\{\sigma\}_r)$ is the equilibrium distribution function without the field (11). With this initial state (14) is the conventional definition of the order parameter relaxation time in linear response.[19] If the same procedure is used to prepare the initial state but with finite conjugate field, then (14) is called the relaxation time in nonlinear response[20] and is denoted by $\tau_n^{(n,1,\cdots)}$.

The existence of critical slowing down is proved by calculating a lower bound for the relaxation time (14) and showing that it diverges at the critical point. The calculation is based on Kawasaki's method[21] applied to the relaxation time.[22,23] Its essence is the following: the relaxation time can be expressed as the expectation value of the inverse of an operator $\hat{W}$, and in purely relaxational systems $\hat{W}$ is a positive semidefinite operator. In this case for the expectation value $(f,\hat{W}^{-1}f)$ the following inequality holds:

$$(f,\hat{W}^{-1}f)(f,\hat{W}f)\geq (f,f)^2 \quad , \tag{16}$$

and since $(f,\hat{W}f)$ is calculated quite easily, one has the desirable lower bound.

To show that the model introduced in Sec. II is also a purely relaxational model, let us rewrite the master equation in operator form:

$$\frac{d}{dt}\,p(\{\sigma\}_r;t)=-\hat{L}p(\{\sigma\}_r;t) \quad , \tag{17}$$

where the operator L is defined by comparing (2) and (17).

Then the relaxation time in linear response is expressed as

$$\tau_n=\frac{\sum_{r,\{\sigma\}_r} n\hat{L}^{-1}\tilde{p}_{eq}n}{\sum_{r,\{\sigma\}_r} n\tilde{p}_{eq}n}$$

$$\equiv\frac{(n\hat{L}^{-1}\tilde{p}_{eq}n)}{(n\tilde{p}_{eq}n)}=\frac{(n\tilde{p}_{eq}^{1/2}\hat{W}^{-1}\tilde{p}_{eq}^{1/2}n)}{(n\tilde{p}_{eq}n)} \quad , \tag{18}$$

where

$$\hat{W}=\tilde{p}_{eq}^{-1/2}L\tilde{p}_{eq}^{1/2} \quad . \tag{19}$$

From the detailed balance condition (9), it follows that for arbitrary functions $f(\{\sigma\}_r)$ and $g(\{\sigma\}_r)$,

$$(f,\hat{W}g)=(g,\hat{W}f) \quad , \tag{20}$$

i.e., $\hat{W}$ is a Hermitian operator which means that all its eigenvalues are real. The stability of the system guarantees that (17) has no infinitely growing solution so all the eigenvalues of $\hat{W}$ must be positive or zero. This proves the positive semidefiniteness of $\hat{W}$ and the purely relaxational character of the model.

To find a lower bound for the relaxation time, one calculates the initial decay time τ_n^i,

$$\frac{1}{\tau_n^i}=-\frac{1}{n(0)}\frac{d}{dt}n(t)\bigg|_{t=0}$$

$$=\frac{(n\hat{L}\tilde{p}_{eq}n)}{(n\tilde{p}_{eq}n)}=\frac{(n\tilde{p}_{eq}^{1/2}\hat{W}\tilde{p}_{eq}^{1/2}n)}{(n\tilde{p}_{eq}n)} \tag{21}$$

and comparing (16), (18), and (21) concludes the inequality valid for every purely relaxational system[23]

$$\tau_n\geq\tau_n^i \quad . \tag{22}$$

The denominator of the right-hand side of (21) is the fluctuation of the order parameter which is proportional to the susceptibility so what remains to be calculated is the numerator. Using lemmas analogous to those of Abe[24] it is found to be a temperature-independent constant:

$$(n\hat{L}\tilde{p}_{eq}n)=\frac{2}{N\tau_0}\left(\tilde{p}_{eq}\sum_a w_a(\{\sigma\}_r)\right)=\frac{2}{N\tau_0} \quad , \tag{23}$$

where in the last equation we have used the normalization of the transition probabilities (8).

Substituting (23) into (21), the inequality (22) takes the form

$$\tau_n\geq\tau_n^i=\frac{\tau_0}{2}N\langle n^2\rangle=\frac{\tau_0}{2}\frac{\langle n^2\rangle}{\langle n^2\rangle_{T=\infty}} \quad , \tag{24}$$

where $\langle n^2\rangle_{T=\infty}=1/N$ is the fluctuation of the order parameter in the noninteracting (infinite temperature) limit. Since $\langle n^2\rangle$ is proportional to the susceptibility, (24) implies that $\tau_n^i\sim\epsilon^{-\gamma}$ where $\epsilon=(T-T_c)/T_c$, T_c being the critical temperature, and γ is the critical index of the susceptibility. It also implies that the relaxation time diverges at T_c and if its divergence can be characterized by an exponent $\tau_n\sim\epsilon^{-\Delta_n}$, then $\Delta_n\geq\gamma$. This completes the proof of the existence of critical slowing down.

IV. MONTE CARLO CALCULATION

The Monte Carlo (MC) method has proved to be a useful tool in analyzing the critical dynamics of the two-dimensional kinetic Ising model.[9,10,25] In addition to the high-temperature expansion[26,27] and Wilson's expansion,[3,4] it provides a third independent way of estimating the critical exponents.

The method is based on the ergodicity of the kinetic Ising model,[11,28] the dynamics of the model is simulated by a computer and the ensemble averages are calculated by averaging in time.

In the vacancy model discussed in the previous sections, the magnetization (the number of A- and B-type atoms) is conserved so phase space consists of subspaces in which the magnetization is constant and the system is ergodic in these subspaces. Since in an antiferromagnet the magnetization is not a relevant quantity,[1] one can neglect its fluctuation by an investigation of the critical properties of the system by means of the MC method in the subspace where the magnetization has the equilibrium value.

We have performed the MC calculation on a 64 $\times$ 64 square-lattice version of the vacancy model. The lattice was subjected to periodic boundary conditions.

The computation is performed in the following way. Initially a completely ordered state with a vacancy at a randomly chosen lattice site is stored in the computer and the temperature is given as the only input parameter. Then the four probabilities $w_a(\{\sigma\}_r)$ of interchanging the vacancy with the neighboring atoms are calculated. In order to move the vacancy according to the probabilities, the interval $[0, 1]$ is divided into four parts representing the values of the probabilities. Then a uniformly distributed random number is picked from $[0, 1]$ and the vacancy moves according to which part of $[0, 1]$ the number is from. The resulting new state serves as the initial state for the next step.

Repeating the process N times a MC step per atom is considered to have been performed and the value of the order parameter is taken as output. Since according to (1) the MC step per atom is proportional to the time unit in this way the time development of the staggered magnetization is generated.

Let L be the number of MC steps necessary for the system to reach equilibrium. Since in equilibrium the order parameter fluctuates around its equilibrium value $n = 0$, the integral determining the relaxation time (14) can be approximated by a finite sum

$$\tau_n^{(n,1,\cdot)} = \int_0^\infty \frac{n(t)}{n(0)}\,dt \simeq \sum_{i=0}^{L} \frac{n(t_i)}{n(0)} , \tag{25}$$

where $n(t_i)$ is the value of the order parameter after the ith MC step and this sum determines the nonlinear relaxation time ($\tau_n^{(n,1,\cdot)}$) since the completely ordered initial state can be prepared either by an infinite field ($\delta h = \infty$) or by a finite temperature change ($\Delta T = T$).

The fluctuation in $n(t)$ restricts the accuracy in determining $\tau_n^{(n,1,\cdot)}$. Near T_c the error goes roughly as the susceptibility.[11] In order to have an idea about the accuracy of the method, four independent runs were performed and the "statistical error" was calculated from the results of those runs.

If initially the system is in equilibrium with an infinitesimal field δh which is turned off at $t = 0$, the relaxation time is calculated not directly from (14) but rather from a formula equal to it to order $(\delta h)^2$ for $T > T_c$:

$$\tau_n = \int_0^\infty \frac{n(t)}{n(0)}\,dt = \int_0^\infty \frac{\langle n(0)n(t)\rangle}{\langle n^2\rangle}\,dt + O(\delta h^2) , \tag{26}$$

where the thermal averages are calculated as time averages

$$\langle n^2\rangle = \frac{1}{t_M - t_L} \sum_{i=L}^{M} n^2(t_i) , \tag{27}$$

$$\langle n(0)n(t_j)\rangle = \frac{1}{t_M - t_j - t_L} \sum_{i=L}^{M-j} n(t_i)n(t_i + t_j) . \tag{28}$$

In calculating (27) and (28), one faces the problem of uncertainty in the limits (L, M) of the sums. It is not trivial to determine how many MC steps are needed to reach the equilibrium starting from a completely ordered state. For example, the fact that the order parameter is settled to its equilibrium value does not necessarily indicate that the system is in equilibrium.

An equally difficult question is how long the time sequences should be, in order that the time averages give a reasonable approximation for the ensemble averages.[11]

At this point the MC calculation is more like an experiment. One sets a starting point in the region where such quantities as the staggered magnetization and the nearest-neighbor correlation have already settled to their equilibrium value. Then longer and longer time sequences are tried until the results of several (in our case, four) independent runs converge.[29]

Fortunately it turns out that, as in the kinetic Ising model,[10] the normalized correlation function $\langle n(0)n(t)\rangle/\langle n^2\rangle$ converges faster than $\langle n(0)n(t)\rangle$ or $\langle n^2\rangle$ alone. In the light of this observation Fig. 2, where $\langle n^2\rangle$ is compared with the extrapolated high-temperature series,[30] looks encouraging. The agreement is very good though the error bar at the nearest temperature to the critical point is large. This gives confidence in the reliability of the estimate of τ_n, although there is one more approximation in (26), the infinite integral is replaced by a

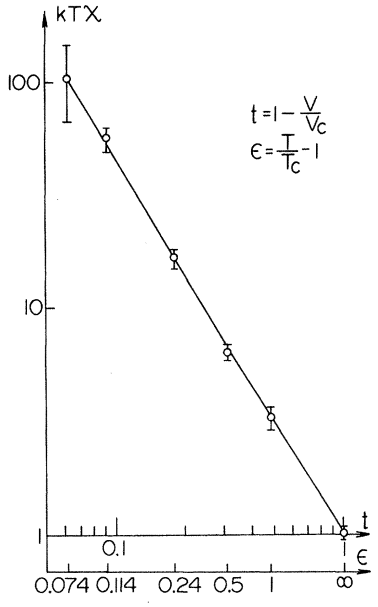

FIG. 2. Temperature dependence of the susceptibility calculated from the order-parameter fluctuation ($kT\chi = \langle n^2\rangle / \langle n^2\rangle_{T=\infty}$). The solid line corresponds to the infinite-lattice case calculated from the extrapolation of the high-temperature series. $v = \tanh(2J/kT)$ is the natural variable of the high-temperature expansion, but the normal temperature scale is also indicated. The error bars are calculated from the results of four independent runs.

finite sum. However, the sum always can be extended so far that actually $\langle n(0)n(t)\rangle / \langle n^2\rangle \sim 0$ and the effect of finiteness of the sum is negligible.

There is another source of inaccuracy following not from the finiteness of the calculated time sequences but from the finiteness of the system and the existence of the vacancy in it. However, for a 64×64 lattice and for the temperature region $0.074 < \epsilon < 1$, even the largest effect, the shift of the critical temperature[31]

$$\Delta T_c/T_c = -0.36/\sqrt{N} \approx 0.006 , \tag{29}$$

is so small that none of the conclusions are altered if it is neglected.

The results of the calculation of the relaxation time in linear and nonlinear response are displayed in Fig. 3. The consequences can be summarized in the following points.

(i) In the temperature region $0.074 < \epsilon < 0.5$ the relaxation time of the linear response is proportional to the susceptibility

$$\tau_n \sim \langle n^2\rangle \sim \chi . \tag{30}$$

Therefore, taking into account the accuracy of the calculation, one concludes that the effective critical exponent of τ_n ($\tau_n \sim \epsilon^{-\Delta_n^{\text{eff}}}$ in the considered temperature region) is given by

$$\Delta_n^{\text{eff}} = \gamma^{\text{eff}} \pm 7\% , \tag{31}$$

where γ^{eff} is found to be 1.6 if the susceptibility is plotted as a function of $\epsilon = (T - T_c)/T_c$. It has been pointed out, however, by Stoll *et al.*[10] that in the high-temperature phase the correction terms are smaller if the quantities are considered as functions of $1 - v/v_c$, where $v = \tanh(2J/kT)$ is the natural variable of the high-temperature expansion. Plotting χ against $1 - v/v_c$ (Fig. 2), it can be seen that in the region $0.074 < \epsilon < 0.5$ $\gamma^{\text{eff}} = 1.7$ which is only slightly less than the limiting value of 1.75. So (31) yields the following estimate:

$$\Delta_n^{\text{eff}} = 1.7 \pm 0.1 . \tag{32}$$

The fact that $\tau_n \sim \chi$ suggests that there is no kinetic slowing down in this model, although one might argue that for $\epsilon < 0.074$ there can be a change-over from $\Delta_n = \gamma$ to $\Delta_n > \gamma$. This question can never be settled finally in a calculation of finite systems. One can hope only that, similarly to the kinetic Ising model, if there is kinetic slowing down it will show up quite far from T_c.

Indeed, in the MC calculation of Stoll *et al.*[10] the kinetic slowing down is found in the region $0.02 < \epsilon < 0.2$ while Ogita *et al.*[9] found it already in the region $0.2 < \epsilon < 1$. The result of Ogita *et al.* $\tau_n^{(n.l.)} \sim \epsilon^{-1.75}$ has been interpreted as $\Delta_n^{(n.l.)} = \Delta_n = \gamma$. In fact in this temperature region $\chi \sim \epsilon^{-\gamma^{\text{eff}}}$ with γ^{eff} varying from 1.0 to 1.5 which clearly indicates that $\Delta_n^{(n.l.)} > \gamma$. It is remarkable that if $\tau_n^{(n.l.)}$ is plotted as a function of $1 - v/v_c$, the resulting $\Delta_n^{(n.l.)} \approx 2.1$ is close to the high-temperature expansion estimate[20] $\Delta_n^{(n.l.)} = 2.0$.

(ii) The relaxation time is greater in the nonlinear regime than in the linear regime

$$\tau_n^{(n.l.)} > \tau_n \quad (T > T_c) . \tag{33}$$

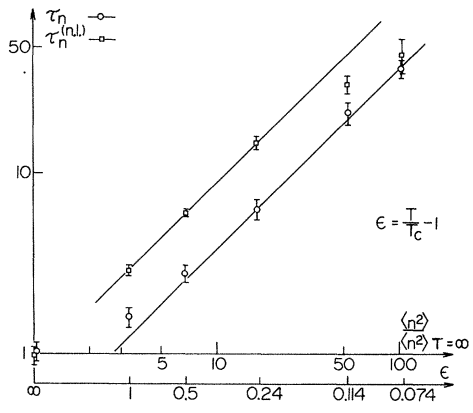

FIG. 3. Relaxation time of linear (τ_n) and nonlinear response ($\tau_n^{(n.l.)}$) plotted against the order-parameter fluctuation. The slope of the solid line is one. The unit of τ is 2.5 Monte Carlo steps.

This shows that the intuitive expectation[20] that $\tau_n^{(n.l.)} < \tau_n$ cannot be valid in general. In the temperature region $0.24 < \epsilon < 1$

$$\tau_n^{(n.l.)} \sim \chi \,, \tag{34}$$

but nearer to T_c, $\tau_n^{(n.l.)}$ approaches the value of τ_n. This approach is expected since close to T_c the diverging fluctuations will submerge the difference between the linear and nonlinear perturbations. Clearly $\tau_n^{(n.l.)}$ cannot be characterized by a single exponent.

V. FINAL REMARKS

In the vacancy model there is only one conserved quantity, the magnetization. Since the magnetization is not a relevant quantity, one expects that as in the case of a uniaxial antiferromagnet,[4] this conservation law does not effect the critical dynamics, i.e., it is the same for the vacancy model and for the one-spin-flip kinetic Ising model[3] where there is no conserved quantity at all. The MC calculation described in the previous section indicates that the critical index of the order-parameter relaxation time is different in the two models. So, if the difference cannot be ascribed to the conservation of magnetization, one is left with the conclusion that the change from the spin-flip mechanism to the vacancy mechanism has changed the critical dynamics. This means that the classification of dynamic critical behavior is not exhausted by specifying whether the relevant quantities are conserved.

The above statement is also illustrated in the infinite-component Bose-gas model[6] and in the lattice model with an infinite number of displacement components.[7] The statics in both models is equivalent to the spherical model and the critical dynamics is reduced to scaled free-field behavior in both cases. However, since the Bose field is complex while the displacement is real, the dispersion relations for the critical modes are $\omega \sim k^2$ and $\omega^2 \sim k^2$ correspondingly, i.e., the dynamic index is different in the two models.

Finally we would like to mention a problem in the vacancy model. In the vacancy mechanism introduced in this paper, the vacancy moves with a certain frequency independent of the configuration around it, i.e., the probabilities of jumps are normalized (10). It would probably shed some light on the nature of the kinetic slowing down if one examined the question of whether lifting this condition would alter the critical dynamics.

ACKNOWLEDGMENTS

This work has been financially supported by the National Research Council of Canada. We would like to thank P. Szèpfalusy for helpful correspondence.

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