

Nonequilibrium Ising models with competing, reaction-diffusion dynamics

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We study the phase diagram and other general macroscopic properties of an interacting spin (or particle) system out of equilibrium, namely, a reaction-diffusion Ising model whose time evolution occurs as a consequence of a combination of spin-flip (Glauber) and spin-exchange (Kawasaki) processes. The Glauber rate at site \mathbf{x} when the configuration is \mathbf{s} , say $c(\mathbf{s}; \mathbf{x})$, satisfies detailed balance at a reciprocal temperature β , while the Kawasaki rate for the interchange between nearest-neighbor sites \mathbf{x} and \mathbf{y} , $\Gamma c(\mathbf{s}; \mathbf{x}, \mathbf{y})$, satisfies detailed balance at temperature β' . We derive hydrodynamic-type macroscopic equations from the stochastic microscopic model for $\beta', \beta \geq 0$ and large Γ when time and space are rescaled by Γ and $\sqrt{\Gamma}$, respectively, and study the homogeneous steady solutions of those equations when $\Gamma \rightarrow \infty$. We state some general theorems for $\beta' = 0$ and solve explicitly the model with different choices $c(\mathbf{s}; \mathbf{x})$ for systems of arbitrary dimension d when $\beta' = 0$ and also for $d = 1$ when $\beta' \neq 0$. We also describe new Monte Carlo data for finite Γ , $\beta' = 0$, and $d = 1, 2$. The latter suggests, in particular, the existence of phase transitions for $d = 1$, finite Γ , and some choices for $c(\mathbf{s}; \mathbf{x})$.

I. INTRODUCTION AND DEFINITION OF MODEL

This paper is one of a series devoted to the study of the nonequilibrium steady states occurring in a model with competing dynamics. We study here an Ising spin (or lattice-gas) system on a simple hypercubic lattice in d dimensions whose spin configurations $\mathbf{s} = \{s_{\mathbf{x}}; \mathbf{x} \in \mathbb{Z}^d, s_{\mathbf{x}} = \pm 1\}$ evolve in time due to a combination of reaction and diffusion processes. That is, \mathbf{s} changes stochastically due to both spin-flip (reaction) processes caused by the contact with a heat bath at temperature $\beta = (k_B T)^{-1}$, the so-called Glauber dynamics,¹ and diffusion processes caused by nearest-neighbor (NN) exchanges, the dynamics introduced by Kawasaki,² which occur as if the associated bath temperature was β' . Those two competing processes are independent in continuous time, with Γ the ratio of attempted exchanges per bond to attempted flips per site. The same model was studied before in the case $\beta' = 0$, i.e., for a completely random diffusion process, by De Masi, Ferrari, and Lebowitz^{3,4} in the limit $\Gamma \rightarrow \infty$, and by means of a mean-field approximation by Dickman⁵ for arbitrary Γ , as a continuation of previous interest on reaction-diffusion stochastic models by both physicists^{6,7} and mathematicians.⁸⁻¹⁰ Further related nonequilibrium lattice models have been studied recently; see, for instance, the bibliography contained in Refs. 11 and 12.

The system configurational probability distribution, say $\mu_{\Gamma}^{\beta\beta'}(\mathbf{s}; t)$, will be assumed to evolve in time according to the Markovian master equation:

$$\frac{\partial \mu_{\Gamma}^{\beta\beta'}(\mathbf{s}; t)}{\partial t} = (\mathbf{L}_G^{\beta} + \Gamma \mathbf{L}_K^{\beta'}) \mu_{\Gamma}^{\beta\beta'}(\mathbf{s}; t). \tag{1.1}$$

Here

$$\mathbf{L}_G^{\beta} \equiv \sum_{\mathbf{x}} (\mathbf{G}_{\mathbf{x}} - 1) c^{\beta}(\mathbf{s}; \mathbf{x}), \quad \mathbf{G}_{\mathbf{x}} g(\mathbf{s}) = g(\mathbf{s}^{\mathbf{x}}), \tag{1.2}$$

$$\mathbf{L}_K^{\beta'} \equiv \sum_{|\mathbf{x}-\mathbf{y}|=1} (\mathbf{K}_{\mathbf{xy}} - 1) c^{\beta'}(\mathbf{s}; \mathbf{x}, \mathbf{y}), \quad \mathbf{K}_{\mathbf{xy}} g(\mathbf{s}) = g(\mathbf{s}^{\mathbf{xy}}), \tag{1.3}$$

$g(\mathbf{s})$ stands for an arbitrary function of the system configuration, $\mathbf{s}^{\mathbf{x}}$ represents the configuration obtained from \mathbf{s} by flipping the spin at site \mathbf{x} , i.e.,

$$(\mathbf{s}^{\mathbf{x}})_{\mathbf{z}} = \begin{cases} s_{\mathbf{z}}, & \mathbf{z} \neq \mathbf{x} \\ -s_{\mathbf{z}}, & \mathbf{z} = \mathbf{x} \end{cases} \tag{1.4}$$

and $\mathbf{s}^{\mathbf{xy}}$ is the configuration obtained from \mathbf{s} after the interchange of the spin variables at sites \mathbf{x} and \mathbf{y} , i.e.,

$$(\mathbf{s}^{\mathbf{xy}})_{\mathbf{z}} = \begin{cases} s_{\mathbf{z}}, & \mathbf{x}, \mathbf{y} \neq \mathbf{z} \\ s_{\mathbf{y}}, & \mathbf{x} = \mathbf{z} \\ s_{\mathbf{x}}, & \mathbf{y} = \mathbf{z}. \end{cases} \tag{1.5}$$

The respective rates $c^{\beta}(\mathbf{s}; \mathbf{x})$ and $c^{\beta'}(\mathbf{s}; \mathbf{x}, \mathbf{y})$ for the Glauber and Kawasaki processes both satisfy detailed balance, but with respect to different heat bath temperatures. As a consequence, one has that

$$\mathbf{L}_G^{\beta} \mu_{\text{eq}}^{\beta}(\mathbf{s}) = 0 \tag{1.6}$$

with

$$\mu_{\text{eq}}^{\beta}(\mathbf{s}) = \left[\sum_{\mathbf{s}} \exp[-\beta H(\mathbf{s})] \right]^{-1} \exp[-\beta H(\mathbf{s})], \tag{1.7}$$

where $H(\mathbf{s})$ represents the system configurational Hamil-

tonian, assumed for simplicity to be $H(\mathbf{s}) = -J \sum'_{x,y} s_x s_y$, where the sum is over NN pairs, and

$$L_K^\beta \mu_{\text{eq}}^\beta(\mathbf{s}; m) = 0 \quad (1.8)$$

with

$$\mu_{\text{eq}}^\beta(\mathbf{s}; m) = Z(\bar{\mu})^{-1} \exp \left[-\beta' H(\mathbf{s}) + \bar{\mu} \sum_{\mathbf{x}} s_{\mathbf{x}} \right]. \quad (1.9)$$

Here, $\bar{\mu} = \bar{\mu}(m)$, namely,

$$m = N^{-1} \left[\frac{\partial}{\partial \bar{\mu}} \right] \ln Z(\bar{\mu}), \quad (1.10)$$

where

$$Z(\bar{\mu}) \equiv \sum_{\mathbf{s}} \exp \left[-\beta' H(\mathbf{s}) + \bar{\mu} \sum_{\mathbf{x}} s_{\mathbf{x}} \right], \quad (1.11)$$

i.e., the Gibbs state at temperature β' has a fixed value for the magnetization m .

The stationary state implied by Eqs. (1.1)–(1.11) is expected to bear a number of interesting properties. For instance, it will not be unique in general but will depend, in a way which is not yet quite well understood, on the parameters β , β' , J , and Γ and on the specific form assumed for the spin-flip and spin-exchange rates $c^\beta(\mathbf{s}; \mathbf{x})$ and $c^\beta(\mathbf{s}; \mathbf{x}, \mathbf{y})$. Also, it may present continuous and discontinuous instabilities leading to nonequilibrium phase transitions in the infinite-volume limit. One may distinguish the following cases.

(i) $\Gamma \equiv 0$ or $c^\beta(\mathbf{s}; \mathbf{x}, \mathbf{y}) \equiv 0$ corresponds to the familiar kinetic Ising model with a nonconserved magnetization.¹ Any spin-flip rate $c^\beta(\mathbf{s}; \mathbf{x})$ satisfying detailed balance, this implying (1.6) in particular, drives the system to the same stationary state. This is the equilibrium Gibbs state (1.7) corresponding to the temperature $\beta = (k_B T)^{-1}$ and to the energy $H(\mathbf{s})$ whose nature is well known, e.g., the system shows a finite critical temperature β_c for any $d \geq 2$. The same follows when $c^\beta(\mathbf{s}; \mathbf{x}) \equiv 0$ for finite Γ . This is the Ising model evolving by the Kawasaki dynamics which conserves the system magnetization.² The steady state is then also an equilibrium Gibbs state, (1.9), with a fixed magnetization, however. This is independent of the rate $\Gamma c^\beta(\mathbf{s}; \mathbf{x}, \mathbf{y})$ when it satisfies detailed balance, which implies (1.8) in particular. Those two limiting, equilibrium situations are a well-known reference for the nonequilibrium situations in which we are interested here.

(ii) The situation is very different when $\Gamma > 0$ and c^β , $c^\beta \neq 0$, e.g., multiplying $c^\beta(\mathbf{s}; \mathbf{x})$ by a constant may dramatically modify the stationary state. This is already implicit in certain versions of the model which were investigated before, namely, when $c^\beta(\mathbf{s}; \mathbf{x}, \mathbf{y}) \equiv 1$ as if the bath temperature controlling the diffusion process was infinite, i.e., the case of a completely random diffusion. That case was found most interesting because, as one rescales time and space by Γ and by $\sqrt{\Gamma}$, respectively, and takes the limit $\Gamma \rightarrow \infty$, it follows rigorously^{3,4,12} that the macroscopic magnetization $m(\mathbf{r}, t)$, $\mathbf{r} \in R^d$, satisfies a hydrodynamic-type, macroscopic equation. Namely, a reaction-diffusion equation:

$$\frac{\partial m(\mathbf{r}, t)}{\partial t} = \frac{1}{2} \nabla^2 m(\mathbf{r}, t) + F\{m(\mathbf{r}, t)\}. \quad (1.12)$$

Here, $F\{m\}$ is a polynomial in m , which may be interpreted as the derivative of a mean-field energy Φ , $F = \partial \Phi(m) / \partial m$, obtained as

$$F\{m\} = -2 \langle s_{\mathbf{x}} c^\beta(\mathbf{s}; \mathbf{x}) \rangle_m, \quad (1.13)$$

$m \equiv \langle s_{\mathbf{x}} \rangle_m$, where the average is taken with respect to a Bernoulli state with uniform magnetization m . The study of the homogeneous steady (nonequilibrium) solutions of (1.12) reveals,^{3,4,13} for instance, the presence of instabilities, even when $d=1$ for some choices $c^\beta(\mathbf{s}; \mathbf{x})$.

(iii) The case of finite Γ , where no exact results are known, was studied for $\beta' = 0$, $d=2$, and for some specific choice $c^\beta(\mathbf{s}; \mathbf{x})$,¹⁴ by means of a mean-field-type approximation⁵ and Monte Carlo (MC) computer simulations.¹³ The main conclusion from those studies concerns the presence of a nonequilibrium phase transition changing, as Γ is increased, from the Ising-type second order to a mean-field-type first order. That is, the phase diagram has a “tricritical point” separating those two behaviors.

(iv) It was shown recently¹⁵ that one may also obtain, as for case (ii), a hydrodynamic-type macroscopic equation when both temperatures, β and β' , remain finite.

It is our purpose here to study some questions related to cases (ii)–(iv). When $\beta' = 0$ and $\Gamma \rightarrow \infty$, we conclude some properties of the d -dimensional stationary state for the rates $c^\beta(\mathbf{s}; \mathbf{x})$ which are more familiar in the literature, and state some general theorems relating the properties of $c^\beta(\mathbf{s}; \mathbf{x})$ to those of the stationary state. In particular, we find the conditions on $c^\beta(\mathbf{s}; \mathbf{x})$ to expect a phase transition for $d=1$ and ferromagnetic-type interactions, and conclude some properties of the antiferromagnetic case. The nature of the phase diagram in the β - Γ plane, with $\beta, \Gamma \in [0, \infty]$, is further investigated by performing computer simulations for ferromagnetic interactions, several choices $c^\beta(\mathbf{s}; \mathbf{x})$, and for $d=1$ and 2. We thus find, in particular, strong evidence for the existence of a phase transition for $d=1$ and finite Γ . When $\beta' > 0$, we study analytically the situation depicted above under case (iv), $\Gamma \rightarrow \infty$, and find explicit steady solutions for $d=1$. Brief reports of some of the results here were presented before;^{13,15} we describe now, in addition to methods and most relevant details of the proofs, some novel analytical results and further numerical, Monte Carlo data.

II. HYDRODYNAMIC LIMIT

The generalized reaction-diffusion model in the preceding section was defined as a microscopic, stochastic model. An important question is whether one may obtain a hydrodynamic-type macroscopic equation from that microscopic description under some scaling limit. We present here such a derivation, and a method to obtain macroscopic equations which generalize in a sense the one obtained before by De Masi *et al.*^{3,4} for $\beta' = 0$.

With that aim, we first multiply Eq. (1.1) by $s_{\mathbf{x}}$ and sum over \mathbf{s} ; it follows immediately that

$$\frac{\partial \langle s_{\mathbf{x}} \rangle}{\partial t} = -2 \langle s_{\mathbf{x}} c^\beta(\mathbf{s}; \mathbf{x}) \rangle + \Gamma \sum_{\mathbf{s}} s_{\mathbf{x}} L_K^\beta \mu^{\beta\beta'}(\mathbf{s}; t). \quad (2.1)$$

The angular brackets indicate here an average with measure $\mu_{\Gamma}^{\beta\beta}(\mathbf{s};t)$. The last term in Eq. (2.1) may be transformed successively as follows:

$$\begin{aligned} & \Gamma \sum_{\mathbf{s}} s_x \sum_{|y-z|=1} [c^{\beta}(s^{yz}; \mathbf{y}, \mathbf{z}) \mu_{\Gamma}^{\beta\beta}(s^{yz}; t) \\ & \quad - c^{\beta}(s; \mathbf{y}, \mathbf{z}) \mu_{\Gamma}^{\beta\beta}(\mathbf{s}; t)] \\ & = \Gamma \sum_{|y-z|=1} \langle [(s^{yz})_x - s_x] c^{\beta}(s; \mathbf{y}, \mathbf{z}) \rangle \\ & = \Gamma \sum_{i=1}^d \sum_{\mathbf{z}=\mathbf{x}\pm\mathbf{i}} \langle [(s^{xz})_x - s_x] c^{\beta}(s; \mathbf{x}, \mathbf{z}) \rangle \end{aligned}$$

where $(s^{xz})_x = s_z$ according to (1.5) and $\mathbf{x}\pm\mathbf{i}$ represents the NN of site \mathbf{x} along the $\pm\mathbf{i}$ direction, $i=1, 2, \dots, d$. Thus one has that

$$\begin{aligned} \frac{\partial \langle s_x \rangle}{\partial t} & = -2 \langle s_x c^{\beta}(s; \mathbf{x}) \rangle \\ & \quad + \Gamma \sum_{i=1}^d \sum_{\mathbf{z}=\mathbf{x}\pm\mathbf{i}} \langle (s_z - s_x) c^{\beta}(s; \mathbf{x}, \mathbf{z}) \rangle. \end{aligned} \quad (2.2)$$

$$\frac{\partial m_{\epsilon}(\mathbf{r}; t)}{\partial t} = -2\epsilon^d \sum_{\mathbf{x} \in \Omega_{\mathbf{r}, \epsilon}} \langle s_x c^{\beta}(s; \mathbf{x}) \rangle + \frac{1}{2}\epsilon^{d-2} \sum_{i=1}^d \sum_{\mathbf{x} \in \Omega_{\mathbf{r}, \epsilon}} \sum_{\mathbf{z}=\mathbf{x}\pm\mathbf{i}} \langle (s_z - s_x) c^{\beta}(s; \mathbf{x}, \mathbf{z}) \rangle, \quad (2.4)$$

where $m_{\epsilon}(\mathbf{r}; t) \equiv \langle m_{\epsilon}(\mathbf{r}; \mathbf{s}) \rangle$.

Most interesting is the limit $\epsilon \rightarrow 0$, where the boxes $\Omega_{\mathbf{r}}$ develop a macroscopic size and $\langle m_{\epsilon}(\mathbf{r}; \mathbf{s}) \rangle$ transforms into the macroscopic, deterministic variable $m(\mathbf{r}; t)$. Simultaneously, $\epsilon \rightarrow 0$ makes the diffusion very fast as compared to the reaction process, i.e., there is an infinite number of spin exchanges within the box (per unit time) for each spin flip, and the corresponding number of exchanges through the box surface becomes negligible. Under those circumstances, when the observation occurs in time units of ϵ^{-2} , one expects some sort of local equilibrium within the box with respect to the fast diffusion process.

More precisely, the original measure $\mu(\mathbf{s}; t) \equiv \mu_{\Gamma}^{\beta\beta}(\mathbf{s}; t)$ satisfies (1.1), i.e.,

$$\frac{\partial \mu}{\partial t} = \mathbf{L}_G \mu + (2\epsilon^2)^{-1} \mathbf{L}_K \mu, \quad (2.5)$$

where

$$\mathbf{L}_G \mu_{\text{eq}}^{\beta}(s) = 0, \quad \mathbf{L}_K \mu_{\text{eq}}^{\beta}(s; m) = 0. \quad (2.6)$$

Let us assume that $\phi(\mathbf{s}; t)$ exists such that

$$\mu(\mathbf{s}; t) = \mu_0(\mathbf{s}; t) + \epsilon^{\alpha} \phi(\mathbf{s}; t) + O(\epsilon^b), \quad (2.7)$$

where $b > \alpha > 0$. By using (2.7) in (2.5), it follows to leading order that

$$\frac{\partial \mu_0}{\partial t} = [\mathbf{L}_G + (2\epsilon^2)^{-1} \mathbf{L}_K] \mu_0 + \frac{1}{2} \epsilon^{\alpha-2} \mathbf{L}_K \phi + O(\epsilon^{b-2}). \quad (2.8)$$

Next, we write $\Gamma \equiv \frac{1}{2}\epsilon^2$ and make a partition of the infinite lattice into (hyper) cubic boxes of side $\epsilon^{-1}a_0$, with a_0 the original lattice spacing. The location of each box is then represented by a discrete vector \mathbf{r} , and two neighboring boxes, at \mathbf{r} and \mathbf{r}' , respectively, are separated by a distance $a = \epsilon^{-1}a_0$ which we shall take as our unit of length. Consequently, we define a coarse-grained magnetization at each box,

$$m_{\epsilon}(\mathbf{r}; \mathbf{s}) = \epsilon^d \sum_{\mathbf{x} \in \Omega_{\mathbf{r}, \epsilon}} s_x, \quad (2.3)$$

where $\Omega_{\mathbf{r}, \epsilon}$ is the part of the original lattice within the box at \mathbf{r} . The quantity m_{ϵ} is determined by a competition between the spin flips occurring within the box and the spin exchanges with the neighboring boxes. Those two mechanisms produce variations of the same order of magnitude in m_{ϵ} , i.e., the variations induced by the former are of the order of the volume of the box, ϵ^{-d} , and the ones induced by the spin interchanges are a surface effect of order $\epsilon^{-(d-1)}$ times the gradient of the magnetization involved at each exchange, $1/\epsilon^{-1}$, times Γ . By combining (2.3) and (2.2) one has that

This reveals in particular that, for ϵ small enough, there will only be a well-behaved solution as far as $L_K \mu_0(\mathbf{s}; t) = 0$. Therefore the relevant measure in the limit $\epsilon \rightarrow 0$, i.e., assuming that surface terms tend to disappear, is simply

$$\mu_0(\mathbf{s}; t) = \prod_{\mathbf{r}} \mu_{\text{eq}}^{\beta}(s_{\mathbf{r}}; m(\mathbf{r}; t)), \quad (2.9)$$

which corresponds indeed to a sort of local equilibrium characterized by the local magnetization $m(\mathbf{r}; t)$; $\prod_{\mathbf{r}}$ represents here a product over boxes and $s_{\mathbf{r}}$ is the configuration within the box at \mathbf{r} .

The measures (2.7) and/or (2.9) are the ones to compute the average involved by (2.4) when ϵ is small enough or zero, respectively. Assuming $\alpha > 1$, we have immediately to leading order in ϵ that

$$\begin{aligned} \frac{\partial m(\mathbf{r}; t)}{\partial t} & = -2 \langle s_x c^{\beta}(s; \mathbf{x}) \rangle_{m(\mathbf{r}; t)} \\ & \quad + \frac{1}{2} \epsilon^{-2} \sum_{i=1}^d \sum_{\mathbf{r}'=\mathbf{r}+\mathbf{a}\mathbf{i}} C(m(\mathbf{r}; t), m(\mathbf{r}'; t)) \\ & \quad + O(\epsilon). \end{aligned} \quad (2.10)$$

Here,

$$C(m(\mathbf{r}; t), m(\mathbf{r}'; t)) \equiv \langle (s_z - s_x) c^{\beta}(s; \mathbf{x}, \mathbf{z}) \rangle_0 \quad (2.11)$$

with $\mathbf{x} \in \Omega_{\mathbf{r}, \epsilon}$ and $\mathbf{z} \in \Omega_{\mathbf{r}', \epsilon}$, and

$$\langle \cdot \rangle_m \equiv \sum_{\mathbf{s}} \cdot \mu_{\text{eq}}^{\beta}(s; m), \quad \langle \cdot \rangle_0 \equiv \sum_{\mathbf{s}} \cdot \mu_0(\mathbf{s}; t). \quad (2.12)$$

Now, take $a = \epsilon^{-1}a_0 = 1$ and the lengths scaled by ϵ , i.e.,

i is replaced by ϵi . Equation (2.10) leads in the limit $\epsilon \rightarrow 0$ to the hydrodynamic-type macroscopic equation:

$$\begin{aligned} \frac{\partial m(\mathbf{r};t)}{\partial t} = & -2 \langle s_{\mathbf{x}} c^{\beta}(\mathbf{s};\mathbf{x}) \rangle_{m(\mathbf{r};t)} \\ & + \frac{1}{2} \sum_{i=1}^d \left[\frac{\partial}{\partial r_i} \right] \left[[\delta_v C(u,v)]_{u=v=m(\mathbf{r};t)} \right. \\ & \left. \times \left[\frac{\partial m(\mathbf{r};t)}{\partial r_i} \right] \right] \end{aligned} \quad (2.13)$$

where δ_v represents a derivative with respect to v . This equation has coefficients which are evaluated in the local equilibrium ensemble (2.9) and depend in general on the details (transition rates) of both the spin-flip and the spin-exchange mechanisms.

Notice also that the measure (2.9) for $\epsilon \rightarrow 0$ reduces as $\beta' \rightarrow 0$ to the factorized one:

$$\mu_{\text{eq}}^0(s; m) = Z^{-1} \exp \left[\bar{\mu} \sum_{\mathbf{x}} s_{\mathbf{x}} \right], \quad (2.14)$$

where $\bar{\mu} = \bar{\mu}(m)$ is defined by Eq. (1.10). This is the Bernoulli measure found previously by De Masi, Ferrari, and Lebowitz^{3,4} for $\beta' = 0$ when the "infinite temperature" (i.e., completely random) diffusion avoids any local correlation. We recover their macroscopic equation for $\beta' = 0$, Eqs. (1.12) and (1.13), after using (2.14) in Eq. (2.13).

III. STATIONARY SOLUTIONS: SOME GENERAL RESULTS

Consider now the case of a homogeneous system in the limit $\epsilon \rightarrow 0$. Then, (2.13) [or (1.12) in the special case $\beta' = 0$] reduces to $\partial m(t)/\partial t = F\{m(t)\}$ where $F\{m\} \equiv -2 \langle s_{\mathbf{x}} c(\mathbf{s};\mathbf{x}) \rangle$ and the averages are computed with measure (2.9). The relevant uniform stationary solutions, say m^* , follow then from

$$F(m^*) = 0, \quad \left[\frac{\partial F(m)}{\partial m} \right]_{m=m^*} \leq 0 \quad (3.1)$$

where the second condition guarantees local stability. We shall first refer to the case $\beta' = 0$; Sec. V will study some stationary solutions when $\beta' > 0$.

The former case is characterized by $c^{\beta}(\mathbf{s};\mathbf{x},\mathbf{y}) \equiv 1$, i.e., the spin-exchange rate is independent of \mathbf{s} , and by the detailed balance condition:

$$c(\mathbf{s};\mathbf{x})/c(\mathbf{s}^{\mathbf{x}};\mathbf{x}) = \exp[-\Delta H(\mathbf{s};\mathbf{x})], \quad (3.2)$$

$\Delta H(\mathbf{s};\mathbf{x}) \equiv H(\mathbf{s}^{\mathbf{x}}) - H(\mathbf{s})$. For simplicity of notation, we are including β in the configurational Hamiltonian, i.e., define $K \equiv \beta J$ and

$$H(\mathbf{s}) = -K \sum_{|\mathbf{x}-\mathbf{y}|=1} s_{\mathbf{x}} s_{\mathbf{y}} = H_0(\mathbf{s}) - K s_{\mathbf{x}} \sum_q s_{\mathbf{y}}, \quad (3.3)$$

where the second sum is over the q NN of site \mathbf{x} , and $H_0(\mathbf{s})$ contains no information about $s_{\mathbf{x}}$. One may write quite generally after using (3.3) that

$$c(\mathbf{x};\mathbf{s}) = f_0(\mathbf{s}) \exp \left[-K s_{\mathbf{x}} \sum_{\mathbf{y}=1}^q s_{\mathbf{y}} \right], \quad (3.4)$$

where $f_0(\mathbf{s})$ is an arbitrary function, except that $f_0(\mathbf{s}) = f_0(\mathbf{s}^{\mathbf{x}}) \geq 0$ as required by (3.2) and by the positivity of the rates. It also turns out convenient to write

$$c(\mathbf{s};\mathbf{x}) = f(\mathbf{s}) [A_+(\mathbf{s}) + s_{\mathbf{x}} A_-(\mathbf{s})] \quad (3.5)$$

where, for simple hypercubic lattices, one has that

$$f(\mathbf{s}) \equiv f_0(\mathbf{s}) \prod_{i=1}^d \cosh[K(s_{\mathbf{x}+i} + s_{\mathbf{x}-i})], \quad (3.6)$$

which also satisfies the symmetry property

$$f(\mathbf{s}) = f(\mathbf{s}^{\mathbf{x}}) \quad (3.7)$$

as a consequence of detailed balance, and

$$\begin{aligned} A_{\pm}(\mathbf{s}) \equiv & \frac{1}{2} \left[\prod_{i=1}^d \left[1 - \frac{\alpha}{2} (s_{\mathbf{x}+i} + s_{\mathbf{x}-i}) \right] \right. \\ & \left. \pm \prod_{i=1}^d \left[1 + \frac{\alpha}{2} (s_{\mathbf{x}+i} + s_{\mathbf{x}-i}) \right] \right], \end{aligned} \quad (3.8)$$

with $\alpha \equiv \tanh(2K)$. Thus, after using (3.5) in (1.13), one has that

$$F\{m\} = -2m \langle f(\mathbf{s}) A_+(\mathbf{s}) \rangle_m - 2 \langle f(\mathbf{s}) A_-(\mathbf{s}) \rangle_m \quad (3.9)$$

where A_{\pm} have no explicit dependence on $s_{\mathbf{x}}$.

Theorem 1. Consider the case $d=1$ and $K>0$ with $f(\mathbf{s}) = 1 + a s_{\mathbf{x}+1} s_{\mathbf{x}-1}$, $a = a(K)$, $|a| \leq 1$. The system undergoes a second-order phase transition if and only if $a > 0$.

Corollary. The critical temperature K_c when $a > 0$ satisfies the equation

$$[1 - \tanh(2K_c)] / \tanh(2K_c) = a(K_c) \equiv a_c, \quad (3.10)$$

and one has that

$$\begin{aligned} m^* = 0 & \quad \text{when } a < a_c, \\ m^* = \pm [(\alpha - 1)a^{-1} + \alpha]^{1/2} & \quad \text{when } a \geq a_c \end{aligned} \quad (3.11)$$

for the magnetization.

Theorem 2. Consider the case $d=1$ and $K>0$ with $f(\mathbf{s}) = 1 + a_2(s_{\mathbf{x}+1} + s_{\mathbf{x}-1})$, $|a_2| \leq \frac{1}{2}$. The system undergoes no phase transition for any value of a_2 but it presents a nonzero spontaneous magnetization given by

$$\begin{aligned} m^* = [2a_2(2-\alpha)]^{-1} \\ \times \{ [(1-\alpha)^2 + 4(a_2)^2 \alpha(2-\alpha)]^{1/2} + \alpha - 1 \}; \end{aligned} \quad (3.12)$$

m^* has the sign of a_2 .

Remarks. The proofs of Theorems 1 and 2 are a simple matter of algebra within the above formalism. Notice that, for $d=1$ and symmetric interactions restricted to NN spins, one has in general that $f(\mathbf{s}) = 1 + a s_{\mathbf{x}+1} s_{\mathbf{x}-1} + a_2(s_{\mathbf{x}+1} + s_{\mathbf{x}-1})$. For instance, $a = a_2 = 0$ is for the rates introduced by Glauber¹ and Kawasaki,² and $a_2 = 0$, $a \neq 0$ correspond to the rates by Metropolis *et al.*¹⁴ and to the ones introduced in Ref. 4. Thus one has in general that

$$F\{m\} = a_2 \alpha + m [\alpha(a+1) - 1] + m^2 a_2 (\alpha - 2) - m^3 a;$$

where $|a| \leq 1$ and $|a_2| \leq \frac{1}{2}(1+a)$ as implied by the positivity of $f(s)$, and stability requires that

$$\alpha(a+1) - 1 + 2a_2(\alpha-2)m^* - 3a(m^*)^2 < 0$$

where $F\{m^*\} = 0$.

Theorem 3. Consider $d=2$, $K>0$, and the general choice

$$f(s) = \sum_{k=0}^5 a_k \alpha_k(s) \quad (3.13)$$

where $a_0 = \alpha_0 = 1$, $\alpha_1 = \sigma_i \sigma_j$, $\alpha_2 = \pi_i \pi_j$, $\alpha_3 = \sigma_i + \sigma_j$, $\alpha_4 = \pi_i + \pi_j$, $\alpha_5 = \sigma_i \pi_j + \sigma_j \pi_i$, with $\sigma_n \equiv \frac{1}{2}(s_{x+n} + s_{x-n})$, $\pi_n \equiv s_{x+n} s_{x-n}$, $\mathbf{n} = \mathbf{i}, \mathbf{j}$. Then,

$$F(m) = m f'(m^2), \quad f'(\phi) = A + B\phi + C\phi^2 \quad (3.14)$$

is the most general F having all solutions of the form $(m^*)^2 = a \geq 0$, and (3.14) occurs when $a_3 = a_5 = 0$ in (3.13).

Corollary. The following relations hold:

$$A = 2(2\alpha - 1) + \alpha(2 - \frac{1}{2}\alpha)a_1 + 4\alpha a_4, \quad (3.15a)$$

$$C = -2a_2 - \frac{1}{2}a_1\alpha^2,$$

$$B = -2\alpha^2 - (\alpha^2 - 2\alpha + 2)a_1 + 2\alpha(2 - \alpha)a_2 - 4(\alpha^2 - \alpha + 1)a_4 \quad (3.15b)$$

between K and the coefficients of Eqs. (3.13) and (3.14).

Remarks. The proofs are a matter of algebra. Notice also that the stable stationary solutions following from (3.14) need to satisfy

$$m^*(A + Bm^{*2} + Cm^{*4}) = 0, \quad (3.16)$$

$$A + 3Bm^{*2} + 5Cm^{*4} \leq 0. \quad (3.17)$$

That is, $m^* = 0$ satisfies both conditions and, when a nonzero solution exists, it will satisfy $A + Bm^{*2} + Cm^{*4} = 0$ and (3.17). Thus one may define two temperatures, say $T_c^{(1)}$ and $T_c^{(2)}$, where the solutions $m^* = 0$ and $m^* \neq 0$, respectively, become unstable, as follows:

$$A(T_c^{(1)}) = 0 \quad (3.18a)$$

and

$$A(T_c^{(2)}) + B(T_c^{(2)})m^{*2} + C(T_c^{(2)})m^{*4} = 0, \quad (3.18b)$$

$$A(T_c^{(2)}) + 3B(T_c^{(2)})m^{*2} + 5C(T_c^{(2)})m^{*4} = 0, \quad (3.18c)$$

where m^* may be nonzero revealing the existence of a first-order phase transition. More precisely, when $T_c^{(1)} = T_c^{(2)}$ it may occur either that $m^* = 0$ (the transition is second order) or else that $m^* \neq 0$ when $B(T_c^{(1)}) = C(T_c^{(1)}) = 0$ (the transition is first order), while m^* is always nonzero (first-order transition) when $T_c^{(1)} \neq T_c^{(2)}$.

Theorem 4. Consider the case $K < 0$, any dimension d , and a dynamics such that $c(\mathbf{s}; \mathbf{x}) = c(-\mathbf{s}; \mathbf{x})$ for all \mathbf{x} , with $c(\mathbf{s}; \mathbf{x})$ depending only on the NN of s_x ; any homogeneous stationary solution is such that $m = 0$.

A proof follows by noticing that

$$mF_+(m) + F_-(m) = 0, \quad (3.19)$$

where $F_{\pm}(m) \equiv \langle f(\mathbf{s}) A_{\pm}(\mathbf{s}) \rangle_m$, as a consequence of Eqs. (3.1) and (3.9). Next one notices that $f(\mathbf{s})$ is positive defined and that one may write

$$A_{\pm} = \pm 2A_0(\mathbf{s}) \left\{ \frac{\cosh}{\sinh} \right\} \left[K \sum_{i=1}^d (s_{x+i} + s_{x-i}) \right] \quad (3.20)$$

where

$$A_0(\mathbf{s}) \equiv \left[\prod_{i=1}^d \cosh[K(s_{x+i} + s_{x-i})] \right]^{-1}. \quad (3.21)$$

Therefore one has from (3.19) that

$$m = -F_-(m)/F_+(m) \leq K|M||K|^{-1}, \quad (3.22)$$

where

$$M \equiv \frac{\left\langle \sinh \left[|K| \sum_i (s_{x+i} + s_{x-i}) \right] A_0(\mathbf{s}) f(\mathbf{s}) \right\rangle_m}{\left\langle \cosh \left[|K| \sum_i (s_{x+i} + s_{x-i}) \right] A_0(\mathbf{s}) f(\mathbf{s}) \right\rangle_m} \quad (3.23)$$

is independent of the sign of K . Then, $m \leq -|M|$ for $K < 0$ and, due to the symmetry property $c(\mathbf{s}; \mathbf{x}) = c(-\mathbf{s}; \mathbf{x})$, both m and $-m$ must be solutions. That is, any solution is such that $m = 0$.

IV. EXPLICIT COMPUTATIONS FOR DIFFERENT SPIN-FLIP RATES

Following with the case $\beta' = 0$, we study now explicit solutions of (3.1) corresponding to the most interesting choices for $c(\mathbf{s}; \mathbf{x})$, i.e., $f(\mathbf{s})$, for arbitrary d and $K > 0$ (ferromagnetic interactions).

Case 1. The rates originally introduced by Glauber¹ correspond to $f(\mathbf{s}) = \text{const} > 0$ in Eq. (3.5). This yields

$$F(m) = (1 + am)^d(1 - m) - (1 - am)^d(1 + m) = m f_1(m^2)$$

[cf. Eq. (3.9)]. Then, $m = 0$ is a stationary solution which remains stable as far as $\alpha \leq \alpha_c$, where

$$\alpha_c \equiv \alpha(T_c^{(1)}) \equiv \tanh(2J/k_B T_c^{(1)}) = d^{-1}. \quad (4.1)$$

Thus $K_c^{(1)} \equiv J/k_B T_c^{(1)}$ is finite for $1 < d < \infty$, $K_c^{(1)} \rightarrow \infty$ as $d \rightarrow 1$, and $2K_c^{(1)} \approx d^{-1} \rightarrow 0$ as $d \rightarrow \infty$. One may also show after some algebra that

$$m^* \approx B \hat{e}^{\beta}, \quad \hat{e} \equiv 1 - K_c/K \rightarrow 0^- \quad (4.2)$$

with $B^2 = 6K_c d$ and $\beta = \frac{1}{2}$.

In particular, one has for $d=1$ that the only stable solution is $m^* = 0$, so that $T_c^{(1)} = 0$ and there is no phase transition. On the contrary, one has that $F(m) = -2m(\alpha^2 m^2 - 2\alpha + 1)$ for $d=2$ implying the stable solutions

$$m^* = 0 \quad \text{when } \alpha \leq \frac{1}{2}, \\ m^* = \pm [(2\alpha - 1)]^{1/2} / \alpha \quad \text{when } \alpha > \frac{1}{2}; \quad (4.3)$$

i.e., there is a second-order transition with $\alpha_c \equiv \tanh(2K_c) = \frac{1}{2}$ (notice that $T_c^{(1)} = T_c^{(2)} = T_c$). For

$d=3$, one has that $F(m)=[2\alpha^2(\alpha-3)m^2+6\alpha-2]$ leading to the stable solutions

$$\begin{aligned} m^* &= 0 \quad \text{when } \alpha \leq \frac{1}{3}, \\ m^* &= \pm[(3\alpha-1)/\alpha^2(3-\alpha)] \quad \text{when } \alpha \geq \frac{1}{3}, \end{aligned} \quad (4.4)$$

and $T_c^{(1)}=T_c^{(2)}=T_c$ with $\alpha_c \equiv \tanh(2J/k_B T_c) = \frac{1}{3}$.

Case 2. Given that the Glauber rates in case 1 produce a zero-temperature critical point when $d=1$, it seems interesting to consider the more general choice:⁴

$$c(\mathbf{x};\mathbf{s}) = 1 - \hat{\alpha} s_x (s_{x-1} + s_{x+1}) + \hat{\alpha}^2 s_{x-1} s_{x+1} \quad (4.5)$$

where $\hat{\alpha} \equiv \tanh(K)$. This may be generalized to arbitrary dimension by using Eq. (3.5) with

$$f(\mathbf{s}) = \prod_{i=1}^d (1 + \hat{\alpha}^2 s_{x+i} s_{x+i}) \quad (4.6)$$

which leads after Eq. (3.9) to

$$F(m) = (1 + m\hat{\alpha})^{2d}(1-m) - (1 - m\hat{\alpha})^{2d}(1+m).$$

This is precisely the same F as for case 1 when one makes the substitutions $d \rightarrow 2d$, $J \rightarrow J/2$, so that one has the same conclusions as for case 1, except that the critical temperature is given now by $\hat{\alpha}_c = \tanh(K_c^{(1)}) = (2d)^{-1}$. Thus there is a phase transition even for $d=1$ with

$$m^* = 0 \quad \text{when } \hat{\alpha} \leq \frac{1}{2}, \quad (4.7)$$

$$m^* = \pm[(2\hat{\alpha}-1)]^{1/2}/\hat{\alpha} \quad \text{when } \hat{\alpha} \geq \frac{1}{2};$$

this is precisely the behavior shown by the Glauber rates in case 1 when $d=2$, i.e., it might be said that (4.6) causes an effective increase in the system dimension. For $d=2$ the stable solutions are

$$\begin{aligned} m^* &= 0 \quad \text{when } \hat{\alpha} \leq \frac{1}{4}, \\ m^* &= \pm[2\hat{\alpha}-3+2(\hat{\alpha}^2-2\hat{\alpha}+2)^{1/2}]^{1/2}\hat{\alpha}^{-2} \end{aligned} \quad (4.8)$$

when $\hat{\alpha} \geq \frac{1}{4}$,

and the critical temperature for the (second-order) phase transition is $\tanh(K_c) = \frac{1}{4}$.

Case 3. The fact that the stationary states of the model strongly depend on the choice for $f(\mathbf{s})$ may also be illustrated by considering f as a function of \mathbf{s} except of s_x and its NN. It follows that

$$F(m) = \langle f(\mathbf{s}) \rangle_m F^{(1)}(m) \quad (4.9)$$

where $F^{(1)}(m)$ represents the polynomial obtained before for case 1. That is, in addition to the solutions characterizing case 1, one has the solutions of $\langle f(\mathbf{s}) \rangle_m = 0$ which may be as varied as one wishes.

Case 4. Most familiar, from equilibrium and time-dependent problems concerning the binary alloy model system in the canonical formalism, are the rates introduced by Kawasaki² which may also be applied to spin-flip processes. These are defined as

$$c(\mathbf{x};\mathbf{s}) = \{1 + \exp[\Delta H(\mathbf{s};\mathbf{x})]\}^{-1} \quad (4.10)$$

or, equivalently, by putting $f(\mathbf{s}) = A_+^{-1}$ in (3.5). It follows that

$$\begin{aligned} F(m) &= -2m - 2 \langle A_-(\mathbf{s})/A_+(\mathbf{s}) \rangle_m \\ &= -2m + 2 \left\langle \tanh \left[K \sum_{i=1}^d (s_{x+i} + s_{x-i}) \right] \right\rangle_m \end{aligned} \quad (4.11)$$

where the average is given by (cf. the Appendix)

$$\left\langle \tanh \left[K \sum_{i=1}^d (s_{x+i} + s_{x-i}) \right] \right\rangle_m = \sum_{n=1}^d B_n m^{2n-1} \left[\frac{2d}{2n-1} \right] \quad (4.12)$$

where

$$B_n = \sum_{s=0}^{d-1} (b^{-1})_{ns} P_s, \quad n=1, \dots, d \quad (4.13)$$

$$P_r \equiv \tanh[2K(d-r)], \quad r=0, \dots, d-1 \quad (4.14)$$

and

$$\begin{aligned} (b^{-1})_m &= \sum_{s=\max(0,2n-r-1)}^{\min(2n-1,2d-r)} (-1)^{s+1} \\ &\quad \times \binom{2d-r}{s} \binom{r}{2n-1-s}. \end{aligned} \quad (4.15)$$

Then $m^*=0$ is always a solution, which is stable when $B_1 \leq (2d)^{-1}$, and $T_c^{(1)}$ is the solution of $B_1(T_c^{(1)}) = 1/2d$; one may also conclude from above that the magnetization critical exponent is $\frac{1}{2}$ (unless $B_2=0$), independent of d .

For $d=1$ one has that $b_{01}=2$, $B_1 = \frac{1}{2}\alpha$, where $\alpha \equiv \tanh(2K)$ as before, $F(m) = 2m(2B_1-1)$, and the only solution is $m^*=0$ which is always stable. For $d=2$ one has

$$b^{-1} = \frac{1}{8} \begin{bmatrix} 1 & 2 \\ 1 & -2 \end{bmatrix}, \quad B_{1,2} = \frac{1}{8} [\tanh(4K) \pm 2\alpha],$$

and

$$F(m) = m(8B_2m^2 + 8B_1 - 2), \quad (4.16)$$

and the only stable solutions are

$$\begin{aligned} m^* &= 0 \quad \text{when } B_1 \leq \frac{1}{4}, \\ m^* &= \pm[(\alpha^3 - \alpha^2 + 2\alpha - 1)\alpha^{-3}]^{1/2} \quad \text{when } B_1 \geq \frac{1}{4}, \end{aligned} \quad (4.17)$$

implying a second-order phase transition with $T_c^{(1)}=T_c^{(2)}=T_c$ the solution of $\alpha_c^3 - \alpha_c^2 + 2\alpha_c - 1 = 0$, i.e., $\alpha_c = 0.5698$ ($K_c = 0.3236$). One has, for $d=3$,

$$(b^{-1}) = \frac{1}{32} \begin{bmatrix} 1 & 4 & 5 \\ 1 & 0 & -3 \\ 1 & -4 & 5 \end{bmatrix},$$

$$B_{1,3} = \frac{1}{32} [\tanh(6K) \pm 4 \tanh(4K) + 5\alpha],$$

$$B_2 = \frac{1}{32} [\tanh(6K) - 3\alpha],$$

and

$$F(m) = -2m(1 - 6B_1 - 20B_2m^2 - 6B_3m^4), \quad (4.18)$$

and the stable solutions are $m^* = 0$ when $B_1 \leq \frac{1}{6}$, and

$$m^* = \pm \left[\frac{1}{6\alpha^3} [5\alpha + 5\alpha^3 - (12\alpha - 11\alpha^2 + 48\alpha^3 - 58\alpha^4 + 36\alpha^5 - 11\alpha^6)^{1/2}] \right]^{1/2} \quad (4.19)$$

otherwise; i.e., there is a second-order phase transition with $T_c^{(1)} = T_c^{(2)} = T_c$ the solution of $B_1 = \frac{1}{6}$ or $3\alpha_c^5 - 3\alpha_c^4 + 9\alpha_c^3 - 4\alpha_c^2 + 3\alpha_c - 1 = 0$: $\alpha_c = 0.3750$ ($K_c = 0.197$).

Case 5. Consider now the familiar Metropolis rates¹⁴ defined as

$$c(\mathbf{x}; \mathbf{s}) = \min[1, \exp[-\Delta H(\mathbf{s}; \mathbf{x})]] \quad (4.20)$$

or equivalently by

$$f(\mathbf{s}) = \exp \left[-K \left| \sum_{i=1}^d (s_{x+i} s_{x-i}) \right| \right] \times \prod_{i=1}^d \cosh[K(s_{x+i} s_{x-i})]. \quad (4.21)$$

Then,

$$F(m) = -2m \langle f(\mathbf{s}) A_+(\mathbf{s}) \rangle_m - 2 \langle f(\mathbf{s}) A_-(\mathbf{s}) \rangle_m$$

where (cf. the Appendix)

$$\langle f A_+ \rangle_m = \sum_{n=0}^d \left[\frac{2d}{2n} \right] B_n^+ m^{2n},$$

$$\langle f A_- \rangle_m = - \sum_{n=1}^d \left[\frac{2d}{2n-1} \right] B_n^- m^{2n-1}$$

with

$$B_n^+ = \sum_{r=0}^d (b')_{nr}^{-1} P_r^+, \quad n=0, 1, \dots, d \quad (4.22)$$

$$B_n^- = \sum_{r=0}^{d-1} (b)_{nr}^{-1} P_r^-, \quad n=0, \dots, d-1$$

$$P_r^\pm = \exp[-2K(d-r)] \left[\frac{\cosh}{\sinh} \right] [2K(d-r)], \quad (4.23)$$

and

$$(b')_m = \sum_{s=\max(0, 2n-r)}^{\min(2n, 2d-r)} (-1)^s \left[\frac{2d-r}{s} \right] \left[\frac{r}{2n-s} \right]. \quad (4.24)$$

Thus

$$F(m) = 2m \left\{ \sum_{n=0}^{d-1} m^{2n} \left[\left[\frac{2d}{2n+1} \right] B_{n+1}^- - \left[\frac{2d}{2n} \right] B_n^+ \right] - B_d^+ m^{2d} \right\}, \quad (4.25)$$

and it follows that $m^* = 0$ is always a solution which is stable when $2dB_1^- - B_0^+ \leq 0$. In particular, for $d=1$:

$$(b')^{-1} = 1/2 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad b=2;$$

then,

$$B_{0,1}^+ = \frac{1}{2} [\bar{\alpha}^{1/2} \cosh(2K) \pm 1], \quad B_1^- = \frac{1}{2} \bar{\alpha}^{1/2} \sinh(2K)$$

where $\bar{\alpha} \equiv \exp(-4K)$, and

$$F(m) = 2m(2B_1^- - B_0^+ - B_1^+ m^2), \quad (4.26)$$

implying that the only stable solution is $m^* = 0$ for all temperatures, i.e., there is no phase transition for $d=1$. For $d=2$, on the other hand, one has

$$(b')^{-1} = \begin{bmatrix} -2 & -8 & -6 \\ -2 & 0 & 2 \\ -2 & 8 & -6 \end{bmatrix},$$

$$(b)^{-1} = \frac{1}{8} \begin{bmatrix} 1 & 2 \\ 1 & -2 \end{bmatrix},$$

$$16B_0^+ = \bar{\alpha}^2 + 4\bar{\alpha} + 11, \quad 16B_1^+ = \bar{\alpha}^2 - 1,$$

$$16B_2^+ = \bar{\alpha}^2 - 4\bar{\alpha} + 3, \quad 16B_1^- = 3 - 2\bar{\alpha} - \bar{\alpha}^2,$$

$$16B_2^- = -(1 - \bar{\alpha})^2,$$

and

$$F(m) = 2m [4B_1^- - B_0^+ + m^2(4B_2^- - 6B_1^+) - B_2^+ m^4]. \quad (4.27)$$

Then, $m^* = 0$ is stable when $\bar{\alpha} > \bar{\alpha}_c^{(1)}$ where the latter is the solution of $5(\bar{\alpha}_c^{(1)})^2 + 12\bar{\alpha}_c^{(1)} - 1 = 0$, i.e., $\bar{\alpha}_c^{(1)} = 0.0806$ ($K_c^{(1)} = 0.6295$). There is also a solution, say m_+ such that

$$(m_+)^2(3 - \bar{\alpha}) = 1 + 5\bar{\alpha} + 2[(1 - 7\bar{\alpha} + 3\bar{\alpha}^2 - 5\bar{\alpha}^3)(1 - \bar{\alpha})^{-1}]^{1/2}, \quad (4.28)$$

which is stable for $\bar{\alpha} < \bar{\alpha}_c^{(2)}$ where

$$5(\bar{\alpha}_c^{(2)})^3 - 3(\bar{\alpha}_c^{(2)})^2 + 7\bar{\alpha}_c^{(2)} - 1 = 0,$$

i.e., $\bar{\alpha}_c^{(2)} = 0.1501$ ($K_c^{(2)} = 0.4741$). Thus $K_c^{(1)} \neq K_c^{(2)}$ and the transition is first order:

$$m(K) = \begin{cases} 0 & \text{when } K < K_c^{(2)} \\ 0 \text{ and } m_+ & \text{when } K_c^{(2)} < K < K_c^{(1)} \\ m_+ & \text{when } K > K_c^{(1)} \end{cases} \quad (4.29)$$

where $m_+(K_c^{(1)}) = 0.9612$ and $m_+(K_c^{(2)}) = 0.6142$. For $d=3$ one has

$$(b')^{-1} = \frac{1}{592} \begin{bmatrix} 56 & 186 & 240 & 110 \\ 16 & 32 & -16 & -32 \\ 16 & -42 & -16 & 42 \\ 56 & -36 & 240 & -260 \end{bmatrix},$$

$$(b)^{-1} = \frac{1}{32} \begin{bmatrix} 1 & 4 & 5 \\ 1 & 0 & -3 \\ 1 & -4 & 5 \end{bmatrix},$$

and

$$F(m) = 2m(a\phi^3 + b\phi^2 + c\phi + d) \quad (4.30)$$

where

$$\phi \equiv m^2, \quad a \equiv -B_3^+, \quad b \equiv 6B_3^- - 15B_2^+,$$

$$c \equiv 20B_2^- - 15B_1^+, \quad d \equiv 6B_1^- - B_0^+,$$

$$592B_0^+ = 28\alpha^3 + 93\alpha^2 + 120\alpha + 351,$$

$$592B_1^+ = 8\alpha^3 + 16\alpha^2 - 8\alpha - 16,$$

$$592B_2^+ = 8\alpha^3 - 21\alpha - 8\alpha + 21,$$

$$592B_3^+ = 28\alpha^3 - 18\alpha^2 + 120\alpha - 130,$$

$$64B_1^- = -\alpha^3 - 4\alpha^2 - 5\alpha + 10, \quad 64B_2^- = -\alpha^3 + 3\alpha - 2,$$

$$64B_3^- = -\alpha^3 + 4\alpha^2 - 5\alpha + 2.$$

That is, $m^* = 0$ is always a solution for $\alpha \geq \alpha_c^{(1)} = 0.3843$ ($K_c^{(1)} = 0.2390$) and, as for $d=2$, there is a jump $|m_c| = 0.7089$ in the magnetization at $K_c^{(1)}$.

Table I collects some results for cases 1-5.

Case 6. Finally, we may consider the action of an external magnetic field, i.e., the original Hamiltonian is now

$$H(\mathbf{s}) = -K \sum_{|x-y|=1} s_x s_y - h \sum_x s_x \quad (4.31)$$

and the transition probability is

$$c(\mathbf{x}; \mathbf{s}) = f(\mathbf{s}) \{ A_+ [\cosh(h) - s_x \sinh(h)] - A_- [\sinh(h) - s_x \cosh(h)] \} \quad (4.32)$$

The corresponding stationary solutions satisfy that

$$\langle f A_+ \rangle_m [m \cosh(h) - \sinh(h)] + \langle f A_- \rangle_m [\cosh(h) - m \sinh(h)] = 0 \quad (4.33)$$

Let us assume that $f(\mathbf{s}) = \text{const}$ as for case 1, and remember that $\alpha_c = d^{-1}$ when $h=0$; it follows that $m \approx Ah^{1/\delta}$ with $\delta=3$ and $A^3 = 3d^2/(d^2-1)$ revealing that $d \rightarrow 1$ is again singular and that $A \rightarrow 0$ as $d \rightarrow \infty$. It also seems interesting to refer to case 2 with $d=1$ in the presence of an external field. One has that

$$m(1-2\alpha + m^2\alpha^2) = \tanh(h)(1-2m^2\alpha + m^2\alpha^2) \quad (4.34)$$

TABLE I. Critical values K_c for the parameter $K \equiv \beta J$ when the transition is second order, or for $K_c^{(1)}$ and $K_c^{(2)}$ (as defined in the text) when it is first order, corresponding to the models designated in the text as cases 1 [Glauber rates (Ref. 1)], 2 [a generalization of case 1 (Ref. 4)], 4 [Kawasaki rates (Ref. 2)], and 5 [Metropolis rates (Ref. 15)].

| Case | $d=1$ | $d=2$ | $d=3$ | Phase transition order |
|------|----------|-------|-------|------------------------|
| 1 | ∞ | 0.275 | 0.173 | Second |
| 2 | 0.549 | 0.255 | 0.168 | Second |
| 4 | ∞ | 0.324 | 0.197 | Second |
| 5 | ∞ | 0.629 | 0.239 | First |
| | | 0.474 | | |

which, for small fields, reduces to $m(1-2\alpha) \approx h - m^3\alpha^2$; that is, one has near α_c that $m = 4^{1/3}h^{1/3} + O(h)$ while far from α_c the prediction is that $m \approx h(1-2\alpha)$ when m is small enough and $\alpha < \frac{1}{2}$.

V. FINITE TEMPERATURE DIFFUSION

We now turn to the computation of $F(m)$ when $\beta' > 0$ (and $\Gamma \rightarrow \infty$). We shall illustrate this by considering two different choices for $c(\mathbf{s}; \mathbf{x})$; one of them induces a (non-equilibrium) phase transition for $d=1$ ($J > 0$).

Consider first the transition probability

$$c(\mathbf{s}; \mathbf{x}) = 1 - \frac{1}{2}\alpha s_x(s_{x+1} + s_{x-1}), \quad (5.1)$$

i.e., case 1 of Sec. IV with $d=1$. It follows that $F(m) = -2m(1-\alpha)$, so that the only solution is $m^* = 0$. More interesting is the one-dimensional choice (4.5), case 2, which produces, after some algebra,

$$F(m) = -2[m(1-2\hat{\alpha}) + \hat{\alpha}^2 \langle s_{x-1} s_x s_{x+1} \rangle] \quad (5.2)$$

The three-spin correlation here, which is defined via the equilibrium measure (1.9), follows (by using a transfer matrix method, for instance) as

$$\langle s_{x-1} s_x s_{x+1} \rangle = m \Theta^{-2} [2\Theta \cosh(\bar{\mu}) - 1 - 3/(\hat{\alpha}')^2], \quad (5.3)$$

where

$$\hat{\alpha} \equiv \tanh(K), \quad \hat{\alpha}' \equiv \exp(2K'), \quad K' \equiv \beta' J, \quad (5.4)$$

$$\Theta \equiv \cosh(\bar{\mu}) + m^{-1} \sinh(\bar{\mu}), \quad (5.5)$$

and $\bar{\mu}$ is related to the magnetization by

$$m = \{1 + [\hat{\alpha}' \sinh(\bar{\mu})]^{-2}\}^{-1/2} \quad (5.6)$$

That is, there is always a solution $m^* = 0$ which remains stable as far as

$$\hat{\alpha} \leq \hat{\alpha}_c \equiv (1 + \hat{\alpha}') / (3 + \hat{\alpha}') \quad (5.7)$$

for any given β' . Otherwise, i.e., when $2K > \ln(2 + \hat{\alpha}')$, there is a stable nonzero solution, namely,

$$m^* = \sigma [\sigma^2 + (1 - \sigma^2)(\hat{\alpha}')^{-2}]^{-1/2} \quad (5.8)$$

with

$$\sigma^2 = 1 - 4\hat{\alpha}^2(1 - \hat{\alpha})^2 [(1 - 2\hat{\alpha} - \hat{\alpha}^2) \sinh(2K') + 2\hat{\alpha}^2 \cosh(2K')]^{-2} \quad (5.9)$$

which corresponds to a second-order phase transition, as one can convince oneself by following the method in the remark after Theorem 3 in Sec. III. As expected, the limits $K' \rightarrow 0$ and $K' \rightarrow \infty$ produce in (5.7) the known results $\hat{\alpha}_c \leq \frac{1}{2}$ (Ref. 4) and $\hat{\alpha}_c \leq 1$ (Ref. 1), respectively.

It also follows from above that, for any given K' , one has a "critical spin-flip temperature" such that $K_c = \frac{1}{2} \ln[2 + \exp(2K')]$, while K needs to be larger than $\frac{1}{2} \ln 3$ in order to have a "critical spin-exchange temperature," namely, $K_c' = \frac{1}{2} \ln[\exp(2K) - 2]$. That is, the system presents a line of critical points, corresponding to

pairs (K, K') related as $2K = \ln[2 + \exp(2K')]$, $K > K'$, which ends at the "special point" $(\frac{1}{2}\ln 3, 0)$. When one approaches that point from the two-phase region by following the line of slope b , i.e., $2K = \ln 3 + 2bK'$, one obtains the classical behavior $m^* = [2(3b-1)K']^{1/2}$ as $K' \rightarrow 0$. One also has a classical critical behavior in the same sense when crossing the line of critical points at fixed $K' > 0$. Thus it follows that such a mean-field type of behavior, which was first found associated to the limit $K' = 0$,³ is a consequence of the diffusion fast-rate limit $\epsilon \rightarrow 0$ ($\Gamma \rightarrow \infty$). This is also supported by the MC results for finite Γ in the next section.

The limit $K' = 0$ is characterized by an essential lack of correlation between sites, as was discussed before. As expected, this is no longer true for finite values of K' . This is illustrated here by computing the spin-spin correlation function for any fixed K' in the case of the one-dimensional choice (4.5). We find that

$$\langle s_0 s_n \rangle = (\Theta_+ + \Theta_-)^{-2} [(\Theta_+^* + \Theta_-^*)^2 - 4(\Theta_- / \Theta_+)^n \Theta_+^* \Theta_-^*] \quad (5.10)$$

where

$$\Theta_{\pm}^* \equiv \Theta_{\pm} - \exp(K + \bar{\mu}) \quad (5.11)$$

and

$$\Theta_{\pm} = (1 - \sigma^2)^{-1/2} \{ (\hat{\alpha}')^{1/2} \pm [\sigma^2 \hat{\alpha}' + (1 - \sigma^2) / \hat{\alpha}']^{1/2} \}. \quad (5.12)$$

In the one-phase region, one has $\bar{\mu} = 0$, $\sigma = 0$, and it follows that

$$\langle s_0 s_n \rangle = \exp(-n / \xi_1), \quad \xi_1 \equiv -1 / \ln[\tanh(K')], \quad (5.13)$$

while, in the two-phase region, an expansion around $m = 0$ ($\sigma = 0$) produces

$$\langle s_0 s_n \rangle = \exp(-n / \xi_1) \exp(-n / \xi_2) + (\sigma \hat{\alpha}')^2 \{ 1 - \exp[-n(\xi_1^{-1} + \xi_2^{-1})] \}, \quad (5.14)$$

with

$$\xi_2 \equiv [\sigma^2 \exp(3K')]^{-1}, \quad (5.15)$$

which diverges as $m \rightarrow 0$. We also find that

$$\langle s_1 s_2 s_3 \rangle = \frac{2e^{K \sinh(\bar{\mu})}}{\Theta_+^* (\Theta_- + \Theta_+)} \times [4 \cosh(2K) + \Theta_+^2 - 4\Theta_+ e^K \cosh(\bar{\mu})] \quad (5.16)$$

for the three-spin correlation function.

VI. COMPUTER SIMULATION RESULTS

Also interesting are the properties of the stationary states of the model for finite Γ , $0 < \Gamma < \infty$. In particular, the relationship between the macroscopic mean-field instability which occurs for random diffusion and $\Gamma \rightarrow \infty$ when $J > 0$ and $d \geq 2$ [and, for some spin-flip rates $c(s; \mathbf{x})$,

also for $d=1$], and the behavior of the stationary state at fixed Γ . We have investigated that relationship by simulating in a computer the model dynamics in Sec. I with $c(s; \mathbf{x}, \mathbf{y}) = 1$, i.e., a completely random diffusion, for two particular spin-flip rates $c(s; \mathbf{x})$, namely, for those corresponding to case 2, where $c(s; \mathbf{x})$ is given by Eq. (4.5), and 5, where $c(s; \mathbf{x})$ is given by Eq. (4.20). The latter choice was motivated by the fact that it is probably the most familiar one in the literature and it is also most efficient when trying to reach the stationary state by means of the MC method, so that it becomes then more simple to simulate true (stabilized) magnetic ordering disturbed by exchanges; also, because (4.20) produces quite different behaviors for $d=1$ than for $d=2$ in the limit $\Gamma \rightarrow \infty$, so that one may also expect important differences for finite values of Γ . We also found it interesting to simulate the behavior of the model for finite Γ when the spin-flip mechanism is governed by the transition probability (4.5) because, in the limit $\Gamma \rightarrow \infty$, this produces a phase transition already for $d=1$. It is questionable whether this may remain true for finite Γ .¹³

Our procedure is essentially the usual one in a MC experiment,¹⁶ except that after a site \mathbf{x} is chosen at random from a given lattice ($d=1, 2$) then with probability p , $0 \leq p \leq 1$, the spin $s_{\mathbf{x}}$ is exchanged with one of its NN as if the system was in contact with a heat bath at infinite temperature, and with probability $1-p$ the spin $s_{\mathbf{x}}$ is flipped with rate $c(s; \mathbf{x})$ computed as if the bath temperature was β^{-1} . As compared with the model discussed in Sec. I, this corresponds, except for a renormalization of time units which is irrelevant for the stationary state, to have $\Gamma = p/d(1-p)$. Periodic boundary conditions and ferromagnetic interactions are always assumed.

Two-dimensional systems. The case $d=2$ was studied for different sizes L^2 , $L \leq 100$, NN interactions, and Metropolis rates. The detailed behaviors of the energy (NN correlation) and magnetization as a function of β for several values of p , and their comparison with a mean-field computation⁵ which essentially produces the same qualitative results, were reported before.¹³ We describe now the behavior of the specific heat C (Fig. 1) and magnetic susceptibility χ (Fig. 2), as given by energy and magnetization fluctuations, respectively, and of the short-ranged order parameter (Fig. 3), defined as $\sigma = (N_{++})(N_{--}) / (N_{+-})^2$, where N_{+-} represents the number of up-down pairs of NN spins in the system, etc. The latter turned out to be a very useful quantity to determine the nature of a phase transition.¹⁷

Figure 2 reveals that the function $\chi(\beta, p)$ for $p \lesssim 0.8$ remains sharp around a transition temperature, say β_*^{-1} , which decreases with increasing p . The characteristic shape of $\chi(\beta, p)$ for a given p ($\lesssim 0.8$) is qualitatively indistinguishable from the one for $p=0$ (i.e., the equilibrium, Onsager case). Moreover, all our data for $p \lesssim 0.8$ are consistent with the Onsager value for the corresponding critical exponent, $\gamma \approx 1.75$, independently of p . Also, the magnetization critical exponent is then always around 0.125.¹³

Figure 1 reveals that $p=0.1$ is characterized by a sharp divergence, apparently the same logarithmic divergence as $p=0$. The cases $p=0.6$ and 0.8 are also consistent

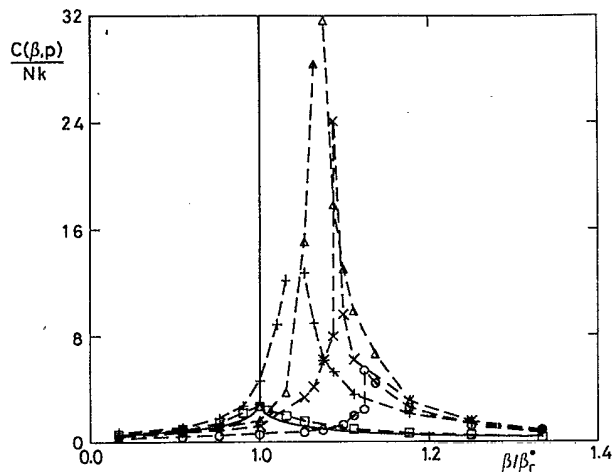


FIG. 1. The specific heat, computed from energy fluctuations, as a function of the inverse temperature β ($\beta_c^0 = 0.441/J$, the equilibrium critical temperature) for the two-dimensional system with NN interactions (Ref. 13) and case-5 rates. The solid line represents the equilibrium ($p=0$) result for the infinite system. The symbols are for $p=0.1$ (empty squares), 0.6 (+), 0.8 (triangles), 0.85 (\times), and 0.95 (\circ); the dashed lines are a guide to the eye.

with a sharp divergence. In any case, there seems to be a symmetry $\alpha \approx \alpha'$ with α very small or zero.

The situation for $p \geq 0.85$ is, however, qualitatively different. That is, long-lived metastable states, which were never present for $p < 0.8$, now frequently appear during the system evolution, the energy and magnetization become discontinuous at some well-defined temperature β_*^{-1} ,¹³ and $C(\beta, p)$ and $\chi(\beta, p)$ are more asymmetric than before. Actually, the data suggest that both C and χ present a finite jump at $\beta_*^{-1}(p)$ which keeps decreasing with increasing p .

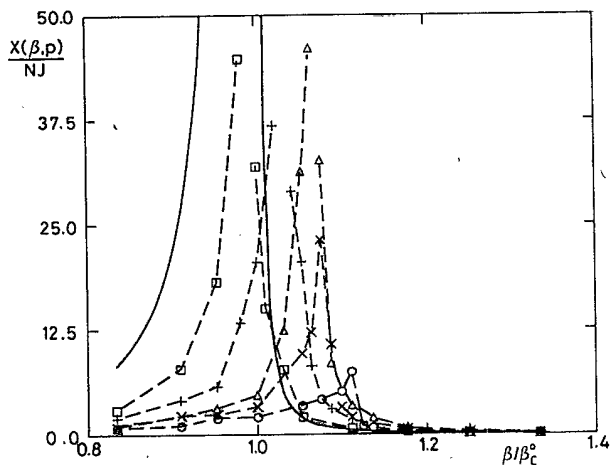


FIG. 2. The magnetic susceptibility, obtained from the fluctuations of the magnetization, as a function of β . Same system and symbols as in Fig. 1.

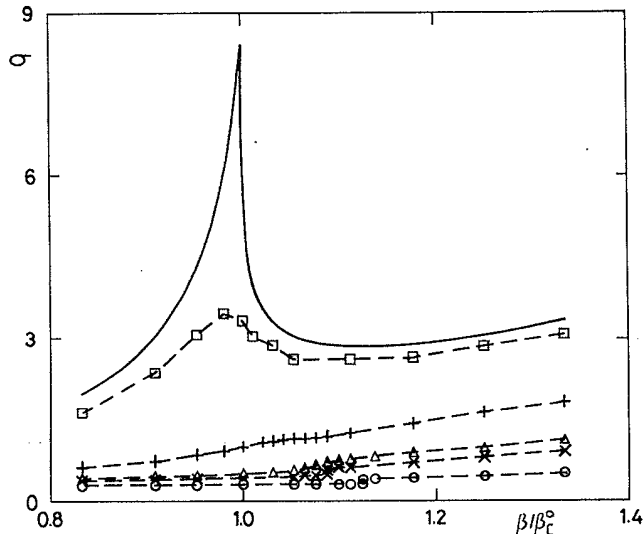


FIG. 3. Short-ranged order parameter, as defined in Sec. VI, as a function of β . Same system and symbols as in Fig. 1.

Figure 3 depicts the behavior of the short-ranged order parameter σ . This confirms our previous observations. In particular, $p=0.1$ is consistent with a second-order phase transition similar to the one for $p=0$, while $p \geq 0.85$ is characterized by a discontinuity. Moreover, the qualitative behavior shown by σ in Fig. 3 allows one to exclude the possibility of having a second-order phase transition with classical exponents for small values of p , say for $p=0.1$.¹⁷

The phase diagram for the two-dimensional system with Metropolis rates, as implied by the above MC data and by the exact results in Sec. IV (see also Ref. 13), is reported in Fig. 7 (main graph): There is a "tricritical point" at $p_t \approx 0.83$ separating two different behaviors for $p < p_t$ and $p > p_t$, respectively. The first one is similar to the situation at equilibrium ($p=0$), i.e., second-order phase transitions with Onsager critical exponents. The second one is characterized by mean-field type first-order transitions. There is also some evidence for a changeover of the critical exponents from the Onsager values towards the classical ones as $p \rightarrow p_t^-$.

One-dimensional systems. The case $d=1$ was studied numerically for Metropolis rates, (4.20), and for the generalized rates defined by Eq. (4.5). The former case was reported before.¹³ The main conclusion there is that a system with $p=0.95$ ($L=2500$) presents no phase transition, as it is also known to occur for $p=0$ (equilibrium) and for $\Gamma \rightarrow \infty$ (Sec. IV, case 5). Actually, the magnetization-temperature curve for $p=0.95$ is identical to the equilibrium one (while the energy differs due to the action of the fast random diffusion process when $p=0.95$). We also performed the experiment for $p=0.95$ when the spin interactions extend up to the next NN. The energy and magnetization curves are then more structured than for $p=0$, but they always depict a monotonous behavior and there is no evidence of a phase transition for a chain with 2500 spins. The same follows by inspection of specific heats and magnetic susceptibilities.

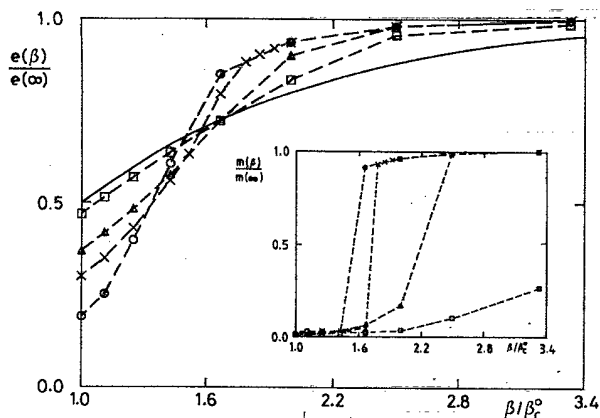


FIG. 4. The energy (main graph) and the magnetization (inset) as a function of β (β_c^0 is the exact value of the transition temperature with $p=1$) for the one-dimensional system with NN interactions and case-2 rates. The symbols are for $p=0.1$ (squares), 0.5 (triangles), 0.75 (\times), and 0.95 (\circ); the dashed lines are a guide to the eye.

The picture revealed by the experiments with the generalized rates (4.5) is more interesting. This is reported in Figs. 4–6 which refer to 10000 spins and $p=0.1, 0.5, 0.75$, and 0.95: As p is increased, the energy curves (Fig. 4) are observed to deviate from the equilibrium result in a way which suggests that the system segregates for $p \gtrsim 0.7$. This is also suggested by the inset in Fig. 4 where the magnetization seems to present a discontinuity for $p \gtrsim 0.75$, and perhaps also for $p=0.5$. Figures 5 and 6 for $C(\beta, p)$ and $\chi(\beta, p)$, respectively, are indeed consistent with the presence of a first-order, mean-field-type phase transition for $p > 0$, perhaps only for $p \gtrsim 0.5$, occurring at a temperature which increases with p .

Finally, let us mention two important features of the temporal evolution of the one-dimensional system with rates (4.5). First, that seems always characterized by a very slow decay rather than by the presence of actual

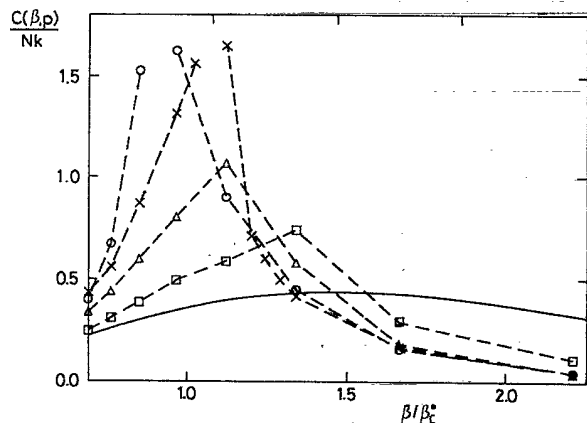


FIG. 5. The specific heat as a function of β . The solid line is the equilibrium result for the infinite system. Same system and symbols as in Fig. 4.

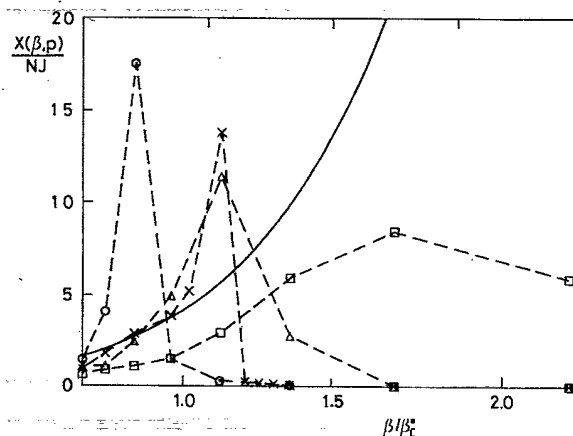


FIG. 6. The magnetic susceptibility as a function of β . Same system and symbols as in Fig. 4.

steady metastable states (as one would expect for a first-order phase transition; cf. the case $d=2$ above). This suggests that, in spite of the abrupt jump manifested by the magnetization (cf. inset for Fig. 4), the discontinuity we are interpreting for $p > 0.5$ is characterized by a very weak energy jump, if any. This is indeed confirmed by the energy curves in Fig. 4. The fact that the energy

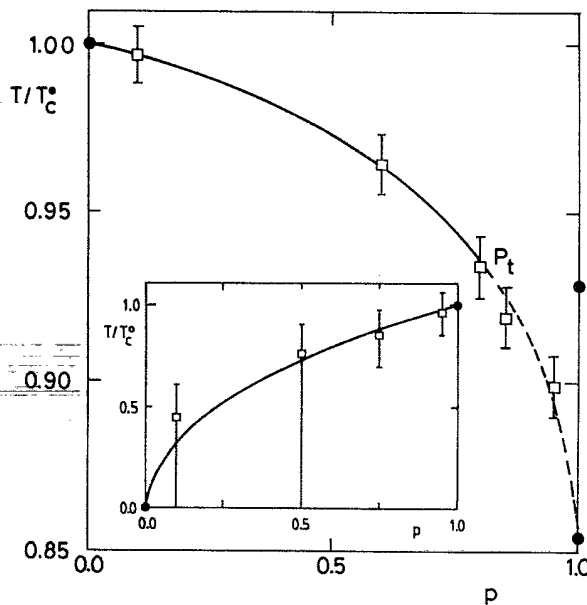


FIG. 7. Monte Carlo (empty squares) and exact (solid circles) results for the phase diagram of the two-dimensional system in Fig. 1 (main graph) and for the phase diagram of the one-dimensional system in Fig. 4 (inset). The MC transition temperatures follow from the analysis of Figs. 1–6; the exact ones are defined in the “Remarks” after Theorem 3 (Sec. III). Both exact and Monte Carlo results (the latter including error bars) when $d=1$ are consistent with the situation described by the curve in the inset, i.e., mean-field-type phase transitions for all $p > 0$, and also with the presence of a phase transition only for $p \gtrsim 0.5$.

discontinuity may be quite negligible, even when the associated magnetization discontinuity is large enough, just reflects the zero measure of the surface of the one-dimensional clusters, where the energy changes take place. This is a feature of $d=1$ which cannot be extrapolated to $d>1$. On the other hand, the relaxation times of the system are larger here than usual, and they increase with decreasing p . As a consequence, we cannot decide definitely from the MC data, as suggested above, whether the phase segregation occurs for all $p>0$ or only for $p>0.5$ (see the inset in Fig. 7).

VII. CONCLUSION

We have studied by different methods a reaction-diffusion Ising model whose dynamics consists of a competition between spin-flip and spin-exchange processes, with $p/d(1-p)$ the relative probability of attempted exchanges per bond to attempted flips per site, both driven by canonical heat baths at (inverse) temperatures β and β' , respectively. It was shown that one may derive macroscopic equations (involving time and spatial derivatives) for large enough p from that microscopic model for all $\beta, \beta' \geq 0$. This generalizes previous results for $p \rightarrow 1$ and $\beta' \rightarrow 0$ which represent the limit of pure mean-field behavior and lack of correlations.

The stable (nonequilibrium) homogeneous steady states predicted by those macroscopic equations depend strongly on the spin-flip rate and less critically on the spin-exchange rate. We concentrated here on the detailed study of the former dependence when $\beta'=0$, i.e., when the diffusion is completely random, and $p \rightarrow 1$. In particular, we determined (A) the conditions on the rate to have a second-order phase transition, and the associated critical temperature, for a one-dimensional system, (B) the most general form of the magnetization curve for a two-dimensional system, and (C) most details of the steady state for systems of arbitrary dimension and for the rates which are familiar in the literature.

In addition, the study of the general case $\beta' \neq 0$ revealed (D) a rich phase diagram for the one-dimensional system, (E) the fact that the resulting classical behavior comes rather associated to the limit $p \rightarrow 1$ than to the random diffusion destroying correlations, and (F) the existence of microscopic correlations for $\beta' > 0$ which decay exponentially in the one-phase region.

Most information concerning the case $p < 1$ was obtained from MC studies for $\beta'=0$. The results are consistent with the exact computations for $p \rightarrow 1$, and with the equilibrium results for $p=0$, while they help in characterizing the whole phase diagram. For $d=2$ and certain familiar rates, there is a "tricritical point" at $p=p_t \equiv 0.83 \pm 0.01$. For $p < p_t$, the system undergoes a second-order phase transition with equilibrium, Onsager critical exponents. The exponents probably become classical as $p \rightarrow p_t$, and the phase transition changes to first order for $p > p_t$. The situation for $d=1$ is more intriguing. For the same rates as before, the one-dimensional system has essentially the same behavior as in equilibrium, i.e., no phase transition exists for any $p \geq 0$. The conclusion remains unchanged when the interactions are ex-

tended to next NN, though one observes then some more definite changes with temperature than for NN interactions. The use of certain generalized rates for the spin-flip process produces, however, phase segregation in one dimension. Two alternative pictures emerge, both contrary to some expectations: (i) equilibrium behavior, i.e., lack of long-range order, for small values of p and first-order phase transitions, as in the limit $p \rightarrow 1$, for large p , or (ii) discontinuous phase transitions for all $p > 0$. The transition temperature increases with p in both cases. The data at hand seem to favor the first picture. We are presently studying further this question and the nature of the situation for $p < 1$ and $\beta' > 0$.

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APPENDIX

This illustrates the computation of Bernoulli averages $\langle g(\mathbf{s}) \rangle_m$, as required in Secs. III and IV, where $g(\mathbf{s})$ represents a function of the system configuration \mathbf{s} . Let us assume that $g(\mathbf{s}) = g(s_1, \dots, s_l)$ and that $g(\mathbf{s})$ remains invariant under the interchange of any two spin variables. Then,

$$g(\mathbf{s}) = g_0 + g_1 \sum_{i=1}^l s_i + g_2 \sum_{\text{NN}} s_i s_j + \dots + g_l s_1 \dots s_l. \quad (\text{A1})$$

Each configuration with l spins has

$$r \text{ spins down and } l-r \text{ spins up,} \quad (\text{A2})$$

and one may write the function g as

$$\begin{aligned} \bar{g}(r, l-r) &= g(s_1 = \dots = s_r = -1, s_{r+1} = \dots = s_l = 1) \\ &= \sum_{n=0}^l a_n g_n \end{aligned} \quad (\text{A3})$$

with $r=0, \dots, l$, where $a_0=1$. Thus the computation of the coefficients a_n determines the unknowns g_n in Eq. (A1).

Denote by $p(s, n-s)$ the probability of having n spins, out from a configuration (A2), such that s are up and $n-s$ are down,

$$\begin{aligned} p(s, n-s) &= \frac{(l-r)! r! (l-n)!}{l!} \binom{n}{s} \\ &\times \frac{1}{(l-r-s)!} \frac{1}{(r+s-n)!} \end{aligned} \quad (\text{A4})$$

where one has the bounds $\max(0, n-r) \leq s \leq \min(n, l-r)$, the symmetry property $p(s, n-s) = p(n-s, s)$, and

$$a_n = \binom{l}{n} \sum_s p(s, n-s) (-1)^{n-s} \quad (\text{A5})$$

such that $a_n(r) = (-1)^n a_n(1-r)$, and $a_n(\frac{1}{2}l) = 0$ for any odd n , i.e., $g_n = 0$ for any even n . Thus

$$\bar{g}(l-r, r) = \sum_{n=0}^l \binom{l}{n} \sum_s p(s, n-s) (-1)^{n-s} g_n. \quad (\text{A6})$$

One may introduce the matrix notation

$$P_r \equiv \bar{g}(l-r, r), \quad B_{rn} \equiv \binom{l}{n} \sum_s p(s, n-s) (-1)^{n-s} \quad (\text{A7})$$

such that

$$g_n = \sum_k (B^{-1})_{nk} P_k, \quad (\text{A8})$$

and

$$\langle g(s) \rangle_m = \sum_{n=0}^l \binom{l}{n} m^n \sum_k (B^{-1})_{nk} P_k, \quad (\text{A9})$$

i.e., the computation of the required Bernoulli averages follows after the inversion of the B matrix and the construction of the elements P_r , both defined in (A7).

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