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Self-organization in a kinetic Ising model

Tânia Tomé and Mário J. de Oliveira
Instituto de Física, Universidade de São Paulo, Caixa Postal 20516, 01498 São Paulo, São Paulo, Brazil
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We have analyzed a self-organization occurring in an open ferromagnetic Ising system on a square lattice in contact with a heat bath and subject to an external source of energy. The system follows a stochastic dynamics composed of two processes: one of the Glauber type, which simulates the contact of the system with the heat bath, and the other of the Kawasaki type, which simulates the continuous flux of energy into the system. When the flux is small, the stationary state is paramagnetic at high temperatures and ferromagnetic at low temperatures. By increasing the flux, the ferromagnetic state is destroyed and the system reaches a new stationary state of high energy identified with the antiferromagnetic ordered state.

I. INTRODUCTION

A system subject to an external source of energy may, in certain circumstances, organize itself. This self-organization results from the amplification of fluctuations and is sustained by itself as long as the nonequilibrium conditions are maintained. The structures arising from self-organization processes, called dissipative structures,[1] have been observed experimentally and are an object of study in the areas of thermodynamics of nonequilibrium systems and nonequilibrium statistical mechanics. Examples of dissipative structures are found in fluid dynamics and physical-chemical reactions.[1,2]

In this paper we analyze a dissipative structure occurring in an open ferromagnetic Ising system in contact with a heat bath and subject to an external source of energy. The Ising system evolves in time according to stochastic dynamics composed of two competing processes: one of the Glauber[3] type, which simulates the contact with the heat bath, and the other of the Kawasaki[4] type, which simulates the continuous flux of energy. When the intensity of the energy source is small we are in the linear regime of the irreversible process and the system displays (at low temperatures) an ordering similar to that occurring in equilibrium. If the intensity is increased, this ordering will be destroyed, and at sufficiently large intensities we reach the nonlinear region of irreversible process where a new order will occur.

We have analyzed the stationary states of the system as a function of the flux of energy for the case of an Ising model in a square lattice with ferromagnetic interactions between nearest neighbors. In the linear regime, when the flux is small, the Glauber process dominates and the system will be in the ferromagnetic state below a certain critical temperature. At high temperatures the stationary state will be the paramagnetic state. By increasing the flux the critical temperature decreases. In other words, the flux of energy destroys the ferromagnetic ordered state. In the nonlinear regime, when the flux is sufficiently large, the Kawasaki process will prevail and the system will be found in a stationary ordered state of high energy which is identified with the antiferromagnetic ordered state.

The problem was solved by using the dynamic pair approximation which leads to equations for the time evolution of the two sublattice magnetizations and the nearest-neighbor pair correlation. At equilibrium this approximation reduces to the Bethe-Peierls approximation.

II. MASTER EQUATION

Consider a lattice of N Ising spins with ferromagnetic interactions. The state of the system is represented by $\sigma=(\sigma_1,\sigma_2,\sigma_3,\ldots,\sigma_N)$, where σ_i, the spin variable at site i, takes the values ± 1. The energy of the system in state σ is given by

$$E(\sigma)=-J\sum_{(ij)}\sigma_i\sigma_j \ , \tag{1}$$

where the summation is over nearest-neighbor pairs and $J>0$.

The state of the system evolves in time according to stochastic dynamics. Let $P(\sigma,t)$ be the probability of state σ at time t. The evolution of $P(\sigma,t)$ is given by the master equation[4]

$$\tau\frac{d}{dt}P(\sigma,t)=\sum_{\sigma'}[P(\sigma',t)W(\sigma',\sigma)-P(\sigma,t)W(\sigma,\sigma')] \ , \tag{2}$$

where $W(\sigma',\sigma)/\tau$ is the probability, per unit time, of transition from state σ' to state σ, *if* the system is in state σ'.

The transition probability $W(\sigma',\sigma)$ is constructed in order to describe the following processes: (a) the contact of the system with a heat bath at temperature T, and (b) the flux of energy into the system. We assume that

$$W(\sigma',\sigma)=pW_A(\sigma',\sigma)+qW_B(\sigma',\sigma) \ , \tag{3}$$

where $W_A(\sigma',\sigma)$ is associated to the process (a) and $W_B(\sigma',\sigma)$ to process (b). The process (a) occurs with probability p and the process (b) with probability $q=1-p$.

The process (a) is simulated by Glauber dynamics[3,4] (one-spin flip) so that

$$W_A(\sigma',\sigma)=\sum_i \delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}\cdots\delta_{\sigma_i-\sigma_i'}\cdots\delta_{\sigma_N\sigma_N'}w_i(\sigma)\ , \tag{4}$$

where $w_i(\sigma)$ is the probability of flipping spin i. The contact with the heat bath at temperature T is obtained by using the Metropolis prescription[5]

$$w_i(\sigma)=\begin{cases}1 & \text{for } \Delta E_i\le 0\\ e^{-\Delta E_i/kT} & \text{for } \Delta E_i>0\ ,\end{cases} \tag{5}$$

where ΔE_i is the change in energy obtained after flipping spin i.

The process (b) is simulated by Kawasaki dynamics[4] (two-spin flips), which describes the exchange of two nearest-neighbor spins. That is,

$$W_B(\sigma',\sigma)=\sum_{(ij)}\delta_{\sigma_1\sigma_1'}\cdots\delta_{\sigma_i\sigma_j'}\cdots\delta_{\sigma_j\sigma_i'}\cdots\delta_{\sigma_N\sigma_N'}\times w_{ij}(\sigma)\ , \tag{6}$$

where $w_{ij}(\sigma)$ is the probability of exchanging the nearest-neighbor spins i and j. The flux of energy into the system is obtained by the prescription

$$w_{ij}(\sigma)=\begin{cases}0 & \text{when } \Delta E_{ij}\le 0\\ 1 & \text{when } \Delta E_{ij}>0\end{cases}, \tag{7}$$

where ΔE_{ij} is the change in energy obtained after exchanging spins i and j.

Let us denote by $\langle f(\sigma)\rangle$ the average of the state function $f(\sigma)$, that is,

$$\langle f(\sigma)\rangle=\sum_\sigma f(\sigma)P(\sigma,t)\ . \tag{8}$$

The equations for the magnetization $\langle\sigma_i\rangle$ of spin i and for the correlation $\langle\sigma_j\sigma_k\rangle$ of the nearest-neighbor spins j and k can be derived in a straightforward way from the master equation. With the notation introduced above we get

$$\tau\frac{d}{dt}\langle\sigma_i\rangle=pA_i+qB_i \tag{9}$$

and

$$\tau\frac{d}{dt}\langle\sigma_j\sigma_k\rangle=pA_{jk}+qB_{jk}\ , \tag{10}$$

where

$$A_i=\langle(-2\sigma_i)w_i(\sigma)\rangle\ , \tag{11}$$

$$A_{jk}=\langle(-2\sigma_j\sigma_k)w_j(\sigma)\rangle+\langle(-2\sigma_j\sigma_k)w_k(\sigma)\rangle\ , \tag{12}$$

$$B_i=\sum_{\substack{l\\(\text{NN of } i)}}\langle(\sigma_l-\sigma_i)w_{li}(\sigma)\rangle\ , \tag{13}$$

$$B_{jk}=\sum_{\substack{l(\neq k)\\(\text{NN of } j)}}\langle(\sigma_l\sigma_k-\sigma_j\sigma_k)w_{jl}(\sigma)\rangle+\sum_{\substack{l(\neq j)\\(\text{NN of } k)}}\langle(\sigma_j\sigma_l-\sigma_j\sigma_k)w_{kl}(\sigma)\rangle\ , \tag{14}$$

where (NN of i) denotes that the summation is over the nearest neighbors of site i.

These equations have a simple interpretation. For example, the quantity $(\sigma_l\sigma_k-\sigma_j\sigma_k)$ inside the bracket $\langle(\sigma_l\sigma_k-\sigma_j\sigma_k)w_{jl}(\sigma)\rangle$ equals the variation of $\sigma_j\sigma_k$ in the (b) process (Kawasaki process) in which spins j and l are exchanged.

The equations for $\langle\sigma_i\rangle$ and $\langle\sigma_j\sigma_k\rangle$ are exact. However, they cannot be solved since their right-hand sides (RHS) involve averages of other combinations of spin variables besides $\langle\sigma_i\rangle$ and $\langle\sigma_j\sigma_k\rangle$.

III. PAIR APPROXIMATION

The right-hand sides of expressions (9) and (10) involve the average of clusters of spins. In the case of the quantities A_i and A_{jk}, the type of cluster to be considered consists of a central spin and its nearest neighbors. In the case of B_i and B_{jk}, the type of cluster to be examined is formed by two nearest-neighbor spins and their nearest neighbors. In order to obtain closed equations for $\langle\sigma_i\rangle$ and $\langle\sigma_j\sigma_k\rangle$ we will use an approximation in which the probability of these clusters are written in terms of the probability of a pair of spins.[6-8] Since the probability of a pair of spins in turn can be obtained from the values of $\langle\sigma_i\rangle$ and $\langle\sigma_j\sigma_k\rangle$, a set of self-consistent equations are therefore obtained.

We apply the results obtained so far to the case of a bipartite lattice. We look for solutions such that $\langle\sigma_i\rangle=m_1$ for any spin belonging to sublattice 1, $\langle\sigma_j\rangle=m_2$ for any spin belonging to sublattice 2, and $\langle\sigma_i\sigma_j\rangle=r$ for any pair of nearest-neighbor spins i and j. Let σ_1 and σ_2 be a pair of nearest-neighbor spins belonging to sublattices 1 and 2, respectively. Then, the pair probability $P_{12}(\sigma_1,\sigma_2)$ and the single-spin probabilities $P_1(\sigma_1)$ and $P_2(\sigma_2)$ are given by

$$P_1(\sigma_1)=\tfrac{1}{2}(1+m_1\sigma_1)\ , \tag{15}$$

$$P_2(\sigma_2)=\tfrac{1}{2}(1+m_2\sigma_2)\ , \tag{16}$$

$$P_{12}(\sigma_1,\sigma_2)=\tfrac{1}{4}(1+m_1\sigma_1+m_2\sigma_2+r\sigma_1\sigma_2)\ . \tag{17}$$

We should examine three types of clusters. The first one consists of a spin σ_1 of sublattice 1 surrounded by spins σ_j of sublattice 2. The probability of such a cluster is approximated by[7]

$$P_1(\sigma_1)\prod_{\substack{j\\(\text{NN of }1)}}\frac{P_{12}(\sigma_1,\sigma_j)}{P_1(\sigma_1)}\ . \tag{18}$$

The second type of cluster has a spin σ_2 of sublattice 2 surrounded by spins σ_i of sublattice 1. The probability of such a cluster is[7]

$$P_2(\sigma_2)\prod_{\substack{i\\(\text{NN of }2)}}\frac{P_{12}(\sigma_i,\sigma_2)}{P_2(\sigma_2)}\ . \tag{19}$$

Finally, the third type of cluster is formed by a pair σ_1,σ_2 of nearest-neighbor spins surrounded by their nearest neighbors. The probability of this cluster is

$$P_{12}(\sigma_1,\sigma_2) \prod_{\substack{j\neq 2\\ (\text{NN of } 1)}} \frac{P_{12}(\sigma_1,\sigma_j)}{P_1(\sigma_1)} \prod_{\substack{i\neq 1\\ (\text{NN of } 2)}} \frac{P_{12}(\sigma_i,\sigma_2)}{P_2(\sigma_2)} . \quad (20)$$

Inserting expressions (18)–(20) in the right-hand side (rhs) of (11)–(14) and taking into account equations (15)–(17) we obtain closed equations for m_1, m_2, and r.

The equations for the evolution of the quantities m_1, m_2, and r are

$$\tau\frac{d}{dt}m_1 = pA_1(m_1,m_2,r) + qB_1(m_1,m_2,r) , \quad (21)$$

$$\tau\frac{d}{dt}m_2 = pA_2(m_1,m_2,r) + qB_2(m_1,m_2,r) , \quad (22)$$

$$\tau\frac{d}{dt}r = pA_{12}(m_1,m_2,r) + qB_{12}(m_1,m_2,r) , \quad (23)$$

where A_1, A_2, A_{12}, B_1, B_2, and B_{12} are given in the Appendix. Notice that the following properties hold: $A_2(m_1,m_2,r) = A_1(m_2,m_1,r)$ and $B_2(m_1,m_2,r) = -B_1(m_1,m_2,r)$.

IV. PHASE DIAGRAM

When the system evolves in time it will eventually reach a stationary state characterized by constant values of magnetization and other thermodynamic variables. Three types of stationary states may occur: the paramagnetic ($m_1=m_2=0$), the ferromagnetic ($m_1=m_2\neq 0$), and the antiferromagnetic ($m_1=-m_2\neq 0$) states.

The paramagnetic state corresponds to the trivial solution of Eqs. (21)–(23). It is given by $m_1=m_2=0$ and $r=r^*$ where r^* is the solution of $pA_{12}(0,0,r^*) + qB_{12}(0,0,r^*)=0$, that is,

$$p(-\eta^2 z^4 - 2\eta z^3 v + 2zv^3 + v^4) - 24q(5z^4v^3 + 4z^5v^2 + z^6 v) = 0 , \quad (24)$$

where $z=(1+r^*)/4$, $v=(1-r^*)/4$, and $\eta=\exp(-4J/kT)$.

The second type of solution that may appear is the ferromagnetic state ($m_1=m_2\neq 0$), described by the order parameter $m_F=(m_1+m_2)/2$. The ferromagnetic ordered state is the equilibrium type of order. It occurs, at low temperatures, not only at equilibrium ($q=0$) but also in the region near equilibrium, that is, for small values of q. If q is increased, at low temperatures, the ferromagnetic state eventually disappears giving place to the paramagnetic state. In other words, the ordered state that occurs at equilibrium is destroyed by the increase in the flux of energy.

If, however, the flux of energy is sufficiently increased, the system will organize itself in another type of ordering. That is, by increasing q the system becomes more and more far from equilibrium until a critical value of q is reached where the paramagnetic state becomes unstable, giving rise to a new stationary state. This new state is identified with the antiferromagnetic ordered state described by the order parameter $m_A=(m_1-m_2)/2$.

The phase diagram shown in Fig. 1 displays the regions

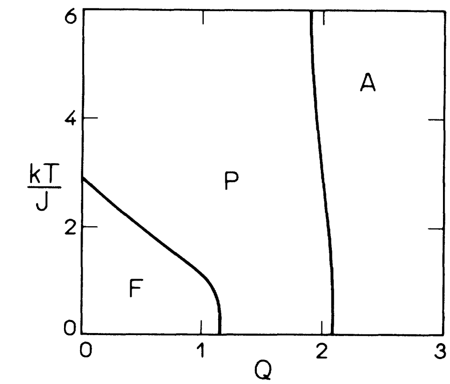

FIG. 1. Phase diagram of the open ferromagnetic Ising system. T is the temperature of the heat bath and the variable $Q=q/(1-q)$ is related to the flux of energy. The system may exhibit one of the three stationary states: paramagnetic (P), ferromagnetic (F), and antiferromagnetic (A). The case $Q=0$ corresponds to the thermodynamic equilibrium.

of occurrence of each type of stationary state. The ferromagnetic state occurs at small values of q and at sufficient low temperatures, whereas the antiferromagnetic state happens at large values of q for any temperature. The ferromagnetic and antiferromagnetic regions are separated by the paramagnetic region. The two transition lines are obtained by the analysis of the stability of the paramagnetic solution. When this solution becomes unstable a symmetry breaking takes place and the system starts to display an ordered state: either a ferromagnetic or an antiferromagnetic state.

The expansion of the rhs of Eqs. (21) and (22) up to linear terms in m_1 and m_2 gives

$$\tau\frac{d}{dt}m_F = \lambda_F m_F , \quad (25)$$

$$\tau\frac{d}{dt}m_A = \lambda_A m_A , \quad (26)$$

where

$$\lambda_F = 16p[\eta^2(6z^4-4z^3) + 4\eta(6z^3-3z^2)v + 6(6z^2-2z)v^2 + 4(6z-1)v^3 + 6v^4] , \quad (27)$$

$$\lambda_A = 16p[\eta^2 6z^4 + 4\eta z^3(6v-1) + 6z^2(6v^2-2v) + 4z(6v^3-3v^2) + (6v^4-4v^3)] + 512q[45z^4(4v^3-v^2) + 12z^5(6v^2-v) + z^6(12v-1)] , \quad (28)$$

with $z=(1+r^*)/4$ and $v=(1-r^*)/4$.

If $\lambda_F<0$ and $\lambda_A<0$, the paramagnetic solution is stable. Therefore $\lambda_F=0$ together with Eq. (24) define the paraferro transition line, and $\lambda_A=0$ together with Eq. (24) give the parantiferro transition line. The two transitions defined by these lines are continuous since the order parameters m_F and m_A vanish continuously when they are crossed.

V. CONCLUSIONS

We have studied an open ferromagnetic Ising system in contact with a heat bath and subject to a continuous flux of energy from an external source. We have found that the stationary states may be one of three types: paramagnetic, ferromagnetic, and antiferromagnetic. The first two states are the only stationary states observed in equilibrium and when the flux of energy is small. We may say then that the ferromagnetic state is of the equilibrium type. The antiferromagnetic ordered state, on the other hand, is the result, in the case considered here, of a far from equilibrium process, namely, the continuous flux of energy into the system. Thus an instability of the usual (equilibrium) solutions leads the system toward states with spatial self-organized structure.

The nonequilibrium antiferromagnetic ordered structure we have found is an indication that the study of stochastic lattice systems may be useful to understand, at the microscopic level, the occurrence of such dissipative structures found in fluid dynamics and physical-chemical reactions. Finally, the system we have studied here can also be interpreted as a kinetic Ising model with competition between ferromagnetic Glauber dynamics at temperature T and antiferromagnetic Kawasaki dynamics at zero temperature.

APPENDIX

Here we write down the quantities A_1, A_2, A_{12}, B_1, B_2, and B_{12} defined in Sec. II as a function of $m_1=\langle\sigma_1\rangle$, $m_2=\langle\sigma_2\rangle$, and $r=\langle\sigma_1\sigma_2\rangle$. Let us define first the quantities $x_1=P_1(+)$, $y_1=P_1(-)$, $x_2=P_2(+)$, $y_2=P_2(-)$, $z=P_{12}(++)$, $v_1=P_{12}(+-)$, $v_2=P_{12}(-+)$, and $w=P_{12}(--)$. From Eqs. (15)–(17) we get

$$x_1=\tfrac{1}{2}(1+m_1)\ , \tag{A1}$$

$$y_1=\tfrac{1}{2}(1-m_1)\ , \tag{A2}$$

$$x_2=\tfrac{1}{2}(1+m_2)\ , \tag{A3}$$

$$y_2=\tfrac{1}{2}(1-m_2)\ , \tag{A4}$$

$$z=\tfrac{1}{4}(1+m_1+m_2+r)\ , \tag{A5}$$

$$v_1=\tfrac{1}{4}(1+m_1-m_2-r)\ , \tag{A6}$$

$$v_2=\tfrac{1}{4}(1-m_1+m_2-r)\ , \tag{A7}$$

$$w=\tfrac{1}{4}(1-m_1-m_2+r)\ . \tag{A8}$$

Using these variable and $\eta=\exp(-4J/kT)$, we have, in the pair approximation,

$$A_1(m_1,m_2,r)=-\frac{2}{x_1^3}(\eta^2z^4+4\eta z^3v_1+6z^2v_1^2+4zv_1^3+v_1^4)+\frac{2}{y_1^3}(\eta^2w^4+4\eta w^3v_2+6w^2v_2^2+4wv_2^3+v_2^4)\ , \tag{A9}$$

$$A_2(m_1,m_2,r)=A_1(m_2,m_1,r)\ , \tag{A10}$$

$$\begin{aligned}A_{12}(m_1,m_2,r)=&\frac{1}{x_1^3}(-2\eta^2z^4-4\eta z^3v_1+4zv_1^3+2v_1^4)+\frac{1}{y_1^3}(-2\eta^2w^4-4\eta w^3v_2+4wv_2^3+2v_2^4)\\&+\frac{1}{x_2^3}(-2\eta^2z^4-4\eta z^3v_2+4zv_2^3+2v_2^4)+\frac{1}{y_2^3}(-2\eta^2w^4-4\eta w^3v_1+4wv_1^3+2v_1^4)\ ,\end{aligned} \tag{A11}$$

$$\begin{aligned}B_1(m_1,m_2,r)=&-\frac{8}{x_1^3y_2^3}(3z^3wv_1^3+3z^3w^2v_1^2+z^3w^3v_1+3zw^3v_1^3+3z^2w^3v_1^2+9z^2w^2v_1^3)\\&+\frac{8}{x_2^3y_1^3}(3w^3zv_2^3+3w^3z^2v_2^2+w^3z^3v_2+3wz^3v_2^3+3w^2z^3v_2^2+9w^2z^2v_2^3)\ ,\end{aligned} \tag{A12}$$

$$B_2(m_1,m_2,r)=-B_1(m_1,m_2,r)\ , \tag{A13}$$

$$\begin{aligned}B_{12}(m_1,m_2,r)=&-\frac{12}{x_1^3y_2^3}(z^3wv_1^3+2z^3w^2v_1^2+z^3w^3v_1+zw^3v_1^3+2z^2w^3v_1^2+3z^2w^2v_1^3)\\&-\frac{12}{x_2^3y_1^3}(w^3zv_2^3+2w^3z^2v_2^2+w^3z^3v_2+wz^3v_2^3+2w^2z^3v_2^2+3w^2z^2v_2^3)\ .\end{aligned} \tag{A14}$$

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