# Monte Carlo simulation of an antiferromagnetic Ising model at two competing temperatures

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We consider a two-dimensional antiferromagnet Ising system interacting with a heat bath at temperature $T$. The dynamics of the system is simulated by two competing stochastic processes: the two-spin-exchange Kawasaki kinetics at temperature $T>0$ and the one-spin-flip Glauber dynamics at $T_G \to 0^-$, which mimics the increase of the energy of the system. These two processes have probabilities $1-p$ and $p$, respectively. Monte Carlo simulations were employed to determine the phase diagram for the stationary states of the model and the corresponding critical exponents. Contrary to the ferromagnetic case, the phase diagram obtained does not exhibit the phenomenon of self-organization: for any nonzero value of the competing parameter $p$, and for any value of $T$, the only stationary phase which remains is the ferromagnetic one. At the phase transition between the antiferromagnetic and paramagnetic phases, at $p=0$, the values found for the critical exponents agree with those of the corresponding equilibrium Ising model. [S1063-651X(99)07205-0]

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When an Ising system is in contact with two heat baths at different temperatures [1,2], it is possible to find it in nonequilibrium steady states. The methods which were employed to deal with this nonequilibrium problem were the Monte Carlo simulations [1,3], the dynamical pair approximation [1,4] and the mean-field renormalization group [5]. In all of these analyses, the stochastic single spin-flip Glauber process was used to drive the spin system towards its nonequilibrium stationary states. In the work of Tomé *et al.* [4], an interesting behavior was observed when the temperature of one of the heat baths is allowed to become negative: this heat bath works like a source of energy to the spin system. Although the exchange interaction between neighboring spins is ferromagnetic, an antiferromagnetic state appears for high values of the flux of energy into the system. This kind of self-organization phenomenon was also observed for the ferromagnetic Ising model when subject to two competing Glauber and Kawasaki dynamic processes [6].

In this work, we used Monte Carlo simulations and finite-size scaling relations [7,8] to determine the phase transition and the critical exponents of the antiferromagnetic two-dimensional (2D) Ising model in contact with two heat baths at distinct temperatures. The system evolves in time according to two independent competing stochastic processes: the one-spin-flip Glauber dynamics [9], with probability $p$, and the two-spin-exchange Kawasaki dynamics [10], with probability $(1-p)$. The role of these two dynamics concerning the symmetries of the system is quite different: the Glauber kinetics always changes the order parameter, while the Kawasaki one conserves the ferromagnetic order parameter but not the antiferromagnetic order parameter. We take for both dynamic processes the transition probability rates given by the Metropolis prescription [11]. In order to simulate an input of energy into the system, we choose the temperature of one of the heat baths as being $T_G \to 0^-$. In this way, the increase of energy of the system is due to the single spin-flip Glauber process. On the other hand, the spin-exchange Kawasaki kinetics accounts for the relaxation of the spin system towards its equilibrium states, at temperature $T$ established by the other heat bath. That is, if $p=0$, the Kawasaki dynamics would drive the magnetic system to its equilibrium state, with a constant value of the ferromagnetic order parameter. On the other hand, the system goes to nonequilibrium stationary states when the Glauber process is present, which occurs for any value of $p$ different from zero. Unlike the work of Tomé *et al.* [4], where the self-organization phenomenon appeared for the ferromagnetic Ising model with two competing Glauber processes, we do not observe it in our simulations: for any value of $p \neq 0$ and for any value of temperature $T$ the only stationary state is the ferromagnetic one. For $p=0$, the system exhibits an order-disorder transition between the antiferromagnetic and paramagnetic phases. The relaxation of the order parameter for the antiferromagnetic Ising model subject to the Kawasaki dynamics is expected to be similar to that of the kinetic Ising ferromagnetic model under Glauber dynamics, where the order parameter is not a conserved quantity [12].

We consider an antiferromagnetic Ising model on a square lattice with $N$ lattice sites. The energy of the system in the state $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_N)$, where the spin variable assumes the values $\sigma_i=\pm 1$, is given by

$$E(\sigma)=J\sum_{(i,j)}\sigma_i\sigma_j . \tag{1}$$

In the summation, only spins that are nearest neighbors are considered and $J>0$. Let $P(\sigma,t)$ be the probability of finding the system in the state $\sigma$ at time $t$. The evolution of $P(\sigma,t)$ is given by the following master equation:

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

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where $W(\sigma',\sigma)$ gives the probability, per unit time, for the transition from the state $\sigma'$ to state $\sigma$. We assume that the two competing processes can be written as

$$W(\sigma',\sigma)=pW_G(\sigma',\sigma)+(1-p)W_K(\sigma',\sigma). \tag{3}$$

In this equation,

$$W_G(\sigma',\sigma)=\sum_{i=1}^{N}\delta_{\sigma_1',\sigma_1}\delta_{\sigma_2',\sigma_2}\cdots\delta_{\sigma_i',-\sigma_i}\cdots\delta_{\sigma_N',\sigma_N}w_i(\sigma) \tag{4}$$

is the single-spin-flip Glauber process, which simulates an input of energy into the system by the heat bath at temperature $T_G\to 0^-$, and

$$W_K(\sigma',\sigma)=\sum_{(i,j)}\delta_{\sigma_1',\sigma_1}\delta_{\sigma_2',\sigma_2}\cdots\delta_{\sigma_i',\sigma_j}\cdots \times\cdots\delta_{\sigma_j',\sigma_i}\cdots\delta_{\sigma_N',\sigma_N}w_{ij}(\sigma) \tag{5}$$

is the two-spin exchange Kawasaki process, which simulates the contact of the system with the heat bath at temperature $T>0$. In the above summation, only pairs of nearest-neighbor spins are considered.

In these equations, $w_i(\sigma)$ is the transition probability of flipping spin $i$, while $w_{ij}(\sigma)$ is the transition probability of exchanging two nearest-neighbor spins $i$ and $j$. We use the following prescriptions for $w_i(\sigma)$ and $w_{ij}(\sigma)$:

$$w_i(\sigma)=\begin{cases}0 & \text{for } \Delta E_i\leqslant 0,\\ 1 & \text{for } \Delta E_i>0,\end{cases} \tag{6}$$

because the temperature $T_G\to 0^-$, and

$$w_{ij}(\sigma)=\exp\left(-\frac{\Delta E_{ij}}{k_BT}\right). \tag{7}$$

$\Delta E_i$ is the change in energy after flipping spin $i$ and $\Delta E_{ij}$ is the change in energy after exchanging the nearest-neighbor spins $i$ and $j$.

We have performed Monte Carlo simulations, with periodic boundary conditions, on a square lattice with $L\times L=N$ sites, with values of $L$ ranging from $L=4$ up to $L=128$. We have started the simulations with different initial states to guarantee that the final stationary states we use in our calculations are the correct ones. For a given temperature $T$ and a selected value of the probability $p$, we choose at random a spin $i$, from a given initial configuration. Then, we generate a random number $\xi_1$ between zero and unity. If $\xi_1\leqslant p$, we choose to perform the Glauber process: we determine the value of $\Delta E_i$ and the corresponding $w_i$ according to the prescription of Eq. (6). If $\xi_1>p$, we go over the Kawasaki process: we again generate another random number $\xi_2$ in order to select one of the four nearest neighbors of the spin $i$, say $j$. Then we find the value of $\Delta E_{ij}$ and the corresponding $w_{ij}$; after generating a random number $\xi_3$, we exchange the selected spins only if $\xi_3\leqslant w_{ij}$. We have discarded the first $10^4N$ Monte Carlo steps in order to achieve the stationary regime, for all lattice sizes we consider. One Monte Carlo step equals $N$ single-spin flips or exchange of spin trials. To estimate the quantities of interest, we used $5\times 10^4$ Monte Carlo steps to calculate the averages for any lattice size.

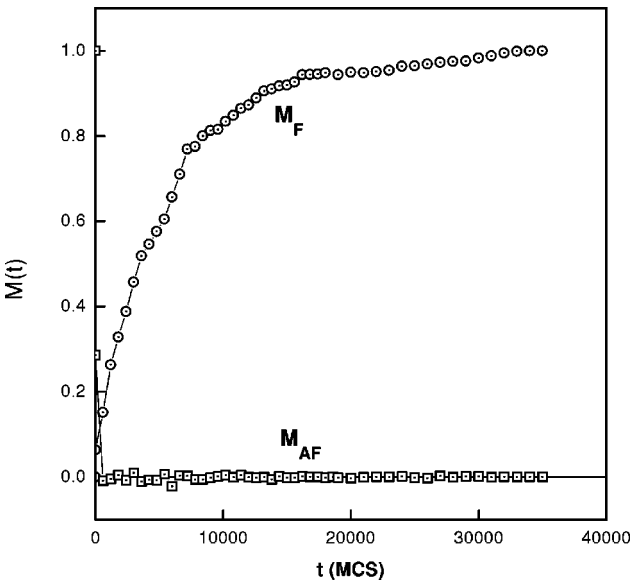


FIG. 1. Ferromagnetic and antiferromagnetic order parameters as a function of $t$, measured in Monte Carlo steps (MCS). We used $p=0.5$, $T=2.0$, in units of $J/k_B$, and $L=64$.

In order to find the transition point, we have plotted, for each value of $p$, the reduced fourth-order cumulant

$$U_L=1-\frac{\langle M^4\rangle}{3\langle M^2\rangle^2} \tag{8}$$

as a function of temperature $T$, for several values of $L$. Once this value is independent of lattice size at the critical temperature $T_c$, the crossing point of these lines [8] gives $T_c$. For any values of $T\neq 0$ and $p\neq 0$, we found, for all values of $L$, that the ferromagnetic order parameter $M_F$ is equal to 1, and that the antiferromagnetic order parameter $M_{\mathrm{AF}}$ is equal to 0. Then, the cumulants never cross themselves. That is, the Monte Carlo simulations showed that the only stationary state of the system is the ferromagnetic one, except for $p=0$. In Fig. 1 we show the behavior of the ferromagnetic and the antiferromagnetic order parameters as a function of the number of Monte Carlo steps. We chose the values $L=128$, $p=0.5$, and $T=2.0$ to exhibit the time evolution of the order parameters. We have also performed analytical calculations employing the dynamical pair approximation [13]: we have also seen that the only stationary phase which appears is the saturated ferromagnetic phase with $M_F=1$ for any value of $p\neq 0$ and for all values of $T$.

We also present the results we obtained for the particular case $p=0$, when the Ising system is only under the spin-exchange Kawasaki dynamics. In this case the antiferromagnetic order parameter relaxes towards its equilibrium value like the nonconservative order parameter of the similar kinetic ferromagnetic Ising model [12]. In this way the model studied here exhibits an order-disorder transition.

We show in Fig. 2 a plot of the antiferromagnetic order parameter $M_{\mathrm{AF}}$ as a function of $1/L$ for different values of temperature. From this plot it is easy to see that the critical

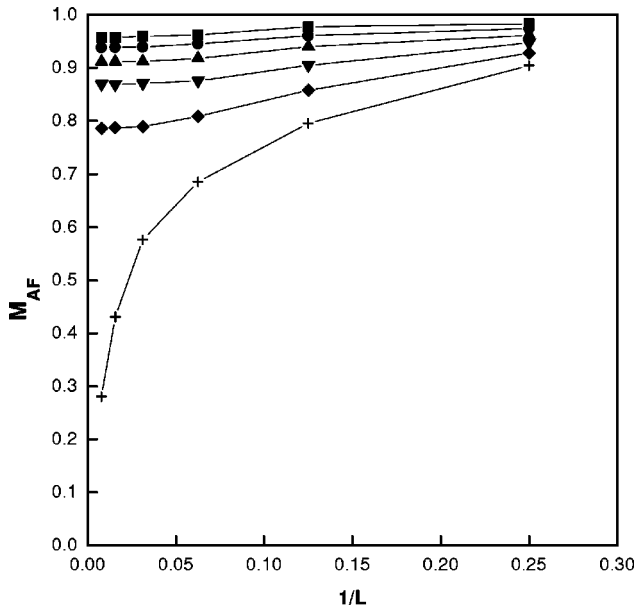


FIG. 2. Antiferromagnetic order parameter $M_{\mathrm{AF}}$ as a function of $1/L$ for several values of $T$ and $p=0$. From top to bottom the values of $T$ are 1.8, 1.9, 2.0, 2.1, 2.2, and 2.3. The transition appears in the range $2.2 \leqslant T \leqslant 2.3$. $T$ is in units of $J/k_B$.

temperature $T_c$ is between 2.20 and 2.30, in units of $J/k_B$. In order to find a more accurate value for the critical temperature, we plot in Fig. 3 the corresponding reduced fourth-order cumulants $U_L(T)$ as a function of $T$ for $L$ ranging from 4 to 128. From the crossing of these curves, we estimate the critical temperature as being $T_c=(2.24\pm0.02)$, in units of $J/k_B$. This value is very close to the well known exact value $T_c=2/\ln(1+\sqrt{2})$. From the finite-size scaling relations [6] obeyed by $U_L(T)$, we can compute the correlation length

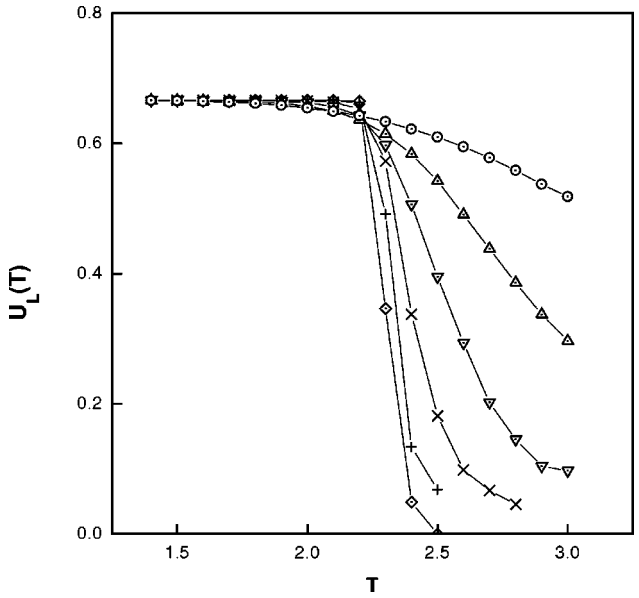


FIG. 3. Reduced fourth-order cumulant $U_L(T)$, for $p=0$, as a function of temperature $T$ for several values of the lattice size $L$. Circles correspond to $L=4$, up triangles to $L=8$, down triangles to $L=16$, crosses to $L=32$, plus signals to $L=64$, and diamonds to $L=128$. The broken lines serve as a guide to the eye. The critical temperature is $T_c=(2.24\pm0.02)$ in units of $J/k_B$.

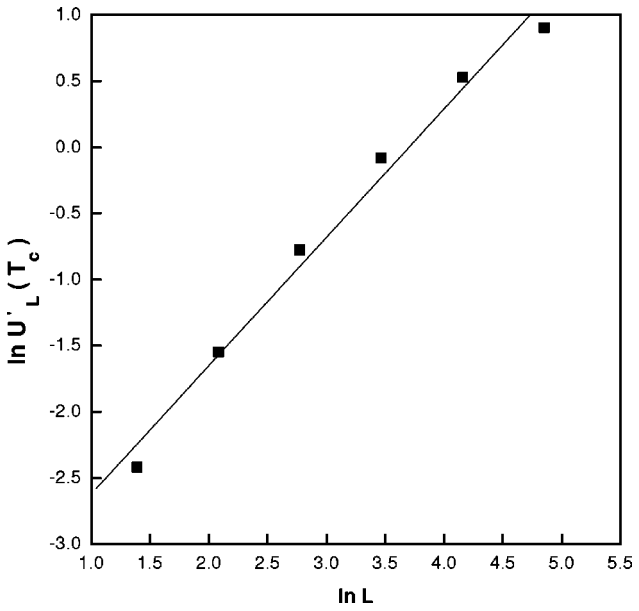


FIG. 4. Log-log plot of $U_L'(T_c)$ versus $L$. The straight line is the best fit to the data, which gives $\nu=1.00\pm0.03$.

exponent $\nu$ by taking the derivative of $U_L(T)$ with respect the temperature at the critical point. This derivative $U_L'(T_c)$ scales as $L^{1/\nu}$. From the best fit of the log-log plot of $U_L'(T_c)$ versus $L$, which can be seen in Fig. 4, we found that $\nu=1.00\pm0.03$. In Fig. 5 we exhibit the log-log plot of the antiferromagnetic order parameter $M_{\mathrm{AF}}$, at the critical temperature $T_c$, versus $L$. As $M_{\mathrm{AF}}(T_c)$ scales as $L^{-\beta/\nu}$, the best fit to the data points of this figure gives us $\beta/\nu=0.124\pm0.002$. We show in Fig. 6 the log-log plot of the susceptibility per spin $\chi_L(T)$ versus $L$, at $T_c$. This quantity scales as $L^{\gamma/\nu}$ at the critical temperature, and from the best fit to the data points we obtain the value $\gamma/\nu=1.75\pm0.05$. As to be expected, this set of critical exponents agrees with the exact

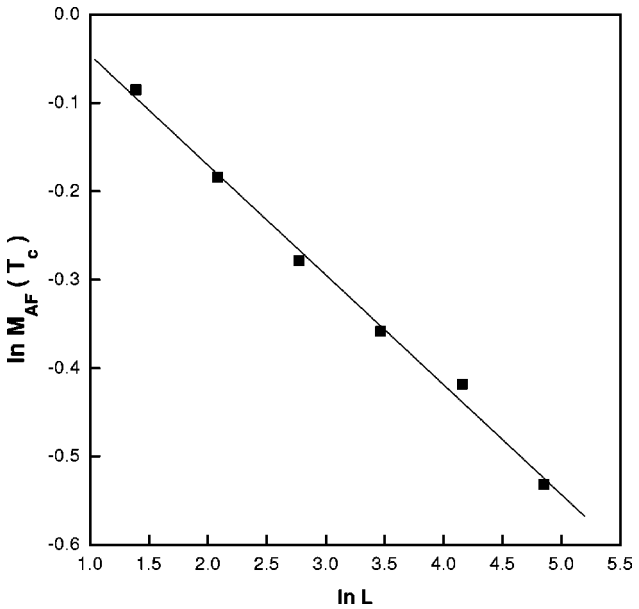


FIG. 5. Log-log plot of the antiferromagnetic order parameter $M_{\mathrm{AF}}(T_c)$ versus $L$. From the slope of the straight line, which is the best fit to the data points, we find $\beta/\nu=0.124\pm0.002$.

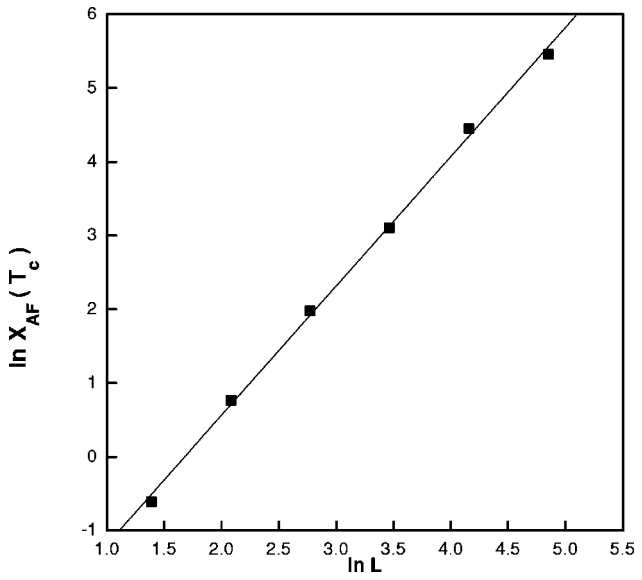


FIG. 6. Log-log plot of the susceptibility $\chi_{\mathrm{AF}}(T_c)$ versus $L$. The straight line is the best fit to the data points. From this slope we find $\gamma/\nu = 1.75 \pm 0.05$.

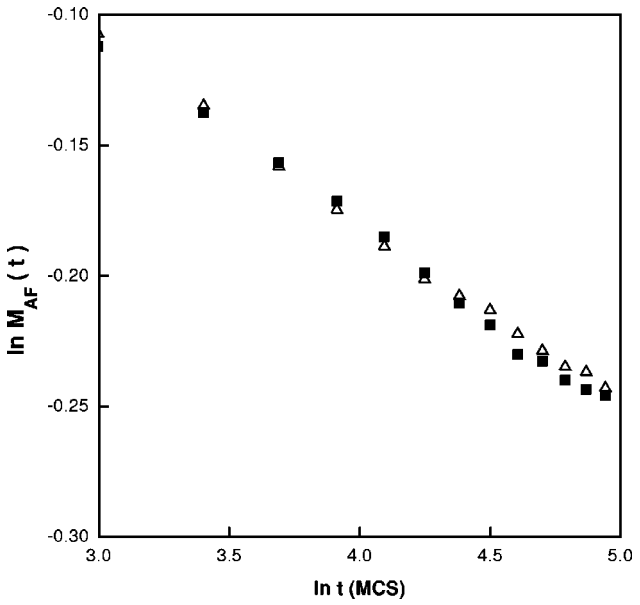


FIG. 7. Log-log plot of the antiferromagnetic order parameter versus time, measured in Monte Carlo steps (MCS), at the determined critical temperature $T_c = 2.24$. Measurements were made every 10 MCS, between 20 and 150 MCS. The lattice sizes are $(160 \times 160)$, triangles; and $(320 \times 320)$, squares. The value of the dynamical critical exponent is $z = 1.98 \pm 0.02$.

values of the two-dimensional Ising model, that is, $\nu = 1$, $\beta = 1/8$, and $\gamma = 7/4$.

Finally, we present our results concerning the dynamical critical exponent $z$ of this model. Following Suzuki [14], the dynamic finite-size scaling theory asserts that the magnetization of a system of linear size $L$, at its critical point, evolves in time according to the following scaling relation:

$$M_{\mathrm{AF}}(t,L) = L^{-\beta/\nu} f(L^{-z} t). \tag{9}$$

It is expected that the magnetization does not depend on the lattice size for very large lattices. Then it is easy to see that [15] $M_{\mathrm{AF}}(t,L)$ can be written as

$$M_{\mathrm{AF}}(t,L) = A t^{-\beta/\nu z}, \tag{10}$$

where $A$ is a constant that does not depend on $L$. The last equation is valid only for very large values of $L$. Therefore, taking into account the latter equation, we can evaluate the exponent $z$, after a log-log plot of $M_{\mathrm{AF}}(t,L)$ versus $t$, for a fixed value of $L$, once we know the value of the ratio $\beta/\nu$. After we prepared the system to be in its antiferromagnetic ground state, we left it to evolve in time, measured in Monte Carlo steps (MCS) per spin, and we recorded the magnetization at each 10 MCS. In Fig. 7 we show the log-log plot of $M_{\mathrm{AF}}(t)$ versus $t$, for $L = 160$ and $L = 320$, at the critical temperature, which we have determined previously. We can see that the decay of $M_{\mathrm{AF}}(t)$ is almost independent of $L$, which allow us to use Eq. (10) to evaluate the dynamical critical exponent $z$. We have considered the decay of the magnetization between 20 and 150 MCS. By fitting the data points to a straight line we obtained $z = 1.98 \pm 0.02$. We have discarded the initial points of the simulation because we want to put the system into the second regime, where a power-law decay of the order parameter is expected [16]. The value we found for $z$ must be compared with the best estimates for this exponent obtained through intensive use of large scale simulations: for instance, Stauffer [17] found $z = 2.18$ for a square lattice with $L = 496\,640$ and Linke *et al.* [18] found $z = 2.16$ for a square lattice with $L = 10^6$. This result also confirms that the relaxation of the antiferromagnetic order parameter for this spin-exchange Kawasaki process is rather similar to that of the kinetic Ising model under Glauber dynamics, where the ferromagnetic order parameter is not constant.

In conclusion, we have studied an antiferromagnetic Ising model subject to two competing dynamical processes: a single-spin flip Glauber dynamics at $T_G \to 0^-$, which simulates the pumping of energy into the system, and the spin-exchange Kawasaki process at finite temperature. We have shown that this model does not exhibit the self-organization phenomenon for any value of the competition parameter $p$ and for any value of temperature. The only stationary state we found was the full saturated ferromagnetic state for all values of $p \neq 0$. At $p = 0$, when only the Kawasaki process is present, and the ferromagnetic order parameter is conserved, we have found an order-disorder transition from the antiferromagnetic to the paramagnetic phase. By using Monte Carlo simulations and finite-size scaling relations in this case, we found the critical exponents of the model. The values we have determined for these exponents agree with those found for the corresponding two-dimensional ferromagnetic Ising model, for which the order parameter does not conserve.

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