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Pair Correlation Function for Ising Spins with Competing Dynamics

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An interacting Ising spin system on a lattice with the competing influence of spin-flip (Glauber) and spin-exchange (Kawasaki) dynamics is studied. The exact nonequilibrium steady-state solution of the pair correlation function in one dimension is derived and compared with the simulation data. The two-dimensional solution, under some Ansatz, is also discussed.

KEY WORDS: Competing dynamics; nonequilibrium steady state; pair correlation function.

1. INTRODUCTION

I investigate a lattice spin model with two competing stochastic dynamics, which has recently been used by De Masi *et al.*[1] to derive a rigorous reaction-diffusion equation. Each dynamics is known to relax the spins into an equilibrium state of the Ising model corresponding to its own temperature (i.e., β^{-1} for the Glauber dynamics and ∞ for the Kawasaki dynamics), while the mixed dynamics will bring the system into a nonequilibrium stationary state. The study of stationary nonequilibrium microscopic states is a problem of great interest.[2] What we would like to know is how these states differ from the corresponding Gibbs states by turning on some nonequilibrium parameters.

Here I consider a simple lattice in d dimensions, $d = 1$ or 2, where at each site there is a spin $\sigma_x = \pm 1$, $\sigma = \{\sigma_x \mid x \in \mathbf{Z}^d\}$. The two mechanisms via which a configuration changes with time are: (i) the Glauber dynamics in which a spin flips at a site x, $\boldsymbol{\sigma} \to \boldsymbol{\sigma}^x$, with a rate $W(\sigma_x)$, and (ii) the

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Kawasaki dynamics, in which unequal nearest neighboring spins σ_x and $\sigma_{x'}$ exchange, $\sigma \to \sigma^{x,x'}$, with a constant rate.

In one dimension, I take the standard rate function[3]

$$W(\sigma_x) = \frac{1}{2}\left[1 - \frac{\gamma}{2}\sigma_x(\sigma_{x-1} + \sigma_{x+1})\right] \tag{1}$$

and in two dimensions, I take[4]

$$W(\sigma_x) = \frac{1}{2}\left[1 - \frac{\gamma_2}{4}\sum_{x'}\sigma_{x'} - \frac{\delta_2}{4}\sigma_x\left(\prod_{x'}\sigma_{x'}\right)\sum_{x'}\sigma_{x'}\right] \tag{2}$$

where the sum runs over the nearest neighbor sites of x; throughout this paper, I use x', y' to indicate the nearest neighbors of x, y, etc.

These rates satisfy detailed balance for the corresponding Gibbs states of the Ising model with the nearest neighbor interaction J at the reciprocal temperature β, provided one chooses

$$\gamma = t_1, \; \gamma_2 = \tfrac{1}{2}(t_2 + 2t_1), \qquad \delta_2 = \tfrac{1}{2}(t_2 - 2t_1) \tag{3}$$

with $t_m \equiv \tanh(2m\beta J)$.

The exchange process, on the other hand, being independent of the neighboring spin configuration, acts as if the system were at infinite temperature. The dynamics of the spin distribution function $P(\sigma, t)$ is described by a master equation of the form

$$\frac{d}{dt}P(\sigma, t) = \sum_x \left[W(-\sigma_x)\, P(\sigma^x, t) - W(\sigma_x)\, P(\sigma, t)\right]$$
$$+ \frac{\varepsilon}{4d}\sum_{\langle x,x'\rangle} V(\sigma_x, \sigma_{x'})[P(\sigma^{x,x'}, t) - P(\sigma, t)] \tag{4}$$

where

$$V(\sigma_x, \sigma_{x'}) = \tfrac{1}{2}(1 - \sigma_x\sigma_{x'}) \tag{5}$$

Notice that I have chosen a time scale such that ε is the only relevant parameter characterizing the ratio of the time scales of the two competing dynamics.

From (4), one obtains the "equation of motion" for the pair correlation function $R_{x,y} = \langle\sigma_x\sigma_y\rangle$, for $|x - y| > 1$,

$$\frac{d}{dt}R_{x,y} = -2\langle\sigma_x\sigma_y[W(\sigma_x) + W(\sigma_y)]\rangle$$
$$-\frac{\varepsilon}{4}\left\langle\sigma_x\sigma_y\left[\sum_{x'}V(\sigma_x, \sigma_{x'}) + \sum_{y'}V(\sigma_y, \sigma_{y'})\right]\right\rangle \tag{6}$$

2. DERIVATION OF THE ONE-DIMENSIONAL PAIR CORRELATION FUNCTION

In one dimension, (6) becomes

$$\frac{d}{dt} R_{x,y} = -2(1+\varepsilon) R_{x,y} + \frac{\gamma+\varepsilon}{2} (R_{x+1,y} + R_{x-1,y} + R_{x,y+1} + R_{x,y-1}) \tag{7}$$

which is true only for $|x-y|>1$. Due to the constraint $R_{x,x} \equiv 1$, the equation for $R_{x+1,x}$ is inhomogeneous,

$$\frac{d}{dt} R_{x+1,x} = -(2+\varepsilon) R_{x+1,x} + \frac{\gamma+\varepsilon}{2} (R_{x+2,x} + R_{x+1,x-1}) + \gamma \tag{8}$$

To find the stationary solution, one seeks a translation-invariant solution of the form

$$R_L \equiv R_{x+L,x} = A_1 \exp(-L/\xi) \tag{9}$$

By substituting (9) into (7), treating (8) as the boundary condition, one gets

$$\xi^{-1} = -\log \frac{1-(1-\Gamma^2)^{1/2}}{\Gamma} \tag{10}$$

and

$$A_1 = \frac{\gamma}{\gamma + \varepsilon[1-\exp(-1/\xi)]} \tag{11}$$

where

$$\Gamma \equiv \frac{\gamma+\varepsilon}{1+\varepsilon} \geqslant \gamma$$

In the limit $\varepsilon \to 0$, $\Gamma \to \gamma$, the correct equilibrium result $R_L = \tanh^L(\beta J)$ is recovered: while in the opposite limit $\varepsilon \to \infty$, which was considered in ref. 1, R_L becomes

$$R_L = [2\varepsilon(1-\gamma)]^{-1/2} \exp\{-[2(1-\gamma)/\varepsilon]^{1/2} L\} \tag{12}$$

This is in accord with the exact scaling behavior obtained in ref. 1 for the same limit.

Figure 1 is a plot of the exact solution (9) against the simulation data, which was done on a one-dimensional periodic chain with 100 lattice sites. The agreement is quite good.

3. DISCUSSION OF THE TWO-DIMENSIONAL PAIR CORRELATION FUNCTION

In two dimensions, the problem becomes much more involved due to multispin correlations. However, for high temperatures, one may neglect δ_2 in (2) and so render the problem trivial again.

Indeed, for $|x-y|>1$ one finds, by setting (6) to zero, that the stationary solution $R_{x,y}$ satisfies the following difference equation [assuming $x=(q_1, q_2)$, $y=(q_3, q_4)$ and denoting $E_1 R_{x,y} \equiv R_{(q_1+1, q_2), y}$, $E_3 R_{x,y} \equiv R_{x,(q_3+1, q_4)}$, etc.]:

$$2R_{x,y} - \frac{\Gamma_2}{4} \sum_{j=1} 4(E_j + E_j^{-1}) R_{x,y} = 0 \tag{13}$$

where $\Gamma_2 = (\gamma_2 + \varepsilon)/(1+\varepsilon)$. The form of (13) is reminiscent of random walks. Indeed, it is precisely that of a two-dimensional isotropic lattice walk with successive steps limited only to nearest neighboring sites. Its solution in that context is well known. I solve it by the lattice Green's

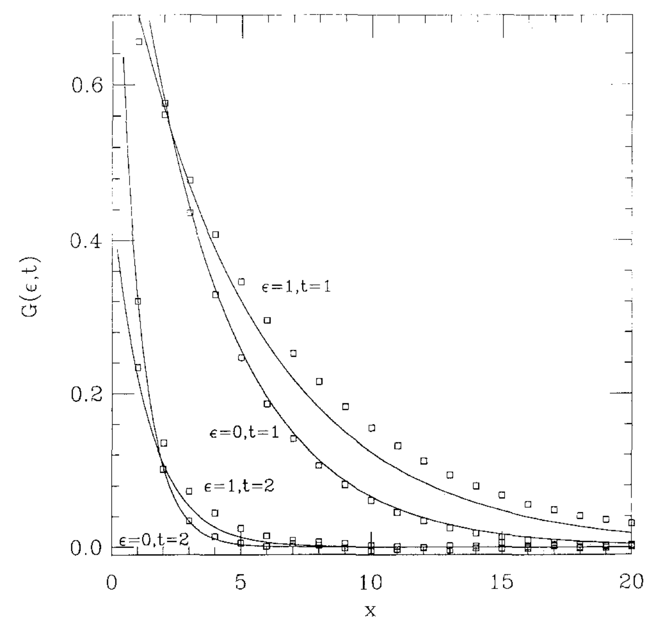

Fig. 1. One-dimensional pair correlation versus distance. The squares are the simulation data on a periodic chain with 100 lattice sites. $t \equiv kT/J$.

function techniques of Montroll.[4] It is easily verified that the solution can be written as $R_{x,y} = A_2 G(x-y)$ for $x \neq y$ with the lattice Green's function

$$G(r) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{\exp(ik \cdot r)}{2 - \Gamma_2(c_1 + c_2)} d^2k \qquad (14)$$
$$c_j = \cos k_j$$

Again A_2 has to be determined by requiring $R_{x,y}$ to satisfy the "boundary conditions," which can be found from (6) by setting $x = (1, 0)$, $y = 0$,

$$\begin{aligned} 0 = {} & \frac{\Gamma_2}{2} - \left(2 + \frac{3}{2}\varepsilon\right) R_{(1,0),0} \\ & + \frac{\gamma_2 + \varepsilon}{4} (R_{(2,0),0} + R_{(1,1),0} + R_{(1,-1),0} + R_{(1,0),(-1,0)} \\ & + R_{(1,0),(0,1)} + R_{(1,0),(0,-1)} \end{aligned} \qquad (15)$$

Solving (15) for A_2, one finds

$$A_2 = \frac{1}{1 + \varepsilon[G(0) - G(1)]/\Gamma_2} \qquad (16)$$

By making use of the identity

$$\frac{1}{z} = \int_0^\infty \exp(-zt)\, dt$$

one can rewrite G in the form

$$G(x = (n, m)) = \frac{1}{2} \int_0^\infty \mathbf{I}_n\left(\Gamma_2 \frac{t}{2}\right) \mathbf{I}_m\left(\Gamma_2 \frac{t}{2}\right) \exp(-t)\, dt \qquad (17)$$

where $\mathbf{I}_n(z)$ is the modified Bessel function of order n. Since $G(0) = (1/\pi)\, \mathbf{K}(\Gamma_2/2)$ with $\mathbf{K}(z)$ the elliptic function of the first kind, and

$$G(1) = \frac{G(0) - 1/2}{\Gamma_2} = \frac{\mathbf{K}(\Gamma_2/2) - 1/2}{\Gamma_2}$$

one may write A_2 more explicitly

$$A_2 = \frac{1}{1 + \varepsilon[1/2 - (1 - \Gamma_2)\, \mathbf{K}(\Gamma_2)(1/\pi)]/\Gamma_2^2} \qquad (18)$$

Once more, in the limit $\varepsilon \to 0$, one recovers the high-temperature solution of the Glauber dynamics, which is exactly the Onsager equilibrium result for small β.[5] In the other limit, $\varepsilon \to \infty$, one can see easily from Eq. (16) or Eq. (18) that $R(x)$ behaves like $\sim 1/\varepsilon$, which is the right scaling form in two dimensions.[1] It turns out that putting $\delta_2 = 0$ reduces the spin-flip dynamics defined by (2) for $\Gamma_2 < 1$ to a voter model with independent spin flips, a well-known stochastic dynamical model in the mathematical literature.[3]

If δ_2 cannot be neglected, one may rewrite the difference equation (6) (setting the right-hand side equal to zero) the following form (for the lattice spacing between x and $y \geqslant 2$):

$$R_{x,y}(\varepsilon) = \frac{\Gamma_2}{4} \sum_e R_{x+e,y}(\varepsilon) + \frac{\tilde{\Delta}_2}{4} \sum_e U_{x+e,y}(\varepsilon) \tag{19}$$

where $\tilde{\Delta}_2 \equiv \delta_2/(1+\varepsilon)$, e is a unit vector, and

$$U_{x+e,y} \equiv \left\langle \sigma_{x+e} \sigma_y \prod_{x'} \sigma_{x'} \right\rangle \tag{20}$$

Due to the identity $\sigma^2 = 1$, these U's contain the four-spin correlation functions. If one uses

$$\Gamma_2 = \frac{\tanh(4\bar{\beta}J) + 2\tanh(2\bar{\beta}J)}{2} \tag{21}$$

to define a new temperature variable $\bar{\beta}(\Gamma_2)$, and defines

$$\Delta_2 = \frac{\tanh(4\bar{\beta}J) - 2\tanh(2\bar{\beta}J)}{2} \tag{22}$$

then the corresponding equilibrium functions defined by

$$\chi_L(\Gamma_2) = R_L(0)|_{\gamma=\Gamma_2} \qquad \text{and} \qquad C_L(\Gamma_2) = U_L(0)|_{\gamma=\Gamma_2}$$

at the new temperature will surely satisfy

$$\chi_L(\Gamma_2) = \frac{\Gamma_2}{4} \sum_e \chi_{L+e}(\Gamma_2) + \frac{\Delta_2}{4} \sum_e C_{L+e}(\Gamma_2) \tag{23}$$

where L denotes the vector connecting a pair of lattice sites.

[3] It was kindly pointed out by C. Maes that it becomes a pure voter model if $\gamma_2 = 1$. It is known, for example, that in two dynamics there are just the two trivial stationary states[6] and I show here that this remains true even if the Kawasaki dynamics is added.

Now suppose one makes an Ansatz (see discussion below) that

$$R_L(\varepsilon) = A(\varepsilon)\,\chi_L(\Gamma_2) \qquad \text{and} \qquad U_L(\varepsilon) = B(\varepsilon)\,C_L(\Gamma_2) \tag{24}$$

Then from (19) and (23), one must have

$$B(\varepsilon) = \frac{\Delta_2}{\tilde{\Delta}_2} A(\varepsilon) \tag{25}$$

To determine $A(\varepsilon)$, one has to substitute (24) and (25) into the following boundary condition resulting from (6) for $|L| = 1$:

$$\left(1 + \frac{3\varepsilon}{4}\right) R_{(1,0)}(\varepsilon) = \frac{\Gamma_2 + \varepsilon}{4} \left[R_{(2,0)}(\varepsilon) + 2R_{(1,1)}(\varepsilon)\right] + \frac{\delta_2}{4} \sum_e U_{(1,0(+e}(\varepsilon) + \frac{\gamma_2}{2} \tag{26}$$

One finally obtains

$$A(\varepsilon) = \frac{\Gamma_2/(1+\varepsilon)}{\Gamma_2 - \varepsilon\chi_{(1,0)}(\Gamma_2) + (\Delta_2 - \tilde{\Delta}_2)(\Delta_2/\tilde{\Delta}_2) \sum_e C_{(1,0)+e}(\Gamma_2)} \tag{27}$$

Actually, the sum of the C's in the denominator can also be expressed entirely in terms of the χ's through Eq. (23).

4. SUMMARY

In summary, by virtue of the above analysis, one sees that the pair correlation function of the stationary state in some cases can be written as $R(x) = AG(x)$, where the β and ε appear in G only through a special combination in the single parameter $\Gamma(d) = [\gamma(d) + \varepsilon]/(1+\varepsilon)$ in dimension d. Therefore, one could say that the long-range behavior is qualitatively the same as the equilibrium Ising model but at some other effective temperature. In particular, the correlation length becomes $\xi(\Gamma)$ instead of $\xi(\gamma)$. Only the amplitude is modified by $A(\beta, \varepsilon)$, which is determined by the short-distance properties of the equilibrium pair correlations at the new effective temperature. Roughly speaking, the long-distance part G is dominated by the Glauber dynamics and the short-distance part A by the Kawasaki.

The result for one dimension is exact for arbitrary ε and β. On the other hand, how far one can extend the two-dimensional results is still unknown. The result for high temperature in two dimensions is valid to order β^2. The exact solution in 2D for arbitrary ε and β can only be found by solving the whole hierarchy of equations which couple all the multispin correlation functions. The solution obtained from the Ansatz (24) will presumably work at least for high temperatures or small ε. A recent 2D Monte Carlo renormalization group study indicated that the phase transition in the stationary state is indeed second order and belongs to the Ising universality class[8]; this seems to support the present results. But if one replaces the rate by the so-called Metropolis instead of Glauber for the "spin-flip" process, one finds a rather different picture. This was first done by computer simulation.[7] It was found that the stationary state undergoes a first-order transition if ε is large enough. This is interpreted in ref. 7 as a crossover from the standard equilibrium phase transition at $\varepsilon = 0$ to a first-order mean field type transition. The existence of a tricritical point (ε^*, β^*) was also confirmed later by Dickman,[9] who used a mean field treatment to show that $T_c(\varepsilon)$ is a decreasing function of ε and magnetization becomes unstable for large ε. Interestingly, there seems to be no crossover for the Glauber rate. Here, only in one dimension is the effective temperature a decreasing function of ε (since $\gamma < 1$, Γ is always $> \gamma$); in two dimensions, since γ_2 in (3) is not necessarily < 1, the effective temperature may or may not be lower than β^{-1}. In fact, when β^{-1} is of the order of the Onsager temperature, γ_2 is actually > 1; therefore, $\Gamma_2 < \gamma_2$, and $\bar{\beta}(\varepsilon) > \beta$. This is also confirmed by the computer simulations.[8]

A more challenging question is whether, in light of Felderhof's work,[10] one could directly diagonalize the master operator and solve the probability distribution $P(\sigma, t)$ exactly. I have tried without success, the major obstacle being the non-Hermiticity of the corresponding evolution operator. As a final remark, I would like to bring to the reader's attention the "discontinuity" of the amplitude at zero distance,

$$R_{x,x} \equiv 1 \geqslant AG(0) = A \qquad \text{for} \quad \varepsilon \neq 0$$

which is caused by a δ potential imposed by the boundary conditions for nonzero ε. This inhomogeneity due to the exclussion effect of the Kawasaki dynamics constitutes the major difficulty in the investigation of the multispin correlation functions.

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