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Diffusion-Annihilation and the Kinetics of the Ising Model in One Dimension

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The relationship between the one-dimensional kinetic Ising model at zero temperature and diffusion-annihilation in one dimension is studied. Explicit asymptotic results for the average domain size, average magnetization squared, and pair-correlation function are derived for the Ising model, for arbitrary initial magnetization. For the case of zero initial magnetization ($m_0 = 0$), a number of recent exact results for diffusion-annihilation with random initial conditions are obtained. However, for the case m_0 not equal to zero, the asymptotic behavior turns out to be different from diffusion-annihilation with random initial conditions and at a finite density. In addition, in contrast to the case of diffusion-annihilation, the domain-size distribution scaling function $h(x)$ is found to depend nontrivially on the initial magnetization. The origin of these differences is clarified and the existence of nontrivial correlations in the initial wall distribution for finite initial magnetization is found to be responsible for these differences. Results of Monte Carlo simulations for the domain size distribution function for different initial magnetizations are also presented.

KEY WORDS: Diffusion-annihilation; Ising model; kinetics.

1. INTRODUCTION

George Weiss has worked on so many different problems that it is not easy to give a presentation about something that he has not studied before. The one problem that we believe George has not worked in is the Ising model. But the problem is how to connect it to the problems that George is interested in. It turns out that there is a close connection between the kinetics of the one-dimensional Ising model and nonclassical kinetics

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This paper is dedicated to George Weiss on the occasion of his 60th birthday.

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occurring in aggregation and annihilation of diffusing particles—a problem associated with random walks in which George has made significant contributions.

The kinetics of diffusion-controlled annihilation in one dimension has been of interest for some time in the context of particle–antiparticle annihilation,[1] binary reactions in one dimension,[2] and exciton fusion kinetics[3] in low-dimensional media. While the exponent ($t^{-1/2}$) characterizing the decay of the particle density in one dimension is well known[1,2] and an asymptotic solution has been given for an initial Poisson distribution in the continuum case,[2] only recently (for certain initial conditions) have explicit solutions been given for diffusion-annihilation on a lattice.[4,5] Because of the equivalence between domain walls in the Ising model and particles in diffusion-annihilation, it has been assumed[5] that there exists an exact duality between the one-dimensional Ising model at zero temperature and diffusion-annihilation. In particular, Rácz has used this analogy to study the kinetics of diffusion-annihilation in the presence of sources.[6] However, until recently,[7] no detailed comparison between the kinetics of the Ising model and diffusion-annihilation in one dimension had been made.

In this paper, we derive exact asymptotic expressions for the average domain size, wall density, and pair-correlation function as a function of the initial magnetization m_0 of the Ising model at zero temperature. Our results are then analyzed in terms of the relationship between the Ising model and diffusion-annihilation. If we interpret the presence of a domain wall (up spin followed by a down spin or vice versa) in the Ising model as equivalent to a particle in diffusion-annihilation, then our results for the wall density turn out to be *identical* to known results[4,5] for the particle density in diffusion-annihilation for the case $m_0 = 0$. However, somewhat surprisingly, for general values of m_0 they appear to differ. In particular, for an initial random distribution with $m_0 \neq 0$, we find that the asymptotic coefficient of $t^{-1/2}$ for the wall (particle) density depends on m_0, in contrast to what is expected for diffusion-annihilation.

Monte Carlo simulation results for the domain size distribution function as a function of m_0 are also presented. Again, there is agreement for the case $m_0 = 0$, while for $m_0 \neq 0$ the domain size distribution function depends on m_0, in contrast to what is expected for the case of diffusion-annihilation. In addition, we study the small-x behavior of the domain size (interparticle) distribution scaling function $h(x)$ as a function of m_0 and show, for both the case of the Ising model and diffusion-annihilation, that the exponent τ is equal to 1.

Finally, we extend our previous work[7] and discuss more fully the connection between the Ising model and diffusion-annihilation. In particular, we explain why for $m_0 \neq 0$, our results *appear* to be different from the known results for diffusion-annihilation. The reason turns out to be that the asymptotic behavior in diffusion-annihilation is sensitive to subtle correlations in the initial conditions, which occur for $m_0 \neq 0$. We also compare our results with a recent formula derived by Balding *et al.*[8] and thus show explicitly that the duality between the zero-temperature Ising model and diffusion-annihilation is exact.

The organization of this paper is as follows. In Section 2, we review the general solution of the kinetic Ising model. Our analytical results at zero temperature are presented in Section 3, and compared with results for diffusion-annihilation. In Section 4, Monte Carlo simulation results for the domain size are compared with the asymptotic predictions and we also study the scaling of the domain size distribution and compare it with results for diffusion-annihilation. In Section 5, we discuss the effects of correlations in the initial state on the asymptotic behavior of the wall/particle density. Finally, in Section 6 we discuss in more detail the relation between diffusion-annihilation and the Ising model and give a summary of our results.

2. ISING DYNAMICS IN ONE DIMENSION

The one-dimensional kinetic Ising model consists of a lattice of spins $s_i = \pm 1$, which interact ferromagnetically with their nearest neighbors. The Hamiltonian for this model (for a chain of length N) is

$$H = -J \sum_{i=1}^{N} s_i s_{i+1} \tag{1}$$

The master equation describing the time evolution of the spin configurations is

$$\begin{aligned} dp(s_1, s_2, ..., s_N, t)/dt = & -\sum_i w(s_i)\, p(s_1, s_2, ..., s_i, ..., s_N, t) \\ & + \sum_i w(-s_i)\, p(s_1, s_2, ..., -s_i, ..., s_N, t) \end{aligned} \tag{2}$$

where $p(s_1, s_2, ..., s_N, t)$ is the probability of configuration $\{s_1, s_2, ..., s_N\}$ at time t and $w(s_i)$—the probability per unit time that a given spin s_i will change sign—satisfies the Maxwell–Boltzmann distribution:

$$w(s_i)/w(-s_i) = [1 - \tfrac{1}{2}\gamma s_i(s_{i+1} + s_{i-1})]/[1 + \tfrac{1}{2}\gamma s_i(s_{i+1} + s_{i-1})] \tag{3}$$

where $\gamma = \tanh(2J/k_B T)$. Assuming $w(s_i)$ of the form

$$w(s_i) = \tfrac{1}{2}[1 - \tfrac{1}{2}\gamma s_i(s_{i+1} + s_{i-1})] \tag{4}$$

Glauber[9] studied the dynamics of the Ising model and was able to write an equation for the expectation value of the spin–spin pair-correlation function $G(k, t) = \langle s_0(t)\, s_k(t)\rangle$ which, when averaged translationally, becomes for $k > 0$

$$\frac{dG(k, t)}{dt} = -2G(k, t) + \gamma[G(k-1, t) + G(k+1, t)] \tag{5}$$

The exact solution to this equation has been given by Glauber[9] as

$$G(k, t) = \eta^k + e^{-2t} \sum_{m=1}^{\infty} [G(m, 0) - \eta^m][I_{k-m}(2\gamma t) - I_{k+m}(2\gamma t)] \tag{6}$$

where $\eta = \tanh(J/k_B T)$ and $I_n(x)$ is the modified Bessel function of the first kind. For large x, $I_n(x)$ has the asymptotic expansion[10]

$$I_n(x) = \frac{e^x}{(2\pi x)^{1/2}} \left\{1 + \sum_{s=1}^{\infty} \frac{(-1)^s \prod_{j=1}^{s} [\mu - (2j-1)^2]}{s!\,(8x)^s}\right\} \tag{7}$$

where $\mu = 4n^2$. For $T > 0$, γ is less than 1 and $G(k, t)$ decays exponentially to its equilibrium value η^k.

The equation for the expectation value of each spin $\langle s_k(t)\rangle$ has also been given by Glauber[9] as follows:

$$\frac{d\langle s_k(t)\rangle}{dt} = -\langle s_k(t)\rangle + \frac{1}{2}\gamma[\langle s_{k-1}(t)\rangle + \langle s_{k+1}(t)\rangle] \tag{8}$$

The solution of this equation is

$$\langle s_k(t)\rangle = e^{-t} \sum_{m=-\infty}^{\infty} \langle s_m(0)\rangle\, I_{k-m}(\gamma t) \tag{9}$$

If we define $m(t) = (1/N) \sum_{k=1}^{N} \langle s_k(t)\rangle$ and sum Eq. (8) over k (subscripts are modulo N), Eq. (8) becomes

$$\frac{dm(t)}{dt} = -(1-\gamma)\, m(t) \tag{10}$$

or $m(t) = e^{-(1-\gamma)t} m_0$. For $T = 0$, $\gamma = 1$, we get the somewhat surprising result: $m(t) = m_0 = \textit{constant}$.

3. RELATIONSHIP TO DIFFUSION-ANNIHILATION

At $T=0$, $\gamma=\eta=1$, and Eq. (4) becomes

$$w(s_i)=1-(1/2)[\delta(s_i, s_{i-1})+\delta(s_i, s_{i+1})] \tag{11}$$

Equation (11) implies that a spin which has one nearest neighbor of the same sign and another of the opposite sign (i.e., a domain wall) has a probability of 1/2 of changing sign (domain wall diffusion), while a spin whose nearest neighbors are both of the opposite sign (two domain walls) will change sign with probability one, eliminating both walls (wall–wall annihilation). Thus, at zero temperature the Ising problem appears to be equivalent to the problem of annihilation-diffusion of particles/walls.

Similarly, at $T=0$, Eq. (6) becomes

$$G(k, t)=1+e^{-2t}\sum_{m=1}^{\infty}[G(m, 0)-1][I_{k-m}(2t)-I_{k+m}(2t)] \tag{12}$$

For a random initial state with magnetization $\langle s\rangle=m_0$, and $G(k, 0)=m_0^2$ for $k\neq 0$, this equation reduces to

$$G(k, t)=1-e^{-2t}\sum_{m=1}^{\infty}(1-m_0^2)[I_{k-m}(2t)-I_{k+m}(2t)] \tag{13}$$

Keeping in mind that $I_n(x)=I_{-n}(x)$ for n integer, $x>0$, this infinite series can be rearranged to obtain

$$G(1, t)=1-e^{-2t}(1-m_0^2)[I_0(2t)+I_1(2t)] \tag{14a}$$

$$G(k, t)=1-e^{-2t}(1-m_0^2)\left[I_0(2t)+I_1(2t)+2\sum_{m=1}^{k-1}I_m(2t)\right] \quad \text{for} \quad k>1 \tag{14b}$$

Thus, the average wall density $n(t)=[1-G(1, t)]/2$, which is equivalent to the particle density in the diffusion-annihilation problem, is

$$n(t)=\frac{1-m_0^2}{2}e^{-2t}[I_0(2t)+I_1(2t)] \tag{15}$$

where $n_0=n(0)=(1-m_0^2)/2$.

For an initial random configuration with $m_0=0$, for which $n_0=1/2$, Eq. (15) is *identical* to the following expression, which was recently derived[5] for one-dimensional diffusion-annihilation on a lattice for the time-dependent concentration of particles $c(t)$ with initial concentration 1/2 and with an initial random distribution:

$$c(t) = (1/2)\exp(-4Dt)[I_0(4Dt) + I_1(4Dt)] \tag{16}$$

if one assumes $D = 1/2$.[2]

Substituting the asymptotic expansion (7) into Eq. (15) yields

$$n(t) = \frac{1 - m_0^2}{2\sqrt{\pi}} t^{-1/2} + O(t^{-3/2}) \tag{17}$$

Thus, the average domain size $L(t) = 1/n(t)$ varies asymptotically as

$$L(t) = \frac{2\sqrt{\pi}}{1 - m_0^2} t^{1/2} \tag{18}$$

Equations (17) and (18) hold in general, if one assumes an initial configuration such that $G(k, 0) = m_0^2 + \xi(k)$ for $k \neq 0$ where $\xi(k) \to 0$ as $k \to \infty$. Thus, the asymptotic expression for domain size depends *only* on the initial

[2] This is clearly reasonable, since the probability per unit time for an isolated domain wall to "diffuse" a distance of one lattice spacing is 1/2, according to Eq. (4).

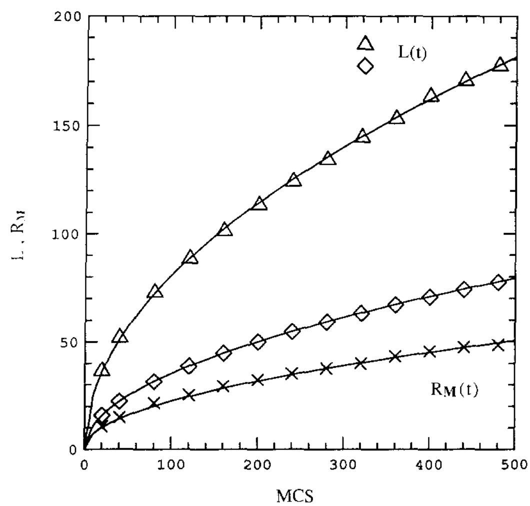

Fig. 1. Comparison of asymptotic predictions for domain size (solid lines) with simulation results (symbols). Top and middle curves correspond to average domain size $L(t)$ with $m_0 = 0.75$ and $m_0 = 0$, respectively. Bottom curve corresponds to another measure of domain size—the mean square magnetization $R_M(t)$—averaged over many runs with $\langle m_0 \rangle = 0$.

magnetization m_0 (assuming no other long-range order at $t=0$) and not on the short-range order of the initial spin distribution.

For an initial nonrandom, antiferromagnetic configuration such that $G(k, 0) = (-1)^k$ (corresponding to a full lattice of walls), Eq. (12) implies

$$n(t) = \exp(-2t)\, I_0(2t) \tag{19}$$

This result agrees with the exact result $c(t) = \exp(-4Dt)\, I_0(4Dt)$ derived by Lushnikov[4] for diffusion-annihilation with an initially full lattice, if one again assumes $D = 1/2$. Thus, for the case $m_0 = 0$, we recover the two known[4,5] exact results for diffusion-annihilation on a lattice.

Using Eq. (14), we have also calculated the asymptotic scaling form of the pair correlation function $G(k, t)$ in the limit $t, k \to \infty$ with $k/\sqrt{t}$ finite. If we insert the asymptotic expansion (7) into (14b), keeping in mind that $\sum_{m=1}^{k-1} m^{2n} = k^{2n+1}/(2n+1) + O(k^{2n})$, we obtain

$$G(k, t) = 1 - \frac{1-m_0^2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n k^{2n+1}}{(2n+1)\, n!\, 2^{2n} t^{n+1/2}} + O(t^{-1/2}) \tag{20}$$

In terms of the scaled variable $z = k/\sqrt{t}$, this may be rewritten as

$$G(k, t) = g(z) = 1 - \frac{1-m_0^2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)\, n!\, 2^{2n}} + O(t^{-1/2}) \tag{21}$$

On inspection this may be seen to be equal to

$$g(z) = 1 - (1-m_0^2) \operatorname{erf}(z/2) = (1-m_0^2) \operatorname{erfc}(z/2) + m_0^2 \tag{22}$$

where $\operatorname{erf}(z) = (2/\sqrt{\pi}) \int_0^z du\, e^{-u^2}$. We note that at $T=0$ ($\gamma = 1$), Eq. (5) for $G(k, t)$ is the discrete version of a one-dimensional diffusion equation $\partial G(x, t)/\partial t = \partial^2 G(x, t)/\partial x^2$. The exact solution of this equation, with boundary conditions $G(0, t) = 1$ and $G(x, 0) = m_0^2$ for $x \neq 0$, is

$$G(x, t) = 1 - (1-m_0^2) \operatorname{erf}(x/2\sqrt{t}) = 1 - (1-m_0^2) \operatorname{erf}(z/2)$$

if one identifies $x/\sqrt{t}$ as z. Thus, the asymptotic result for $g(z)$ is the same as in the continuum approximation. We note, as before, that Eq. (22) holds for an arbitrary initial configuration with $G(k, 0) = m_0^2 + \xi(k)$ with $\xi(k)$ going to 0 as $k \to \infty$.

4. MONTE CARLO SIMULATIONS

In order to test the convergence to asymptotic behavior, we have conducted Monte Carlo simulations (on a lattice of size $N = 128{,}000$) for several values of m_0 with initial random configurations. We found that our results[7] for $L(t)$ versus time (Monte Carlo steps) from Monte Carlo simulations with $m_0=0$ and $m_0=0.75$ were in excellent agreement with (17) after only a few Monte Carlo steps (MCS). Similar good agreement with Eq. (22) for the pair-correlation function $g(z)$ was also found after only a few MCS.

We have also studied the asymptotic distribution of domain sizes $N(k, t)$, where $N(k, t)$ is the density of domains of size k at time t. This is equivalent to the interparticle distribution function in the case of diffusion-annihilation. If one defines $\rho(k, t)=N(k, t)/n(t)$ as the fraction of domains of size k at time t, and assumes scaling with the average domain size $L(t)$, one obtains

$$h(x)=\rho(k, t)\, L(t) \tag{23}$$

where $x=k/L(t)$, $L(t)=[2\pi^{1/2}/(1-m_0^2)]\, t^{1/2}$, and $h(x)$ is a scaling function satisfying $\int_0^\infty dx\, h(x)=1$. Figure 2 shows a plot of the scaling function $h(x)$, obtained from Monte Carlo simulations, for two different values of the initial magnetization m_0. We note that the scaling function $h(x)$ for $m_0=0$ has a peak near $x=1/2$ rather than at $x=1$. The scaling function for $m_0=0.75$ has a peak which is higher and narrower than that for $m_0=0$

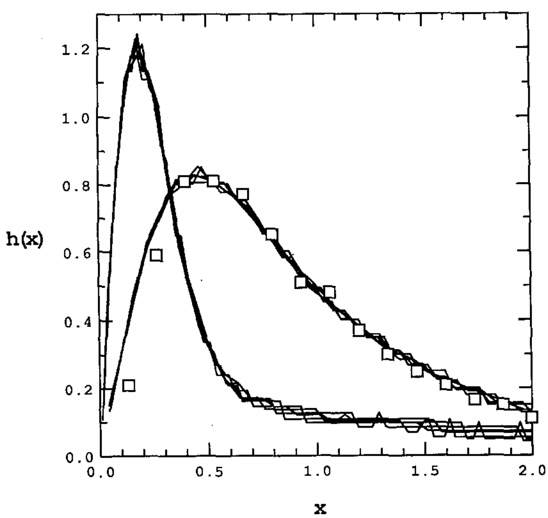

Fig. 2. Domain size distribution scaling function $h(x)$ for $m_0=0$ (lower solid curves) and $m_0=0.75$ (upper solid curves) from Monte Carlo simulations. Data shown are for increments of 20 MCS up to 100 MCS. (The scaling function for $m_0=0.75$ has been reduced by a factor of 2/3 for clarity.) Squares show data from simulations of diffusion-annihilation.[11]

and its location is at a smaller value of x. Thus, the scaling function $h(x)$ is seen to depend nontrivially on the initial magnetization m_0, unlike what is expected in the case of diffusion-annihilation. We note, however, that for $m_0 = 0$, our numerical results for the domain distribution scaling function for the Ising model are almost identical to numerical results obtained by Doering and ben-Avraham[11] for the interparticle distribution scaling function for one-dimensional diffusion-annihilation.

We have also studied the small-x behavior of $h(x)$ as a function of m_0. If one assumes that $h(x) \sim x^{\tau}$ as x goes to 0, then one expects $N(k, t) \sim \rho(k, t)\, t^{-1/2} \sim t^{-(1+\tau/2)}$. Analysis of data for late times indicates that $N(k, t) \sim t^{-3/2}$, i.e., $\tau = 1$. We note that this same behavior ($\tau = 1$) has been seen in simulations of coagulation in one dimension[12] (for the behavior of the number of clusters of size k) and has been obtained in a recent paper[11] on the interparticle distribution function for the one-dimensional irreversible one-species coagulation model $A + A \rightarrow A$.

We now derive the small-x behavior of $h(x)$ as a function of m_0 and the exponent τ as follows. If we define the wall density at site i as

$$w_i = (1/2)(s_i - s_{i+1}) \tag{24}$$

then $w_i = 1$ corresponds to a $+|-$ wall, $w_i = -1$ to a $-|+$ wall, and $w_i = 0$ to no wall. We may then in general calculate the (signed) wall correlation function[3]

$$\langle w_0 w_x \rangle = (1/4)[2G(x, t) - G(x-1, t) - G(x+1, t)] \tag{25}$$

In particular,

$$N(1, t) = -\langle w_0 w_1 \rangle = -(1/4)[2G(1, t) - G(2, t) - 1]$$

Substituting the asymptotic form for $G(k, t)$, we obtain

$$N(1, t) = \frac{1 - m_0^2}{8\sqrt{\pi}}\, t^{-3/2} + O(t^{-5/2}) \tag{26}$$

for the density of domains of size one. Thus, $\rho(1, t) = N(1, t)/n(t) = 1/(4t)$ and $h(x) \rightarrow \pi x/(1 - m_0^2)^2$ as x goes to zero. Good agreement with this form in the limit of small x is found from our simulations for both values of m_0 (see Fig. 2). Thus, we have shown explicitly that $\tau = 1$, and for small x, found the dependence of $h(x)$ on m_0.

[3] We note that we may, in general, write the following expression for the domain distribution function: $N(k, t) = (-1)^k \langle w_0 \prod_{i=1}^{k-1} (1 - w_i)\, w_k \rangle$. Evaluation of this expression requires the evaluation of spin-correlation functions of orders 1 to $k + 1$.

5. EFFECT OF INITIAL CORRELATIONS

We note that, in contrast to the case of one-dimensional diffusion-annihilation with an initially random distribution of particles, for which the asymptotic form[1,2] for the density of particles $n(t)=(8\pi Dt)^{-1/2}$ is *independent* of the initial density of particles/walls, Eq. (17) *depends* on the initial wall density (magnetization). However, as already pointed out, for the case $m_0=0$ ($n_0=1/2$, $D=1/2$), we recovered two recent results[4,5] for diffusion-annihilation on a lattice. Similarly, our numerical results for the domain size distribution scaling function $h(x)$ were in excellent agreement for $m_0=0$ with simulation results[11] for the interparticle distribution scaling function in the case of diffusion-annihilation.

We now address the question of the apparent discrepancy with the known results for diffusion-annihilation for $m_0 \neq 0$. Previously, we had thought that this discrepancy might be due to a subtle difference in the dynamics of annihilation in the two models. It turns out, however, that it is not due to any lack of duality between the two models, but rather to subtle correlations in the initial distribution of walls at $t=0$ which occur for $m_0 \neq 0$.

In particular, if we consider an initial random Ising spin configuration with magnetization m_0, the probability for a spin to be "up" is $p=(1+m_0)/2$, while the probability for a spin to be "down" is $1-p=(1-m_0)/2$. The probability of a wall then is $P_W=2p(1-p)$ ($=1/2$ for $m_0=0$). Thus, for an initial random spin configuration with $m_0=0$, which corresponds to an initial wall density of 1/2, the corresponding initial distribution of walls/particles is also random and it is not surprising that exact agreement is found with the known asymptotic results for diffusion-annihilation.

However, for $m_0 \neq 0$, the initial distribution of walls turns out to be correlated. This may be seen by considering the probability P_2 of two consecutive walls in the initial configuration. If the walls are randomly distributed with probability $P_W=2p(1-p)$ (as above), then $P_2=4p^2(1-p)^2$. However, for a spin system with initial magnetization $m_0=2p-1$, the probability P'_2 of two consecutive walls equals the probability of either a $(-+-)$ or a $(+-+)$ configuration, so $P'_2=p^2(1-p)+(1-p)^2 p=p(1-p)$. Except for the case $m_0=0$ ($p=1/2$), P'_2 is not equal to P_2, and thus for $m_0 \neq 0$, the wall distributions are correlated in the initial configuration. These initial correlations are long-ranged enough so that both the asymptotic scaling function $h(x)$ and the asymptotic coefficient of $t^{-1/2}$ depend on m_0. Thus, the asymptotic behavior of the diffusion-annihilation problem in one dimension turns out to be remarkably sensitive to the initial conditions.

6. CONCLUSION

We have already noted the equivalence between a domain wall in the Ising model at zero temperature and a particle in diffusion-annihilation. The existence of an *exact* duality between the zero-temperature Ising model and diffusion-annihilation may be shown by comparing our results with recent results obtained by Balding, Clifford, and Green (BCG)[8] for diffusion-annihilation with a continuous-time random walk on a lattice. For diffusion-annihilation, BCG obtained [$D=1/2$, see Eqs. (1) and (2) of ref. 8]

$$n(t)=\sum_{m=1}^{\infty} e^{-2t}O_m(0)[I_{m-1}(2t)-I_{m+1}(2t)] \tag{27}$$

where $n(t)$ is the particle density at time t, and $O_m(0)$ is the probability that initially an interval of m sites contains an *odd* number of particles. We note that for an initially random distribution of particles with density p, one has[8] $O_m(0)=[1-(1-2p)^m]/2$, so that, rearranging Eq. (27) and inserting the asymptotic expansion (7), one obtains $n(t)=(4\pi t)^{-1/2}+O(t^{-3/2})$, independent of p, as expected.

Recalling that $n(t)=[1-G(1,t)]/2$, and noting that for the Ising model, $O_m(t)=[1-G(m,t)]/2$ [where $O_m(t)$ refers to an odd number of domain walls], we see that Eq. (12) is equivalent to Eq. (27) above, further supporting the exact duality between the two models. More generally, Eq. (12) also implies

$$O_k(t)=\sum_{m=1}^{\infty} e^{-2t}O_m(0)[I_{k-m}(2t)-I_{k+m}(2t)] \tag{28}$$

which is, as far as we know, a new result. This result may be useful in studying the interparticle distribution function $h(x)$ for diffusion-annihilation as a function of initial conditions.

In conclusion, we have derived exact results for the zero-temperature, one-dimensional Ising model, which we have used to study the relationship between the kinetics of the Ising model and diffusion-annihilation. In particular, a number of recently obtained exact results for diffusion-annihilation were recovered. We have also conducted Monte Carlo simulations and found good agreement at early time with our asymptotic results. In addition, we have clarified the connection between the zero-temperature Ising model and diffusion-annihilation by showing explicitly an exact equivalence between the two models. Finally, we have pointed out the important role of initial correlations in determining the asymptotic dynamics and form of the asymptotic distribution functions.

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