Diffusion annihilation in one dimension and kinetics of the Ising model at zero temperature

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(Received 29 March 1989)

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. These results are compared with known results for diffusion annihilation, and it is shown that there is only partial equivalence between the Ising model and diffusion annihilation. The results of Monte Carlo simulations for the domain-size distribution function for different initial magnetizations are also presented. 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 exponent τ characterizing the small-x behavior of $h(x)$ is determined exactly and is shown rigorously to be the same for both the Ising model and diffusion annihilation.

I. INTRODUCTION

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 characterizing the decay of the particle density in one dimension is well known[1,2] and an exact solution has been given for an initial Poisson distribution in the continuum case,[2] only recently have explicit solutions (for certain initial conditions) 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, no direct comparison between the kinetics of the Ising model and diffusion annihilation in one dimension has been made.

In this paper we derive exact asymptotic expressions for the average domain size, wall density, and pair-correlation function for the one-dimensional kinetic Ising model at zero temperature, as a function of the initial magnetization (m_0). Our results turn out to be identical to known results[4,5] for diffusion annihilation in the case $m_0=0$. However, for general values of m_0 they differ. Monte Carlo simulation results for the domain-wall distribution function as a function of m_0 are also presented. Again, there is agreement for the case $m_0=0$, while for $m_0\neq0$ our results depend on m_0, in contrast to what is expected for the case of diffusion annihilation. This demonstrates that the duality between the kinetic Ising model and diffusion annihilation is only partial. Finally, we study the small-x behavior of the domain-size 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.

The organization of this paper is as follows: In Sec. II we review the general solution of the kinetic Ising model. Our analytical results at zero temperature are presented in Sec. III and compared with results for diffusion annihilation. In Sec. IV Monte Carlo simulation results for the domain size are compared with the asymptotic predictions. In Sec. V we study the scaling of the domain-size distribution and compare it with results for diffusion annihilation. A summary of the results and a discussion are given in Sec. VI.

II. MODEL AND GENERAL SOLUTION

The one-dimensional kinetic Ising model consists of a lattice of spins $s_i=\pm1$, which interact ferromagnetically with their nearest neighbors. The Hamiltonian for this model (for a chain of length N) is

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

while the master equation is

$$\frac{dp(s_1,s_2,\ldots,s_N,t)}{dt} = -\sum_i w(s_i)p(s_1,s_2,\ldots s_i \ldots,s_N,t) + \sum_i w(-s_i)p(s_1,s_2,\ldots -s_i \ldots s_N,t) , \tag{2}$$

where $p(s_1,s_2,\ldots,s_N,t)$ is the probability of configuration $\{s_1,s_2,\ldots,s_N\}$ 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:

$$w(s_i)/w(-s_i)=\frac{1-\frac{1}{2}\gamma s_i(s_{i+1}+s_{i-1})}{1+\frac{1}{2}\gamma s_i(s_{i+1}+s_{i-1})} , \tag{3}$$

where $\gamma=\tanh(2J/k_BT)$. 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[7] 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 $k>0$,

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

The exact solution to this equation has been given by Glauber[7] as

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

where $\eta=\tanh(J/k_BT)$ and $I_n(x)$ is the modified Bessel function of the first kind. For large x, $I_n(x)$ has the asymptotic expansion[8]

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

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[7] as follows:

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

The solution of this equation is

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

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

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

or $m(t)=e^{-(1-\gamma)t}m_0$. For $T=0$, $\gamma=1$, we get the somewhat surprising result:[9] $m(t)=m_0=\text{const}$.

III. SOLUTION AT ZERO TEMPERATURE

At $T=0$, $\gamma=\eta=1$ and Eq. (6) becomes

$$G(k,t)=1+e^{-2t}\sum_{m=1}^{\infty}[G(m,0)-1]\times[I_{k-m}(2t)-I_{k+m}(2t)] . \quad (11)$$

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

$$G(k,t)=1-e^{-2t}\sum_{m=1}^{\infty}(1-m_0^2)\times[I_{k-m}(2t)-I_{k+m}(2t)] . \quad (12)$$

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

$$G(1,t)=1-e^{-2t}(1-m_0^2)[I_0(2t)+I_1(2t)] , \quad (13a)$$

$$G(k,t)=1-e^{-2t}(1-m_0^2)\left[I_0(2t)+I_1(2t)+2\sum_{m=1}^{k-1}I_m(2t)\right] \quad \text{for } k>1 . \quad (13b)$$

Thus, the average wall density $n(t)=[1-G(1,t)]/2$ is

$$n(t)=\frac{(1-m_0^2)}{2}e^{-2t}[I_0(2t)+I_1(2t)] , \quad (14)$$

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

It is interesting to note that for an initial random configuration with $m_0=0$, for which $n_0=\frac{1}{2}$, Eq. (14) 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 $\frac{1}{2}$ and with an initial random distribution

$$c(t)=(\tfrac{1}{2})\exp(-4Dt)[I_0(4Dt)+I_1(4Dt)] , \quad (15)$$

if one assumes $D=\frac{1}{2}$.[10]

Substituting the asymptotic expansion Eq. (7) into Eq. (14) yields

$$n(t)=\frac{1-m_0^2}{2\sqrt{\pi}}t^{-1/2}+O(t^{-3/2}) . \quad (16)$$

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

$$L(t)=\frac{2\sqrt{\pi}}{1-m_0^2}t^{1/2} . \quad (17)$$

Equations (16) and (17) 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 $k\to\infty$. (This is because, as one may see by substituting the asymptotic expansion (7) into the sum $e^{-2t}\sum_{m=1}^{\infty}\xi(m)[I_{k-m}(2t)-I_{k+m}(2t)]$, terms of order $O(t^{-1/2})$ cancel.) Thus, the asymptotic expression for domain size depends *only* on the initial magnetization m_0 (assuming no other long-range order at $t=0$) and not on the short-range order of the initial spin distribution.

We note that, in contrast to the case of one-dimensional diffusion annihilation, 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, (16) *depends* on the initial wall density (magnetization). However, as already pointed out, in the case $m_0=0$ ($n_0=\frac{1}{2}$, $D=\frac{1}{2}$), the two results agree. Thus, for the case $m_0=0$ our results appear to be equivalent to those obtained for diffusion annihilation, while for $m_0 \neq 0$ they are not.

It is interesting to note that for an initial nonrandom, antiferromagnetic configuration such that $G(k,0) = (-1)^k$ (corresponding to a full lattice of walls), Eq. (11) implies

$$n(t) = \exp(-2t) I_0(2t) . \tag{18}$$

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 $D=\frac{1}{2}$. Thus, for the case $m_0=0$, we recover the two known[4,5] exact results for diffusion annihilation on a lattice.

Using Eq. (13) we may also calculate 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 (13b), keeping in mind that $\sum_{m=1}^{k-1} m^{2n} = k^{2n+1}/(2n+1) + O(k^{2n})$, we obtain

$$G(k,t) = 1 - \frac{1-m_0^2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n k^{2n+1}}{(2n+1) n! 2^{2n} t^{n+1/2}} + O(t^{-1/2}) . \tag{19}$$

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

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

On inspection this may be seen to be equal to

$$\begin{aligned} g(z) &= 1 - (1-m_0^2)\operatorname{erf}(z/2) \\ &= (1-m_0^2)\operatorname{erfc}(z/2) + m_0^2 , \end{aligned} \tag{21}$$

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. (21) holds for an arbitrary initial configuration with $G(k,0) = m_0^2 + \xi(k)$ with $\xi(k)$ going to zero as $k \to \infty$.

IV. MONTE CARLO SIMULATIONS

In order to study the approach to the 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. Figure 1 shows plots of $L(t)$ versus time (Monte Carlo steps) from Monte Carlo simulations with $m_0=0$ and $m_0=0.75$. We see that after only a few Monte Carlo steps (MCS) there is good agreement with Eq. (17).

Figure 2 shows the scaled pair-correlation function $g(z)$ along with the asymptotic result [Eq. (21)] for an initial random configuration ($m_0=0$). Again after a short time there is very good agreement between our simulation results and the asymptotic results.

We have also looked at another measure of domain size, $R_M(t)$, corresponding to the mean-square magnetization, where

$$R_M(t) = N[\langle m^2(t) \rangle - \langle m(t) \rangle^2] . \tag{22}$$

This measure of domain size is not self-averaging,[11] i.e., the error in $R_m(t)$ does not depend on system size and depends only on the number of independent runs. Thus, the brackets in Eq. (22) correspond to an average over a large number of runs. Recalling that $\langle m(t) \rangle = m_0$, and the fluctuation-susceptibility relation, we obtain in the asymptotic limit,

$$\begin{aligned} R_M(t) &= \int_{-\infty}^{\infty} [G(x,t) - m_0^2] dx \\ &= (1-m_0^2)\sqrt{t} \int_{-\infty}^{\infty} \operatorname{erfc}(z/2) dz , \\ R_M(t) &= 4(1-m_0^2) t^{1/2}/\sqrt{\pi} . \end{aligned} \tag{23}$$

At first sight, it might seem surprising that, if $\langle m(t) \rangle = m_0 = \text{const}$, that $\langle m^2(t) \rangle$ should not be constant as well. This has to do with the fact that $R_M(t)$ is not a direct measure of domain size but rather of fluctuations about a mean, and in this case consists in averaging

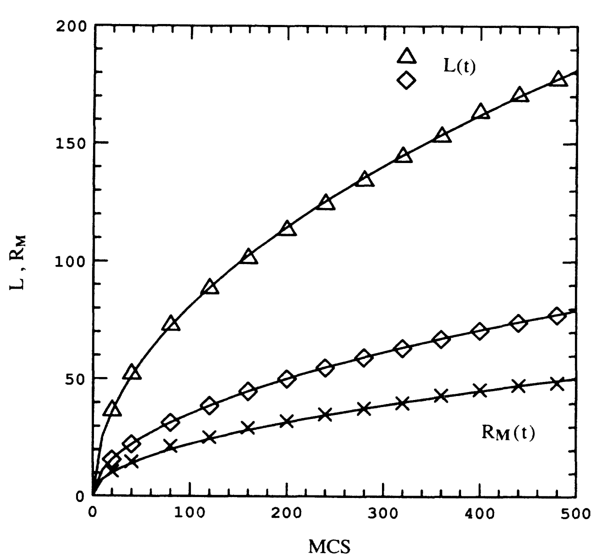

FIG. 1. Comparison of asymptotic predictions for domain size [Eqs. (17) and (23), solid curves] with simulation results (symbols). Top and middle curves correspond to average domain size $L(t)$ with $m_0=0.75$ and $m_0=0$, respectively. Bottom curve corresponds to $R_M(t)$ for the case $m_0=0$, for which the simulation results consist of an average over 1000 runs.

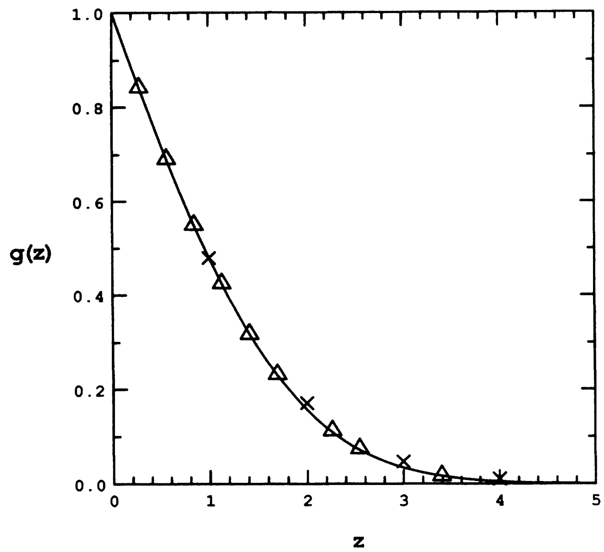

FIG. 2. Scaling form for the pair-correlation function $g(z)$ for the case $m_0=0$ [solid curve, Eq. (21)] compared with simulation results at 1 MCS (X's) and 200 MCS (triangles).

over an ensemble of runs (with different initial configurations) for which the average magnetization is m_0, and $\langle G(k,0)\rangle = m_0^2$ for $k>0$. We get excellent agreement in our simulations for $m_0=0$ (Fig. 1) even after only a few MCS.

V. DOMAIN-SIZE DISTRIBUTION FUNCTION

We have also looked at the asymptotic distribution of domain sizes $N(k,t)$ where $N(k,t)$ is the density of domains of size k at time t. 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

$$h(x)=\rho(k,t)L(t) , \tag{24}$$

where $x=k/L(t)$, $L(t)=[2\sqrt{\pi}/(1-m_0^2)]t^{1/2}$, and $h(x)$ is a scaling function satisfying $\int_0^\infty dx\, h(x)=1$. Figure 3(a) 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 $x=\frac{1}{2}$ rather than at $x=1$. The scaling function for $m_0=0.75$ has a peak which is higher and narrower than that for $m_0=0$ 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 (except possibly below the peak) to numerical results obtained by Doering and ben-Avraham[12] for the interparticle distribution scaling function for one-dimensional diffusion annihilation [see Fig. 3(a)]. This is perhaps not surprising given that our results for the domain size (wall density) for $m_0=0$ were also identical.

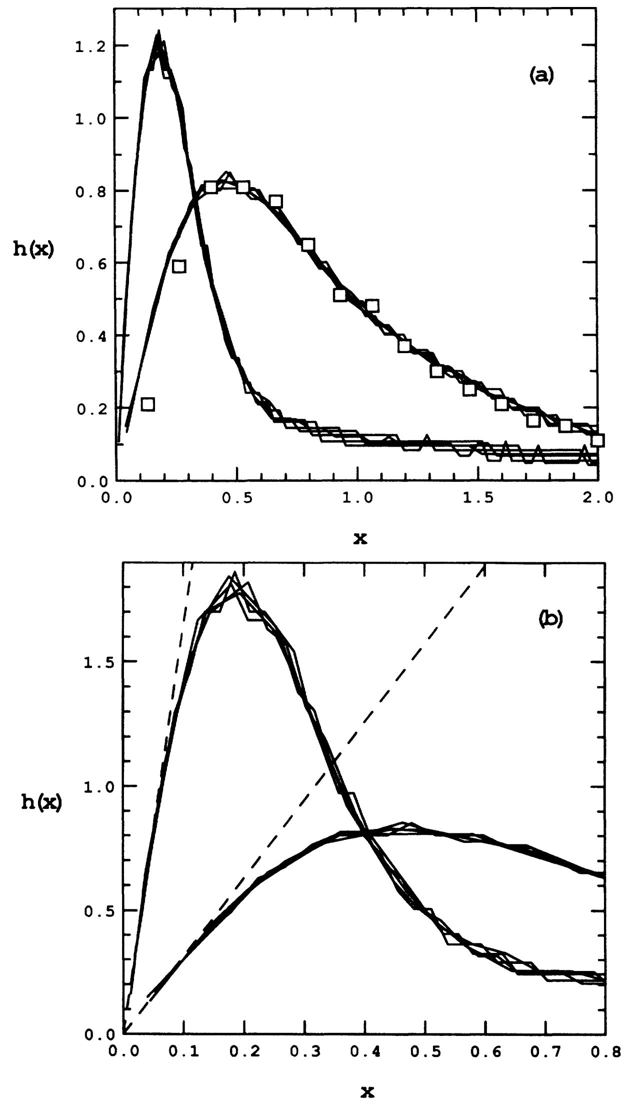

FIG. 3. (a) Domain-size distribution scaling function $h(x)$ for the cases $m_0=0$ (curves with squares imposed) and $m_0=0.75$ (upper peak) from Monte Carlo simulations. Data shown are for increments of 20 MCS up to 100 MCS. (The scaling function for $m_0=0.75$ has been reduced by a factor of $\frac{2}{3}$ for clarity.) Squares show data from Ref. 12. (b) Enlargement of (a) comparing the asymptotic result $h(x)\rightarrow \pi x/(1-m_0^2)^2$ derived in the text (dashed lines) with simulation results.

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 zero, 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[13] (for the behavior of the number of clusters of size k) and has been obtained in a recent paper[12] on the interparticle distribution function for the one-dimensional irreversible one-species coagulation model $A+A\rightarrow A$.

The small-x behavior of $h(x)$ as a function of m_0 and the exponent τ may be derived as follows. If we define the wall density at size i as

$$w_i = \tfrac{1}{2}(s_i - s_{i+1}) , \quad (25)$$

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,[14]

$$\langle w_0 w_x \rangle = \tfrac{1}{4}[2G(x,t) - G(x-1,t) - G(x+1,t)] . \quad (26)$$

In particular, we have $N(1,t) = -\langle w_0 w_1 \rangle = -\frac{1}{4}[2G(1,t) - G(2,t) - 1]$. Substituting the asymptotic form for $G(k,t)$, we obtain

$$N(1,t) = \frac{1-m_0^2}{8\sqrt{\pi}} t^{-3/2} + O(t^{-5/2}) \quad (27)$$

for the density of domains of size 1. Thus $\rho(1,t) = N(1,t)/n(t) = 1/4t$ and $h(x) \to \pi x/(1-m_0^2)^2$ as x goes to zero. Thus, we have shown explicitly that $\tau = 1$, and for small x, found the dependence of $h(x)$ on m_0. Figure 3(b) shows a comparison with this asymptotic form for small x.

VI. DISCUSSION

We have calculated explicit asymptotic expressions for the average domain size, density of walls, mean-square magnetization, and pair-correlation function, as a function of initial magnetization m_0, for the one-dimensional kinetic Ising model at zero temperature. We have carried out Monte Carlo simulations and find that the results converge rapidly to the asymptotic solutions. We have also studied the domain-wall distribution scaling function $h(x)$ for different values of m_0, and derived the small-x behavior of $h(x)$ and the exponent τ.

For the case $m_0 = 0$, our results for the wall density turn out to be identical to results recently derived for the particle density in the case of one-dimensional diffusion annihilation. In fact, we recover the two known exact solutions[4,5] for diffusion annihilation on a lattice. Similarly, our numerical results for the domain-size distribution scaling function $h(x)$ with $m_0 = 0$ are in excellent agreement with simulation results[12] for the interparticle distribution scaling function in the case of diffusion annihilation. However, for general m_0 we find, in contrast to the case of diffusion annihilation, that the coefficient of $t^{-1/2}$ in the asymptotic expression for the domain-wall (particle) density for the Ising model depends on the initial magnetization (concentration). Similarly, we find that the domain-size distribution scaling function $h(x)$ depends in a nontrivial manner on the initial magnetization.

The above results show that the duality between the one-dimensional Ising model at zero temperature and diffusion annihilation is only partial. This is due to the fact that, while the correspondence between the diffusion of walls in the Ising model and the diffusion of particles in the diffusion annihilation model is exact, the dynamics of annihilation in the two models is slightly different. Although this duality may be used to determine exponents for diffusion annihilation, such as τ, it does not apply to nonuniversal quantities such as the interparticle distribution scaling function. In systems in which the annihilation process differs from that of ordinary diffusion annihilation, as in the case of the Ising model, a nontrivial dependence on the initial particle density would also be expected.

ACKNOWLEDGMENTS

We would like to acknowledge useful discussions with Tamás Vicsek and J. L. Spouge. This work was supported by the U.S. Office of Naval Research and the Petroleum Research Fund Administered by the American Chemical Society.

[1] D. Toussaint and F. Wilczek, J. Chem. Phys. **78**, 2642 (1983).
[2] D. C. Torney and H. M. McConnell, J. Phys. Chem. **87**, 1941 (1983).
[3] S. J. Parus and R. Kopelman, Phys. Rev. B **39**, 889 (1989).
[4] A. A. Lushnikov, Phys. Lett. **120A**, 135 (1987).
[5] J. L. Spouge, Phys. Rev. Lett. **60**, 871 (1988).
[6] Z. Rácz, Phys. Rev. Lett. **55**, 1707 (1985).
[7] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[8] G. Arfken, *Mathematical Methods for Physicists*, 3rd ed. (Academic, New York, 1985), pp. 618 and 619.
[9] This may be seen to be in agreement with the solution given by Eq. (9) if one sums Eq. (9) over k and divides by N and recalls that $\langle s_m(0) \rangle = m_0$ and that $\sum_{m=-\infty}^{\infty} I_m(t) = e^t$.
[10] This is clearly reasonable since the probability per unit time for an isolated domain wall to "diffuse" a distance of one lattice spacing is $\frac{1}{2}$, according to Eq. (4).
[11] A. Milchev, K. Binder, and D. W. Heermann, Z. Phys. B **63**, 521 (1986).
[12] C. R. Doering and D. ben-Avraham, Phys. Rev. A **38**, 3035 (1988).
[13] K. Kang and S. Redner, Phys. Rev. A **30**, 2833 (1984).
[14] 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 $k+1$.