

Propagation and extinction in branching annihilating random walks

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We investigate the temporal evolution and spatial propagation of branching annihilating random walks (BAWs) in one dimension. Depending on the branching and annihilation rates, a few-particle initial state can evolve to a propagating finite density wave, or an extinction may occur, in which the number of particles vanishes in the long-time limit. The number parity conserving case where two offspring are produced in each branching event can be solved exactly for a unit reaction probability, from which qualitative features of the transition between propagation and extinction, as well as intriguing parity-specific effects, are elucidated. An approximate analysis is developed to treat this transition for general BAW processes. A scaling description suggests that the critical exponents that describe the vanishing of the particle density at the transition are unrelated to those of conventional models, such as Reggeon field theory.

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I. INTRODUCTION

In the branching annihilating random walk (BAW), a single random walk branches at some specified rate and two random walkers annihilate at another rate when they meet [1–4]. As a function of these rates, the number of random walkers may grow without bound, reach a finite limiting number, or vanish asymptotically. Our goal, in this paper, is to determine some of the long-time properties of this BAW process. We are particularly interested in understanding the kinetics and density distribution when the initial state consists of a small number of localized particles.

Interest in this process has several motivations. First, considerable theoretical effort has been devoted to establishing the existence of and quantifying the nonequilibrium phase transition between “propagation” and “extinction” for a variety of interacting particle systems [5] which are closely related to BAW’s. Here the term extinction refers to the situation where annihilation dominates over branching and an initially localized population of particles ultimately disappears. In the complementary case, branching dominates over annihilation and an initially localized population evolves into a propagating wave front which advances into the otherwise empty system. Typical examples of these phenomena include the contact process [6] and Schlögl models [7], as well as directed percolation and Reggeon field theory [8]. The propagation phenomenon is also a discrete realization of the “Fisher wave” [9,10], which describes the continuum dynamics of an initially localized single-species population whose evolution is influenced by diffusion, as well as by both (linear) birth and (quadratic) death mechanisms. The relation between the continuum description of the Fisher wave and the corresponding BAW is tenuous and comprehensive investigations of discrete BAW models

would be helpful to understand better the relation with the continuum counterpart. Second, there is a direct correspondence between the two-offspring BAW and the interface dynamics in the reaction-limited monomer-monomer surface reaction model in one dimension [11,12]. For the surface reaction, a lattice is filled with A and B particles and the ensuing dynamics is defined by randomly and repeatedly selecting a nearest-neighbor AB pair and changing it to either AA , BB , AB , or BA at specified rates. The dynamics of AB interfaces is identical to that of the individual particles in the two-offspring BAW.

In addition to connections with various nonequilibrium systems, the BAW model is amenable to theoretical analysis. Somewhat surprisingly, we find that the transition between propagation and extinction is controlled by detailed features of the underlying discrete process. In particular, the exact solution of the two-offspring BAW model in one dimension reveals that propagation occurs only for infinite branching rate and the parity of the initial number of particles essentially influences the long-time kinetics.

In the next section, we outline several basic facts about the BAW process. The general conditions which lead to propagation or extinction are discussed. In Sec. III, we present an exact solution for the evolution of the two-offspring BAW processes $A \rightarrow 3A$ and $2A \rightarrow 0$, in the case where the probability of reaction when two particles meet, k , is unity. For this case, extinction is paradoxically found to occur for all nonzero values of the diffusion rate. When there is only branching, a behavior intermediate to propagation and extinction occurs. In Sec. IV, we present an approximate description for the transition between propagation and extinction by solving a truncated hierarchy of rate equations for multiparticle correlation functions. The primary result of this treat-

ment is that the transition emerges naturally at the next level of approximation beyond mean-field theory. In Sec. V, we present numerical simulation results to support our various theoretical predictions, and then conclude in Sec. VI.

II. MODELS AND PHENOMENOLOGY

We define the branching annihilating random walk on a lattice as follows. A particle is picked at random. It can either undergo nearest-neighbor diffusion or it may branch with respective rates D and r . In a diffusion attempt, a random direction is picked and the particle moves to the target site if it is unoccupied. If the target site is occupied, then annihilation of the incident and target particles occurs with probability k . Otherwise, the incident particle remains at its original position. The details of the branching step depend on the number of offspring produced. In the two-offspring BAW, if a branching attempt is selected (at rate r), then branching to the two nearest-neighbor sites occurs with probability 1 if both neighbors are empty. If one or both neighbors are occupied, then branching to both neighbors occurs with probability k . In this branching, if a newly created particle is placed on a previously occupied site, then both particles are removed. An analogous procedure is employed for the one-offspring process; namely, in a branching event, if the target is occupied, then branching occurs with probability k . This branching entails immediate annihilation of the newly created and target particles. While these microscopic rules are somewhat involved when both branching and a finite reaction rate are operative, any reasonable discrete realization of the continuum process is anticipated to give qualitatively similar results. (An exception is the case of parallel dynamics, as opposed to the serial updating assumed here.) Since D and r have dimensions of inverse time and k is dimensionless, two dimensionless parameters which characterize the system are D/r and k .

As mentioned above, the BAW process with an initially localized particle population generically exhibits a transition from extinction (which is of one of two types; see below) to propagation. However, this transition appears to be at odds with a standard mean-field treatment of the model. Indeed, such a description of the BAW leads to the reaction-diffusion equation

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = a\rho(\mathbf{r}, t) - b[\rho(\mathbf{r}, t)]^2 + D\Delta\rho(\mathbf{r}, t), \quad (2.1)$$

where $\rho(\mathbf{r}, t)$ is the particle density at position \mathbf{r} at time t . Here a , b , and D correspond roughly to the branching rate, the reaction rate, and the diffusion rate, respectively. This equation admits a propagating Fisher wave solution of asymptotic density $\rho_\infty = a/b$ which advances into the low-density region with a velocity proportional to \sqrt{aD} , whenever $a > 0$. Since a is implicitly positive in this description, there appears to be no mechanism for extinction.

To generate a transition to extinction, a mechanism which changes the sign of a is needed. Such a mechanism, however, is easily realizable. At low densities, mean-field theory erroneously postulates that the encounter probability varies as the square of the particle density, since all spatial correlations are neglected. However, a more complete treatment of correlations leads to an encounter probability which is *linear* in the particle density in the low-density limit. This follows from the exact reaction-diffusion equation

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = a_{\text{exact}}\rho(\mathbf{r}, t) - b_{\text{exact}}\rho_2(\mathbf{0}, t) + D\Delta\rho(\mathbf{r}, t), \quad (2.2)$$

where $\rho_2(\mathbf{0}, t)$ denotes the two-point correlation function at zero separation, and branching is accounted for by $a_{\text{exact}} > 0$. However, for $\rho \ll \sqrt{a_{\text{exact}}/D}$, any reasonable theory must give $\rho_2(\mathbf{0}, t) \approx \langle \rho \rangle + \langle \rho \rangle^2$ because the birth mechanism produces nearby *pairs* of particles. Thus, extinction may arise in low spatial dimension because branching and annihilation terms are of comparable magnitude in Eq. (2.1); in particular, the sign of the coarse-grained branching rate $a \equiv a_{\text{exact}} - b_{\text{exact}}$ may change as external parameters are varied. In the following, we shall use r for the branching rate and k for the annihilation probability.

In numerical simulations, a transition from propagation to extinction generically occurs as the ratio of diffusion to branching increases (Fig. 1). As the annihilation probability (equivalent to the reaction rate) increases, the extinction transition is shifted to lower values of D/r . A crucial determinant for extinction is the "parity" of the branching event. For example, an even-offspring BAW process which starts with an odd number of particles cannot exhibit true extinction. Rather, the number of particles remains bounded when D/r is large. Thus extinction comes in two versions: In parity nonpreserving models (odd-offspring BAW), or in parity

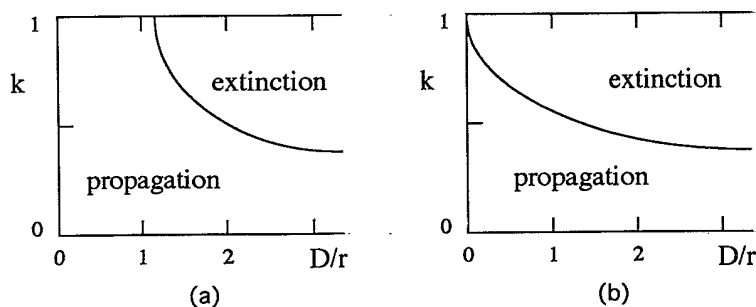


FIG. 1. Phase diagram of the BAW process as a function of the reaction probability k and the ratio of the diffusion to branching rate D/r . In (a) the phase diagram appropriate for BAW processes with parity nonconserving branching is indicated. This behavior should be taken as representative of the continuum limit of the BAW process. In (b), the phase diagram for the two-offspring BAW is schematically indicated. In this case, the nature of the "extinct" phase depends on whether the initial number of particles is even or odd.

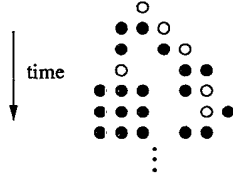


FIG. 2. Illustration of the space-time evolution of the two-offspring BAW in one dimension in the pure branching limit, $D/r=0$ and $k=1$. In this case, an isolated nearest-neighbor pair of particles remains bound and executes a simple random walk. The particle which branches at the next step is indicated by the open circle.

preserving models with an even number of particles initially, there is true extinction, whereas in the complementary cases, the particle number remains bounded.

The special case of the two-offspring BAW in the limits of pure branching, $D/r=0$, and also complete reaction, $k=1$, deserves emphasis because of its peculiar and easily visualized features (Fig. 2). The crucial aspect of this situation is that a pair of nearest-neighbor particles diffuses rigidly under the action of the branching process. Through the branching process, a single initial particle spawns rigid pairs at a finite rate which then diffuse freely. In this situation, the number of particles grows as \sqrt{t} . It is only when there is nonzero diffusion that extinction can occur.

III. EXACT SOLUTION FOR THE TWO-OFFSPRING BAW IN ONE DIMENSION

In this section, we derive the exact solution for the one-dimensional two-offspring BAW in the case of unit reaction probability. This provides a complete description of the transition between extinction and propagation. Our approach is based on solving for the time evolution of $P_{j,k}(t)$, the probability that there is an odd number of particles in the interval $[j,k]$. [Notice that the particle density at site j is simply $P_{j,j}(t)$.] In a spatially homogeneous system, $P_{j,k}(t)$ is a function of $j-k$ only and satisfies a soluble single-variable diffusion equation [12] while for the heterogeneous system, $P_{j,k}(t)$ is a function of both j and k . In the continuum limit, the master equation for $P_{j,k}(t)$ can be written as a two-dimensional diffusion equation with a radiation boundary condition.

To write the master equation for $P_{j,k}(t)$, define D_0 and r_0 as the hopping and branching rates, respectively, in an elemental event. In a single time step, the parity of the number of particles within $[j,k]$ can change only by hopping or branching events at $j-1, j, k$, or $k+1$. From straightforward but somewhat tedious bookkeeping of all these microscopic processes (Fig. 3), we obtain the following equations for $P_{j,k}$ for $j \leq k+1$:

$$P_{j,k}(t+1/N) - P_{j,k}(t) = \frac{D_0 + r_0}{N} [P_{j+1,k}(t) + P_{j,k+1}(t) + P_{j,k-1}(t) + P_{j-1,k}(t) - 4P_{j,k}(t)], \quad (3.1)$$

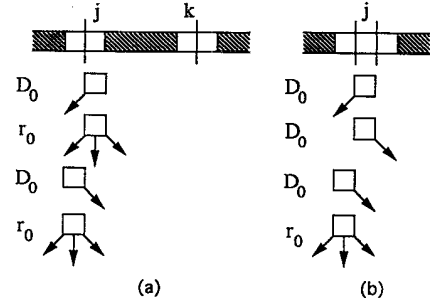


FIG. 3. Enumeration of the processes which can change the parity of the number of particles contained in the interval $[j,k]$ under the action of the two-offspring BAW. Shown are the various microscopic events and their corresponding statistical weights. The cases of (a) $k > j$ and (b) $k = j$ are somewhat different and therefore need to be treated separately.

while for $j=k$

$$P_{j,j}(t+1/N) - P_{j,j}(t) = \frac{D_0 + r_0}{N} [P_{j-1,j}(t) + P_{j,j+1}(t) - 2P_{j,j}(t)] - \frac{2D_0}{N} P_{j,j}(t). \quad (3.2)$$

The first equation can be extended to include $j=k$ by introducing the boundary condition

$$(D_0 + r_0)[P_{j,j-1}(t) + P_{j+1,j}(t)] = 2_0 P_{j,j}(t). \quad (3.3)$$

Here we have taken the time increment for an individual birth or diffusion event to be of the order of the inverse system size so that each particle will typically be updated once in a unit time step.

These equations can be simplified by transforming to the coordinates $x = j+k$ and $y = j-k$. After taking continuous time derivatives, one finds, for $y \geq 1$,

$$\dot{P}_{x,y}(t) = (D_0 + r_0) \times [P_{x+1,y+1}(t) + P_{x+1,y-1}(t) + P_{x-1,y+1}(t) + P_{x-1,y-1}(t) - 4P_{x,y}(t)], \quad (3.4)$$

while for $y=0$ one has

$$\dot{P}_{x,0}(t) = (D_0 + r_0)[P_{x+1,1}(t) + P_{x-1,1}(t) - 2P_{x,0}(t)] - 2D_0 P_{x,0}(t). \quad (3.5)$$

These two equations can again be unified by imposing the boundary condition

$$(D_0 + r_0)[P_{x+1,-1}(t) + P_{x-1,-1}(t) - 2P_{x,0}(t)] = -2D_0 P_{x,0}(t). \quad (3.6)$$

To obtain a nonsingular continuum limit for these master equations, $(D_0 + r_0)$ must be of order $(\Delta x)^{-2}$, whereas, from the boundary condition, $(D_0 + r_0)/D_0$ should be of order $(\Delta x)^{-1}$. These two restrictions, in turn, imply that $r_0 \sim (\Delta x)^{-2}$ and $D_0 \sim (\Delta x)^{-1}$. That is, an infinitely large

microscopic birth rate is needed to counteract the instant recombination of newly formed pairs in the continuum limit, thus ensuring a finite continuum birth rate. In the following, we simply replace the microscopic combination $D_0 + r_0$ by r_0 —since r_0 is infinitely larger than D_0 —and then take the continuum limit. Denoting the continuum limits of $(\Delta x)D_0$ and $(\Delta x)^2 r_0$ as D and r , respectively, the equation of motion for the interval occupation probability $P(x, y)$ becomes

$$\frac{\partial P(x, y)}{\partial t} = r \nabla^2 P(x, y), \quad (3.7)$$

with the corresponding boundary condition

$$\frac{\partial P(x, y)}{\partial y} \Big|_{y=0} = \frac{D}{r} P(x, y) \Big|_{y=0}. \quad (3.8)$$

When $D/r=0$, a slightly different line of reasoning must be used to determine the equation of motion, but the diffusion equation given above remains valid.

This equation can be solved by writing the solution as a superposition of incoming and outgoing modes in y in Fourier space, and imposing the boundary condition to relate the amplitudes of these incoming and outgoing modes. Upon inverting the Fourier transform, one finds

$$P(x, y; x_0, y_0; t) = \int \frac{dk_1 dk_2}{(2\pi)^2} e^{ik_1(x-x_0) - r(k_1^2 + k_2^2)t} \times \left[e^{ik_2(y-y_0)} + \frac{k_2 + iD/r}{k_2 - iD/r} e^{-ik_2(y+y_0)} \right], \quad (3.9)$$

where $P(x, y; x_0, y_0; t)$ denotes the propagator from (x_0, y_0) to (x, y) in time t . For computing the total number of particles, we only need the propagator with final spatial coordinate $y=0$. In the long-time limit, this restricted propagator has the form

$$P(x, 0; x_0, y_0; t) \approx \frac{y_0}{4\pi D r t^{3/2}} \exp \left\{ -\frac{(x-x_0)^2 + y_0^2}{4rt} \right\}, \quad (3.10)$$

which arises by neglecting the dimensionless “radiation” length r/D compared to the diffusion length \sqrt{Dt} .

For a single particle present initially at the origin, $P(x_0, y_0; t=0)$ is zero for $y_0 < |x_0|$ and is equal to 1 for $y_0 \geq |x_0|$. This corresponds to

$$P(x_0, y_0; t=0) = \Theta(y_0 - |x_0|),$$

where $\Theta(x)$ is the Heaviside step function. Thus for the density distribution we find

$$c(x, t) = \int_0^\infty dy_0 \int_{-y_0}^{y_0} dx_0 P(x, 0; x_0, y_0; t) = \frac{e^{-x^2/(8rt)}}{(D/r)\sqrt{2\pi rt}}, \quad (3.11)$$

For the case of two particles which are originally separated by a distance d , $P(x_0, y_0; t=0)=1$ when $||x_0| - y_0| < d$, and $P(x_0, y_0; t=0)=0$ otherwise. This initial condition leads to an expression of a similar form to Eq. (3.11), except that there is an additional multiplicative factor of d/\sqrt{rt} . Thus the total number of particles $N(t) \equiv \int c(x, t) dx \rightarrow 2r/D$ as $t \rightarrow \infty$ when one particle is initially present, and $N(t) \sim (rt)^{-1/2}$ when two particles are initially present. Generally, an initially localized group with an odd number of particles leads to a finite number of particles as $t \rightarrow \infty$, while a localized initial population with an even number of particles leads to $N(t) \propto t^{-1/2}$.

If there is no diffusion, then Eq. (3.8) reduces to a Neumann boundary condition. With this simplification, one finds the following density distribution for a single-particle initial condition, after several straightforward steps and without any approximations other than those involved in the continuum limit:

$$c(x, t) = \int_0^\infty dy_0 \int_{-y_0}^{y_0} dx_0 P(x, 0; x_0, y_0; t) = \frac{1}{4} \left[1 - \operatorname{erf}^2 \left[\frac{x}{2\sqrt{rt}} \right] \right]. \quad (3.12)$$

Thus for a single-particle initial condition, $N(t) \propto \sqrt{t}$, intermediate to the limiting cases of Fisher wave propagation, where the particle number grows linearly in t , and extinction, where the particle number either remains constant (through parity effects) or else decays as $t^{-1/2}$. Another interesting feature of the distribution is that it qualitatively resembles a Gaussian. This can be made plausible by consideration of the underlying discrete process. When there is only branching, it is easy to verify that a nearest-neighbor particle pair propagates diffusively as a rigid unit (Fig. 2). When two such solitonlike excitations meet, they merely “scatter” without any change in their form. As a single initial particle evolves, there is production of pairs at a finite rate which then diffuse freely within a region of length \sqrt{rt} . Conversely, for an even number of particles initially, “interference” between the offspring of the initial seed particles leads to the density vanishing as $t^{-1/2}$ in the long-time limit.

When the reaction rate $k < 1$, then the transition between extinction and Fisher wave propagation can be observed numerically, and the transition line between these two states has the qualitative form in the $D/r - k$ phase plane indicated in Fig. 1. Our exact analysis also provides a basis for a scaling description of this transition. For the total number of particles, we make the following scaling ansatz:

$$N(t) \sim t^\beta \Phi(\epsilon t^\alpha), \quad (3.13)$$

where $\epsilon(k)$ is the deviation of D/r from its critical value. This parameter will be considered positive in the region where propagation occurs and negative otherwise. From the fact that $N(t)$ grows linearly with time for $\epsilon > 0$ and decays as $t^{-1/2}$ otherwise (for the more generic case of parity nonconserving dynamics for an even number of in-

itial particles and parity conserving dynamics), one obtains

$$\Phi(x) \sim \begin{cases} x^{(1-\beta)/\alpha}, & x > 0, \\ |x|^{-(1+2\beta)/2\alpha}, & x < 0. \end{cases} \quad (3.14)$$

Since the exact solution shows that $N(t)$ remains bounded as $t \rightarrow \infty$ for $\epsilon = 0$, β must equal 0. (As above, we consider the case where parity is not conserved, or that the initial number of particles is even for parity conserving dynamics.) Further, for small values of D/r , this ratio appears in the exact solution in combinations of the form $D\sqrt{t}/r$, implying that $\alpha = \frac{1}{2}$. It therefore follows that $N(t) \propto \epsilon^2 t$ for small positive ϵ . This cannot be checked against our exact solution, since the $\epsilon > 0$ regime cannot be reached when $k = 1$. On the other hand, for negative ϵ , the behavior $N(t) \propto (|\epsilon|\sqrt{t})^{-1}$ is predicted, in agreement with Eq. (3.11).

IV. FACTORIZATION OF THE MULTIPARTICLE RATE EQUATIONS

As mentioned in Sec. II, the single-particle reaction-diffusion equation cannot account for the transition between extinction and propagation unless there is a sign change in the coefficient of the linear term in the concentration. Although such a sign change can be justified heuristically, it is worthwhile to present a systematic continuum approach which leads to this mechanism. Our approximate treatment of the multiparticle rate equations accomplishes this task. This approach has also the advantage that it can be applied straightforwardly to different microscopic branching and reaction mechanisms. In contrast, while the exact solution of the last section provides a complete description of the transition in a special case, this method is neither generalizable nor physically intuitive. Given the nature of the approximation in the multiparticle rate equations, we anticipate that our results will not depend quantitatively on the number of offspring in a branching event (except for parity-specific features), but, rather, will be generic to the transition between extinction and propagation.

For simplicity, we study the one-offspring BAW in one dimension which can be represented as



It should be mentioned that the one-offspring BAW with a unit reaction probability has been investigated by rigorous mathematical techniques [1]. These approaches have established the existence of a transition between propagation and extinction and provided weak bounds for the critical value of D/r . Our approximate method locates the transition for all values of the reaction probability. We first determine the first two in the hierarchy of rate equations for the multiparticle densities in this process. These equations will be closed by factorizing three-particle densities as products of two-particle densities. To write the hierarchy of rate equations, define $\rho_{\{k\}}$ as the probability that the set $\{k\}$ is occupied. Thus ρ_0 is the probability that site 0 is occupied, $\rho_{0,i}$ is the probability that sites 0 and i are simultaneously occupied, $\rho_{0,i,j}$ is

the probability that 0, i , and j are simultaneously occupied, etc. The rate equation for ρ_0 is found by enumerating all configurations in which an elemental event changes the occupancy of site 0. For example, if site 0 is empty and site 1 is occupied (which occurs with probability $\rho_1 - \rho_{0,1}$, which, by translation invariance, is also the same as $\rho_0 - \rho_{0,1}$), then, by either branching or hopping to the left, site 0 can become occupied. There is a similar contribution if site -1 is occupied. Similarly, there are three elemental events which lead to a decrease in the occupancy of site 0, as illustrated in Fig. 4(a). Summing these contributions leads to the rate equation

$$\dot{\rho}_0 = r\rho_0 - [r + (2D + r)k]\rho_{0,1}. \quad (4.2a)$$

The rate equation for $\rho_{0,1}$ is obtained by enumerating all three-site configurations for which an elemental event changes the occupancy of sites 0 or 1. These configurations and the associated rates of the processes which change $\rho_{0,1}$ are shown in Fig. 4(b) and lead to

$$\begin{aligned} \dot{\rho}_{0,1} = & r\rho_0 - (D + r)(1 + k)\rho_{0,1} + (D + r)\rho_{0,2} \\ & - [r + (2D + r)k]\rho_{0,1,2}. \end{aligned} \quad (4.2b)$$

The equations for $\rho_{0,i}$ for $i \geq 2$ are obtained similarly [Fig. 4(c)],

$$\begin{aligned} \dot{\rho}_{0,i} = & (D + r)\rho_{0,i-1} - 2D\rho_{0,i} + (D + r)\rho_{0,i+1} \\ & - [r + (2D + r)k](\rho_{0,i,i+1} + \rho_{0,i-1,i}). \end{aligned} \quad (4.2c)$$

To be soluble, these exact equations must now be closed by a suitable truncation. A standard approach is to truncate the equations at the two-particle level by the ansatz

$$\rho_{0,1,i+1} = \rho_{0,1}\rho_{1,i+1}/\rho_0 = \rho_{0,1}\rho_{0,i}/\rho_0. \quad (4.3)$$

While heuristic, this approximation yields reasonable results and turns out to be simpler than the standard Kirkwood truncation.

To establish the existence of propagation, we investi-

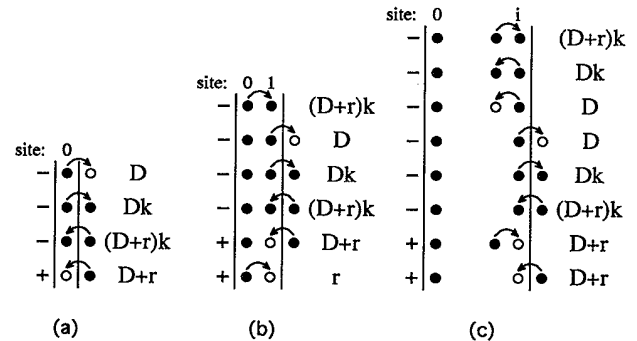


FIG. 4. Enumeration of the processes which can change the occupancy of a selected set of sites in the one-offspring BAW. In (a) the set consists of a single site ρ_0 , while in (b) the set consists of two adjacent sites $\rho_{0,1}$. In (c), the set consists of two nonadjacent sites $\rho_{0,i}$. The signs to the left denote whether a process increases (+) or decreases (-) ρ . The rate of the processes (and their kind) is indicated to the right. Solid and empty circles denote occupied and empty sites, respectively.

gate the existence of a nonzero time-independent solution to the truncated rate equations. The transition between propagation and extinction is then identified by the locus where this steady-state density vanishes as k and D/r are varied. To streamline the notation, let $x \equiv D/r$ and $\rho(i) \equiv \rho_{0,i}/\rho_0$. The steady-state rate equations reduce to

$$1 - [1 + (1 + 2x)k] \rho(1) = 0,$$

$$1 - (1 + x)(1 + k)\rho(1) + (1 + x)\rho(2) - [1 + (1 + 2x)k][\rho(1)]^2 = 0, \quad (4.4)$$

$$(1 + x)\rho(i - 1) - 2x\rho(i) + (1 + x)\rho(i + 1) - [1 + (1 + 2x)k][\rho(i) + \rho(i - 1)] = 0.$$

From the first of these equations,

$$\rho(1) = \frac{1}{1 + (1 + 2x)k}. \quad (4.5)$$

Using this in the second equation then gives

$$\rho(2) = \frac{1 + x - xk}{(1 + k + 2xk)(1 + x)}. \quad (4.6)$$

Substituting the static value for $\rho(1)$ into the last of the rate equations, a constant coefficient recursion equation for $\rho(i)$ results. Using the boundary conditions supplied by the equations for $\rho(1)$ and $\rho(2)$, the solution is

$$\rho(i) = \rho + \frac{xk}{1 + k + 2xk} \left(\frac{x}{1 + x} \right)^{i-1}, \quad (4.7)$$

with

$$\rho = \frac{1 - xk}{1 + k + 2xk}. \quad (4.8)$$

Here $\rho = \lim_{i \rightarrow \infty} \rho(i)$ is just the equilibrium single-particle density. Thus a positive solution for ρ exists only when $x < 1/k$, corresponding to the propagating phase of the one-offspring BAW. When $x = x_c = 1/k$, the equilibrium density vanishes; this defines the phase boundary between propagation and extinction. Note further that the decay of the equilibrium concentration is linear in ϵ as $\epsilon \equiv x - x_c \rightarrow 0+$. If the scaling predictions of the preceding section are correct, the particle number should grow as $\epsilon^2 t$, for $\epsilon \rightarrow 0-$. On the other hand, the total particle number is the particle density multiplied by the

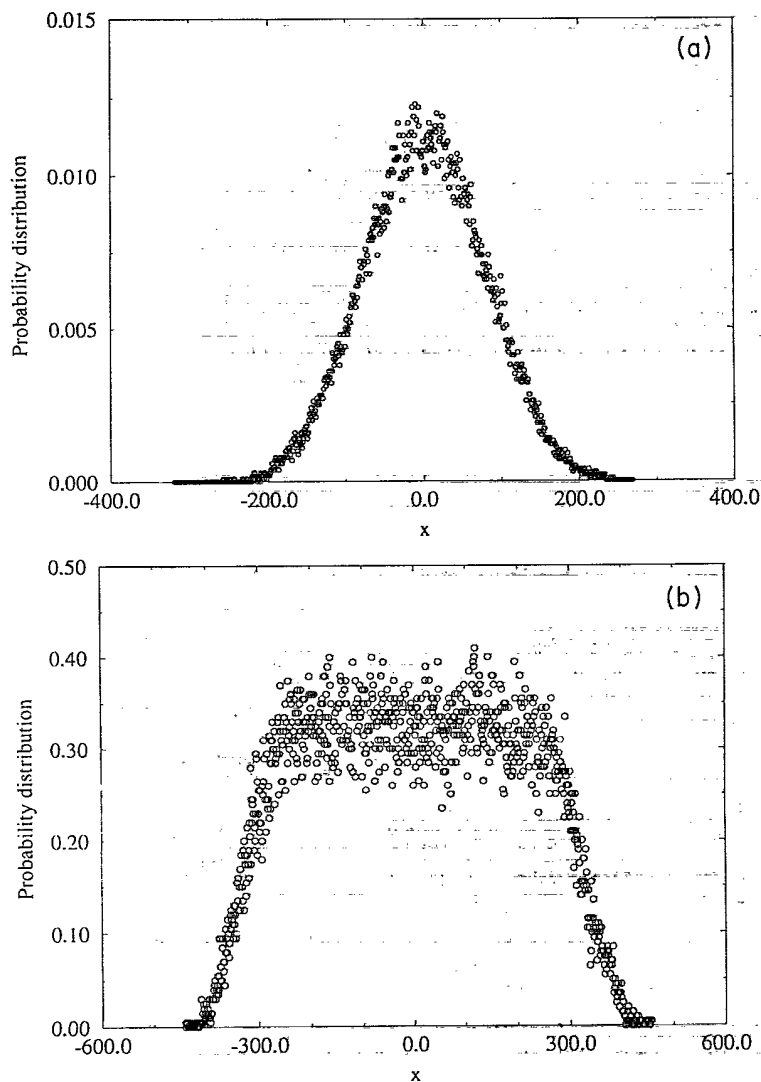


FIG. 5. Spatial distribution for the one-offspring BAW in one dimension at $t = 1.5^{19} \approx 2217$. The cases shown are (a) 25000 configurations at $D/r = 1/0.88$, where the survival probability has decreased to approximately 0.11 and (b) 200 configurations at $D/r = 1/0.95$, where the survival probability has saturated at approximately 0.81.

width of the propagating wave. This latter quantity should grow as ϵt , that is, the front velocity goes linearly to zero as the critical value of x is approached.

V. NUMERICAL SIMULATIONS

To confirm the above analytical results and visualize the evolution of the system, we have performed numerical simulations of the one- and two-offspring BAW in one dimension according to the rules outlined in Sec. II. For concreteness, we have fixed the hopping rate to be unity so that the variables in the simulation are the branching rate r and the reaction probability k .

First consider the one-offspring BAW for which it is known [1,2] that a transition between propagation and extinction occurs for a nonzero value of D/r . Starting with a single particle at the origin and with the parametrizations of our lattice model, the transition occurs at $x \equiv D/r \approx 1/0.89$. For slightly larger values of x , the number of particles initially increases, but ultimately decays to zero. For example, for $x = 1/0.88$, the average number of particles gradually increases to 4.8 for $t \approx 400$, but then decreases to 0 for longer times. By $t = 1.5^{23} \approx 11\,223$, only about 0.1% of the initial configurations are still active. For $400 \lesssim t \lesssim 10\,000$, the spatial distribution of the ensemble of surviving particles appears visually to be well approximated by a Gaussian [Fig. 5(a)]. In this time range, the reduced moments of the spatial distribution are $m_4 \equiv \langle x^4 \rangle / \langle x^2 \rangle^2 \approx 2.8 - 3.02$ and $m_6 \equiv \langle x^6 \rangle / \langle x^2 \rangle^3 \approx 13.0 - 13.9$, while for a Gaussian, the corresponding values are $m_4 = 3$ and $m_6 = 15$. This behavior suggests that the effect of branching is irrelevant in the scaling sense, and that the spatial evolution of the one-offspring BAW coincides with that of a single purely random walk. On the other hand for $x = 1/0.95$, the simulations clearly show that a Fisher-like wave front forms which then propagates at a finite velocity [Fig. 5(b)].

For the two-offspring BAW, we have approximately mapped out the phase boundary between extinction and propagation [Fig. 1(b)]. Simulations clearly indicate that the phase boundary intersects the line $k = 1$ at $D/r = 0$. Thus for $k = 1$ there is extinction for all D/r except when $D/r = 0$. At this special point, our exact solution showed that the number of particles grows as \sqrt{t} for a single-particle initial state. Another amusing feature of the two-offspring BAW that we have verified numerically is the essential dependence on parity. For example, if the initial state consists of two widely separated particles, then propagation associated with two independent particles is observed for early times, followed ultimately by a decay in which the number of particle goes to zero.

Finally, in the course of simulations we discovered an interesting difference between serial and parallel updating. When all lattice sites are updated simultaneously, the two-offspring BAW exhibits propagation, that is, a Fisher wave, even for finite values of D/r . Thus the BAW process is an example of a system where the method of updating, whether parallel or serial, leads to nontrivial differences in the resulting dynamics. We chose to focus on serial updating, since it is more physically motivated.

VI. CONCLUSIONS

In summary, we have analyzed the dynamical behavior of branching annihilating random walks in one dimension. Typically this system exhibits (i) propagation, where a localized population of particles spreads ballistically for large branching and/or small reaction rates, and (ii) extinction, where a localized population eventually disappears for the complementary range of parameters. For parity nonconserving rules, there is a continuous transition between these two behaviors which occurs at a finite value of the branching rate when the reaction probability is unity. This transition appears to have a universal character and can be accounted for by analysis of a truncated hierarchy of rate equations for multiparticle distribution functions, as well as by scaling.

When the branching and reaction mechanisms conserve parity, rather different behavior arises. In particular, for the two-offspring BAW with a unit reaction probability, an exact analysis of the master equation for the parity of the particle number in a fixed length interval shows that the transition between propagation and extinction occurs for infinite branching rate. The long-time behavior also depends fundamentally on the parity of the initial number of particles. When this number is odd, extinction corresponds to a long-time state where the particle number is bounded, while the particle number vanishes as $t^{-1/2}$ for an even number of initial particles, i.e., extinction is complete. In the limit of infinite branching rate, a single initial particle gives rise to a Gaussian-like density distribution where the particle number grows as $t^{1/2}$. Numerical studies confirm many of these analytical predictions.

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