Statistical Description of Contact-Interacting Brownian Walkers on the Line

Ibrahim Fatkullin^{1,3} and Eric Vanden-Eijnden^{2,3}

Received January 7, 2003; accepted February 14, 2003

The distribution of interval lengths between Brownian walkers on the line is investigated. The walkers are independent until collision; at collision, the left walker disappears, and the right walker survives with probability p. This problem arises in the context of diffusion-limited reactions and also in the scaling limit of the voter model. A systematic expansion in correlation between neighbor intervals gives a series of approximations of increasing accuracy for the probability density functions of interval lengths. The first approximation beyond mere statistical independence between successive intervals already gives excellent results, as established by comparison with direct numerical simulations.

KEY WORDS: Brownian walkers; voter model; diffusion-limited reactions.

1. INTRODUCTION

Consider the following problem. An infinite collection of walkers move on the real line. Each walker follows an independent Brownian motion until collision. At collision, the left walker disappears, and the right walker survives with probability p. If the walkers are distributed homogeneously at initial time, what is their distribution at time t > 0? As special cases, note that for p = 1, the right walkers always survive a collision and the resulting process is called diffusion-coalescence process; for p = 0, both walkers disappear at collision and we get the so-called diffusion-annihilation process. Here we investigate the situation with arbitrary $p \in [0, 1]$.

This problem arises in the context of diffusion-limited reactions in onedimension, where the reactants move randomly before reacting instantaneously as $A+A \rightarrow A$ with probability p and $A+A \rightarrow \emptyset$ with probability 1-p.

¹ Rensselaer Polytechnic Institute, New York, New York 12180.

² Courant Institute, New York University, New York, New York 10012.

³ Institute for Advanced Study, Princeton, New Jersey 08540; e-mail: eve2@ias.edu

This problem also arises in the scaling limit of the voter model (see, e.g., refs. 2, 5, 8, and 10), i.e., a system of spins (or voters) equipped with the following dynamics. Each spin has a random clock with a Poisson distribution with rate 1; when its clock rings the spin updates its opinion to the one of its left or right neighbor picked at random. The positions of the interfaces between blocks with equal spins move as the random walkers in the problem above if one rescales space as $\lambda^{-1/2}$ and time as λ^{-1} , and takes the limit as $\lambda \to \infty$; the number of possible opinions that a spin can take corresponds to (2-p)/(1-p) and it is assumed that the opinions of the initial blocks are randomly chosen.

In this paper, we propose a statistical theory for the problem of random walkers on the line. Our approach is based on a systematic expansion in correlation between neighbor intervals which provides a series of approximations of increasing accuracy for the probability density functions of interval lengths. As shown below, the first approximation beyond mere statistical independence between successive intervals already gives results which are in excellent agreement with the numerical simulation of the original model—see below.

It is worth pointing out that the voter model has been studied by many authors for specific values of p and under various simplifying assumptions (see, e.g., refs. 2-5, 8, 11, and 12). One of the most complete analysis is that of Derrida and Zeitak⁽⁶⁾ (see also Ref. 7), who have shown that the voter model with an infinite number of colors (corresponding to diffusioncoalescence in the scaling limit) can be reduced to the problem of computing the Pfaffians of a family of matrices of increasing sizes; in particular, the positions of the N interfaces between consecutive blocks of spins can be deduced from an $2N \times 2N$ matrix. Furthermore, if the positions of all the interfaces between successive blocks are known, one can in principle deduce the positions of the N interfaces between consecutive blocks in the voter model with finite number of colors. Practically, this is of course undoable, and Derrida et al. (6,7) had to make simplifying assumptions or asymptotic expansions to proceed further. They also observed that the system with two colors (corresponding to diffusion-annihilation in the scaling limit) is the hardest situation to handle by their approach, in the sense that the series they obtain diverge as $p \to 0$. Our approach is an alternative to Derrida et al.'s which illuminates different aspects of the problem by providing explicit and closed master equations for the first nprobability density functions of interval lengths.

Finally, a word about the numerical experiments we use to check the statistical theory. The exact solution is inferred by simulating N Brownian walkers with an independent noise, moving on a ring of size L, and interacting appropriately at collision. We make sure that the effects of the finiteness of

the ring do not affect the dynamics by keeping the largest of the distance between the walkers, say, λ , much less than the length of the ring L. We kept $\lambda/L < 10^{-4}$ and as a rule we started with $N=10^6$ walkers. Statistics were computed by averaging over the ensemble of walkers on the ring; in particular, the density n was obtained by bin-counting the interval lengths.

2. STATISTICAL DESCRIPTION AND CLOSURE APPROXIMATIONS

Let $\{L_k(t)\}_{k\in\mathbb{Z}}$ denote the lengths between successive intervals between the surviving walkers at time t. A statistically homogeneous system is such that the interval length between any two walkers is on the average independent of the walker positions along the line, i.e., $\{L_k(t)\}_{k\in\mathbb{Z}}$ and $\{L_{k+N}(t)\}_{k\in\mathbb{Z}}$ have the same law for arbitrary $N\in\mathbb{Z}$. This property is conserved for all times if it is true initially, which we shall assume. In this case, the single-time statistical properties of the walkers can be described by the family of probability density functions, $\{n^{(k)}(l_1,...,l_k,t)\}_{k=1}^{\infty}$, defined so that

$$\int_{0}^{l_{1}} \cdots \int_{0}^{l_{k}} n^{(k)}(l'_{1}, l'_{2}, ..., l'_{k}) dl_{k} \cdots dl_{1} = \mathbf{P}\{L_{1}(t) \leq l_{1}, ..., L_{k}(t) \leq l_{k}\}.$$
 (1)

It is not difficult to show that the $\{n^{(k)}\}$'s satisfy the following hierarchy of equations:

$$n_{t}^{(k)} = \Delta_{\ell}^{(k)} n^{(k)} + p \sum_{i=1}^{k-1} n^{(k+1)}(\dots, l_{i}, \downarrow, l_{i+1}, \dots)$$

$$+ (1-p) \left(\sum_{i=1}^{k} \int_{0}^{l_{i}} n^{(k+2)}(\dots, l_{i-1}, l, \downarrow, l_{i} - l, l_{i+1}, \dots) dl - n^{(k+1)}(\downarrow, l_{1}, \dots) - n^{(k+1)}(\dots, l_{k}, \downarrow) \right) + (2-p) n^{(1)}(\downarrow) n^{(k)}.$$
(2)

where the arrow " \downarrow " designates derivative with respect to the corresponding argument evaluated at 0; terms like $n^{(k+1)}(...,l_i,\downarrow,l_{i+1},...)$ give the probability rates of respective collisions. We also defined

$$\Delta_{\ell}^{(k)} = \partial_{l_1 l_1}^2 - \partial_{l_1 l_2}^2 + \partial_{l_2 l_2}^2 - \dots - \partial_{l_{k-1} l_k}^2 + \partial_{l_k l_k}^2. \tag{3}$$

The mixed-derivative terms in this operator appear after a change of variables from locations of the walkers to distances between them, and the term $\Delta_{\ell}^{(k)} n^{(k)}$ in (2) accounts for diffusive motion of the intervals. The two terms involving sums on the first and second lines correspond to creation of a given state (i.e., a finite sequence of intervals with given lengths) in the

process of collision of two walkers. Such a collision results either in their coalescence (the first sum) or in their mutual annihilation (the convolution terms). The first two terms in the equation on the third line correspond to destruction of a given state via collision with an external walker from the left or from the right. The last term is a simple renormalization term which guarantees that integrals in (1) can be interpreted as probabilities (otherwise there is a probability flux out of the system which arises because the intervals disappear when the walkers collide). Since intervals of zero length disappear, (7) must be solved with the absorbing boundary condition $n|_{l=0} = 0$. The infinite set of equations in (2) is not practical since the equation for the density of order k involve the densities of order k+1 and k+2. Notice however that (2) admits self-similar solution of the type

$$n^{(k)}(l_1,...,l_k,t) = (4t)^{-k/2} m^{(k)}(l_1/\sqrt{4t},...,l_k/\sqrt{4t}).$$
 (4)

These solutions describe the long-time coarsening in the system and indicate that the characteristic length grows as \sqrt{t} .

A systematic class of closure approximations for (2) with increasing accuracy can be obtained as follows. At fixed time t, $\{L_k(t)\}_{k\in\mathbb{Z}}$ can be thought of as a stochastic process with discrete "time" k. We shall assume that this process is s-Markov, where $s \in \mathbb{N}$ is a parameter which can be increased to get better approximations, i.e., for any $q \in \mathbb{N}$,

$$\mathbf{P}\left\{L_{0}(t) \in I \mid L_{\pm 1}(t) = l_{\pm 1}, \dots, L_{\pm (s+q)}(t) = l_{\pm (s+q)}\right\} \\
= \mathbf{P}\left\{L_{0}(t) \in I \mid L_{\pm 1}(t) = l_{\pm 1}, \dots, L_{\pm s}(t) = l_{\pm s}\right\}, \tag{5}$$

where $P\{L_0(t) \in I \mid C\}$ denotes the probability that $L_0(t) \in I$, conditional on C. Next we show that for any $s \ge 0$ (5) allows one to obtain from (2) a closed set of equations for the s+1 first probability density functions.

3. STATISTICAL INDEPENDENCE APPROXIMATION

For s = 0, it is easy to see that (5) implies statistical independence of successive interval lengths,

$$n^{(k)}(l_1,...,l_k,t) = n(l_1,t)\cdots n(l_k,t),$$
 (6)

where $n(l, t) \equiv n^{(1)}(l, t)$ is the probability density function of the length of an interval between two nearest walkers. Approximations of similar nature

were previously used, e.g., in refs. 1, 4, and 9. Equation (6) allows to derive from (2) the following equation for n:

$$n_{t} = n_{ll} + (1 - p) \, n(\downarrow, t) \int_{0}^{l} n(l', t) \, n(l - l', t) \, dl' + pn(\downarrow, t) \, n(l, t), \tag{7}$$

where as earlier the down arrow indicates derivative over the corresponding argument evaluated at zero, $n(\downarrow, t) = n_l(0, t)$. Equation (7) admits a self-similar solution of the form $n(l, t) = (4t)^{-1/2} m(l/\sqrt{4t})$, with m satisfying

$$m'' + 2\xi m' + \frac{2 - 2p}{2 - p} \int_0^{\xi} m(\zeta) m(\xi - \zeta) d\zeta + \frac{4}{2 - p} m = 0,$$
 (8)

where we used m'(0) = 2/(2-p), which can be obtained directly from the hierarchy (2) with substitution (4) (this condition is also easily derived by taking the first moment of (8) and using the normalization condition $\int_0^\infty m \, d\xi = 1$). The analytical solution of (8) is not readily available, but it is rather elementary to solve this equation numerically. The results are shown in Fig. 1 for p = 0 (annihilation), in Fig. 2 for p = 2/3 (corresponding to the scaling limit of the 4-color voter model), and in Fig. 3 for p = 1 (coalescence).

The equation in (7) turns out to be exact if p = 1 (coalescence), but is unsatisfactory for all $p \in [0, 1)$. Furthermore the independence assumption

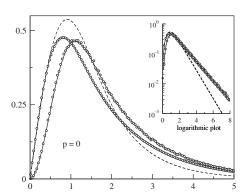


Fig. 1. The self-similar density functions m and m_c for the diffusion-annihilation process (p=0). The dashed line corresponds to the statistical independence approximation, the solid line to the nearest-neighbor approximation, and the circles, to direct simulation. There is only one dashed curve since the independence approximation erroneously predicts that $m=m_c$; in contrast, the nearest-neighbor approximation correctly distinguishes between m and m_c (the graph of m_c being shifted to the right compared to the one of m).

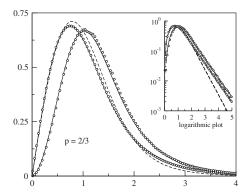


Fig. 2. Same as in Fig. 1 for the 4-color Potts model (p = 2/3).

(6) is always (i.e., for all $p \in [0, 1]$) a poor approximation. Here, we quantify the quality of an approximation via the probability density of colliding intervals, i.e., the conditional probability density of an interval if its neighbor is about to disappear,

$$n_c(l,t) = \lim_{l' \to 0} \frac{n^{(2)}(l,l',t)}{n(l',t)} = \frac{n^{(2)}(l,\downarrow,t)}{n(\downarrow,t)}.$$
 (9)

As can be seen from Figs. 1–3, n_c is not equal to n, indicating the presence of correlations between successive intervals. These correlations are completely missed by the statistical independence approximation.

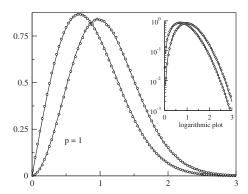


Fig. 3. Same as in Fig. 1 for the diffusion-coalescence process (p=1); in this case, the predictions for m by both the independence and the nearest neighbour approximations are exact, and the dashed line coincides with the solid line.

4. NEAREST-NEIGHBOR APPROXIMATION

The next approximation beyond statistical independence amounts to taking s = 1 in (5); this is equivalent to assume that the conditional probability density to observe an interval of length l_1 with left (or right) neighbors of respective lengths l_2 , l_3 ,... depends on l_2 only, and it is easy to see that under this assumption any $n^{(k)}$ with k > 2 can be expressed as follows in terms of $n^{(2)}$:

$$n^{(3)}(l_1, l_2, l_3) = \frac{n^{(2)}(l_1, l_2) n^{(2)}(l_2, l_3)}{n(l_2)},$$

$$n^{(4)}(l_1, l_2, l_3, l_4) = \frac{n^{(2)}(l_1, l_2) n^{(2)}(l_2, l_3) n^{(2)}(l_3, l_4)}{n(l_2) n(l_3)},$$
(10)

and so on for higher order density functions. An approximation of this sort applied to a different hierarchy of equations for correlation functions —which do not allow to deduce the domain-size distributions in any simple manner—was proposed by Lin *et al.*⁽¹¹⁾ Inserting (10) in (5) for k = 2 yields the following closed equation for $n^{(2)}$:

$$n_{t}^{(2)}(l_{1}, l_{2}) = n_{l_{1}l_{1}}^{(2)} - n_{l_{1}l_{2}}^{(2)} + n_{l_{2}l_{2}}^{(2)} + pn(\downarrow) n_{c}(l_{1}) n_{c}(l_{2})$$

$$+ (1-p) n(\downarrow) \left(\int_{0}^{l_{1}} n_{c}(l_{1}-l) n_{c}(l) n(l_{2}|l) dl \right)$$

$$+ \int_{0}^{l_{2}} n(l_{1}|l) n_{c}(l) n_{c}(l_{2}-l) dl - n(l_{1}|l_{2}) n_{c}(l_{2}) - n_{c}(l_{1}) n(l_{2}|l_{1}) \right)$$

$$+ (2-p) n^{(1)}(\downarrow) n^{(2)}, \qquad (11)$$

where $n_c(l) = n^{(2)}(l,\downarrow)/n(\downarrow)$, $n(l_1 | l_2) = n^{(2)}(l_1, l_2)/n(l_2)$. In self-similar form, $n^{(2)}(l_1, l_2, t) = (4t)^{-1} m^{(2)}(l_1/\sqrt{4t}, l_2/\sqrt{4t})$, this equation becomes

$$m_{\xi\xi}^{(2)} - m_{\xi\eta}^{(2)} + m_{\eta\eta}^{(2)} + 2\xi m_{\xi}^{(2)} + 2\eta m_{\eta}^{(2)} + 6m^{(2)}$$

$$+ \frac{2 - 2p}{2 - p} \left(\int_{0}^{l_{1}} m_{c}(l_{1} - l) m_{c}(l) m(l_{2} | l) dl \right)$$

$$+ \int_{0}^{l_{2}} m(l_{1} | l) m_{c}(l) m_{c}(l_{2} - l) dl$$

$$- m(l_{1} | l_{2}) m_{c}(l_{2}) - m_{c}(l_{1}) m(l_{2} | l_{1}) + \frac{2p}{2 - p} m_{c}(l_{1}) m_{c}(l_{2}) = 0.$$

$$(12)$$

 $m(\xi \mid \eta) = m^{(2)}(\xi, \eta)/m(\eta)$, $m_c(\xi) = m^{(2)}(\xi, \downarrow)/m(\downarrow)$ are the self-similar conditional probability densities.

Equation (12) is not hard to solve numerically. As can be seen from Figs. 1-3, the nearest-neighbor approximation is in excellent agreement with the direct numerical experiments. It captures correctly both m and m_c for all values of ξ , including the large values in the tails of the density functions where the correct exponential decay is obtained.

As a further test of the nearest-neighbor approximation, we studied a situation out of the self-similar regime. Namely, we solved (11) as an initial value problem, with an initial condition chosen so that $n_0(l)$ has two well defined peaks and there is no correlation initially between successive intervals (such correlations will be built by the dynamics). Figure 4 shows snapshots in time of n(l,t) obtained from direct simulation and those predicted by the nearest-neighbor approximation. As one can see there is virtually no difference between the curves. The initial condition was chosen to illustrate an interesting phenomenon. It is easy to notice that the solution has pronounced humps at lengths equal to the multiples of the length of the second peak. This happens because the walkers separated by a short interval have a high probability to collide before the walkers separated by a long interval; when this happens, the short interval disappears, and the two long intervals merge and create an interval of double length.

5. CONCLUDING REMARKS

Based on (5), higher order closures are possible (which provide a systematic expansion in correlation). We didn't pursue this any further since the nearest-neighbor approximation is already excellent for description of

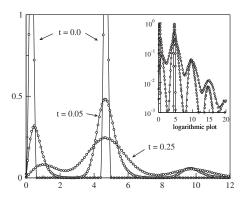


Fig. 4. Relaxation of n(l, t) from some initial condition $n_0(l)$ for the diffusion-annihilation process (p = 0). The solid line corresponds to the nearest-neighbor approximation, circles—to direct simulation.

the domain-length statistics. Furthermore, this approximation captures not only the long time self-similar regime, but also the evolution from an initial configuration; this is unlike most approximations in the literature which focus only on the self-similar regime.

Finally, we note that a class of more complicated models can also be analyzed by means of the domain-length densities slightly modifying the proposed framework. For example one can consider the systems with nucleation where new walkers are injected in the system. Such modifications, however, require a closer look and will be considered elsewhere.

ACKNOWLEDGMENTS

We thank Weinan E, Bob Kohn, Chuck Newman, and especially Gregor Kovačič for useful discussions. I.F. is partially supported by DOE via Grant DE-FG02-88ER25053, by NSF via Grants DMS-0101439, and DMS-9729992, and by AMIAS (Association of Members of the Institute for Advanced Study). E.V.-E. is partially supported by NSF via Grants DMS-0101439, DMS-0209959, and by AMIAS.

REFERENCES

- 1. P. A. Alemany and D. ben-Avraham, Inter-particle distribution functions for one-species diffusion-limited annihilation, $A + A \rightarrow 0$, *Phys. Lett. A* **206**:18–25 (1995).
- J. G. Amar and F. Family, Diffusion annihilation in one dimension and kinetics of the Ising model at zero temperature, *Phys. Rev. A* 41:3258–3262 (1989).
- 3. D. ben-Avraham, M. A. Burschka, and C. R. Doering, Statics and dynamics of a diffusion-limited reaction: Anomalous kinetics, nonequilibrium self-ordering and dynamics transition, *J. Stat. Phys.* **60**:695–728 (1990).
- E. Ben-Naim and P. L. Krapivsky, Domain number distribution in the nonequilibrium Ising model, J. Stat. Phys. 93:583

 –601 (1998).
- A. J. Bray, Universal scaling function for domain growth in the Glauber-Ising chain, J. Phys. A 23:L67-L72 (1990).
- B. Derrida and R. Zeitak, Distribution of domain sizes in the zero temperature Glauber dynamics of the one-dimensional Potts model, *Phys. Rev. E* 54:2513–2525 (1996).
- B. Derrida, V. Hakim, and V. Pasquier, Exact exponent for the number of persistent spins in the zero-temperature dynamics of the one-dimensional Potts model, *J. Stat. Phys.* 85:763-797 (1996).
- L. R. Fontes, M. Isopi, C. M. Newman, and D. L. Stein, Aging in 1D discrete spin models and equivalent systems, *Phys. Rev. Lett.* 87:11201–11204 (2001).
- P. L. Krapivsky and E. Ben-Naim, Domain statistics in coarsening systems, *Phys. Rev. E* 56:3788–3798 (1997).
- 10. T. M. Liggett, Interacting Particle Systems (Springer-Verlag, New York, 1985).
- J-C. Lin, C. R. Doering, and D. ben-Avraham, Joint density closure schemes for a diffusion-limited reaction, *Chem. Phys.* 146:335–371 (1990).
- 12. T. Masser and D. ben-Avraham, Kinetics of coalescence, annihilation and the *q*-state Potts model in one dimension, *Phys. Lett. A* **275**:382–385 (2000).