Ballistic random walker

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We introduce and investigate the scaling properties of a random walker that moves ballistically on a two-dimensional square lattice. The walker is scattered (changes direction randomly) every time it reaches a previously unvisited site, and follows ballistic trajectories between two scattering events. The asymptotic properties of the density of unvisited sites and the diffusion exponent can be calculated using a mean-field theory. The obtained predictions are in good agreement with the results of extensive numerical simulations. In particular, we show that this random walk is subdiffusive. [S1063-651X(96)04007-X]

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I. INTRODUCTION

Random motion has been a subject of constant interest in the history of modern physics. Since critical phenomena made us appreciate the presence of power laws in nature, random walks became a paradigm of various models involving stochastic motion and disorder [1]. In recent years, much attention has been focused on *interacting random-walk* models that differ from traditional random-walk models, such as Brownian motion (BM) [2], in that the walker's motion at a given time depends on its previous trajectory. Examples include the self-avoiding random-walk model [3], which describes the statistics of polymer growth, the ''true'' self-avoiding random walk [4], in which the probability of stepping to a previously visited site depends on the number of times that the site has been visited in the past, the interacting walk of Stanley *et al.* [5], and the Domb-Joyce model [6]. For a comparative study of these models, see Duxbury *et al.* [7].

In order to understand the scaling properties of random walks, one usually studies the time dependence of the mean-square displacement (end-to-end distance of the walk after t time steps), $\langle R^2(t)\rangle$, and the mean number of distinct sites visited, $\langle S(t)\rangle$. For BM, these quantities behave asymptotically as $\langle R^2(t)\rangle \sim t$ and $\langle S(t)\rangle \sim t/\ln t$ [8].

Using the critical exponent ν, defined by $\langle R^2(t)\rangle \sim t^{2\nu}$, random walks can be classified according to their diffusive behavior. Models for which self-intersections are unfavored are superdiffusive, with $\nu > 1/2$. Including self-intersecting dynamics favors subdiffusive behavior, for which $\nu < 1/2$.

In this paper we introduce and study a model describing the ballistic motion of a non-Markovian random walker, which we call the ballistic random-walk (BRW) model. We investigate how the ballistic trajectory affects the dynamics of the motion, the scaling exponents, and the number of visited sites. The scaling exponents are calculated using a mean-field theory and the obtained predictions compared to numerical simulations.

The model is defined on a two-dimensional (2D) square lattice with size $L \times L$ (generalization to higher dimensions and other geometries is straightforward). At time $t=0$, each lattice site is occupied with a particle of type A, except for the site at the center of the lattice, where we place a random walker (particle B). The walker B moves ballistically on the surface, following a straight trajectory along the x or y direction. When B meets an A particle, it desorbs it from the surface, leaving behind an empty site. After every desorption event, the walker B changes its direction of motion randomly, continuing its ballistic motion in any of the four possible directions starting from the newly emptied site. Alternatively, the model described corresponds to the reaction-diffusion process of type $A+B \rightarrow B$, for which the density of the diffusing B particles is constant $(1/L^2)$, while the number of A particles decreases monotonically from the initial value, L^2 [9].

The model has two ingredients that make analytical progress particularly difficult. First, the model is neither deterministic nor completely random, and therefore the conventional approaches available to study random or deterministic systems need to be combined somehow. Second, the dynamics is non-Markovian because the distribution of random scatterers (A particles) changes with time.

We now present numerical calculations and theoretical arguments to understand the diffusion of particle B. We carry out simulations on square lattices of linear sizes up to $L=22\,528$. Each simulation ends when the B particle reaches the boundary. In Fig. 1(a), we show the surviving particles (unvisited sites) after $10^{9.75}$ time steps [10], when the B particle has not yet reached the boundary. We observe that, for long enough times ($t>10^7$), the visited sites form a roughly circular cluster. Moreover, the density of visited sites is close to 1 for a large area around the starting point. Thus, the connected cluster formed of the visited sites is compact, in contrast to fractal clusters generated by BM, as illustrated in Fig. 1(b).

II. SUBDIFFUSIVE BEHAVIOR

To investigate the scaling properties of the system, we evaluate $\langle R^2(t)\rangle$ for the walker B. As shown in Fig. 2, we

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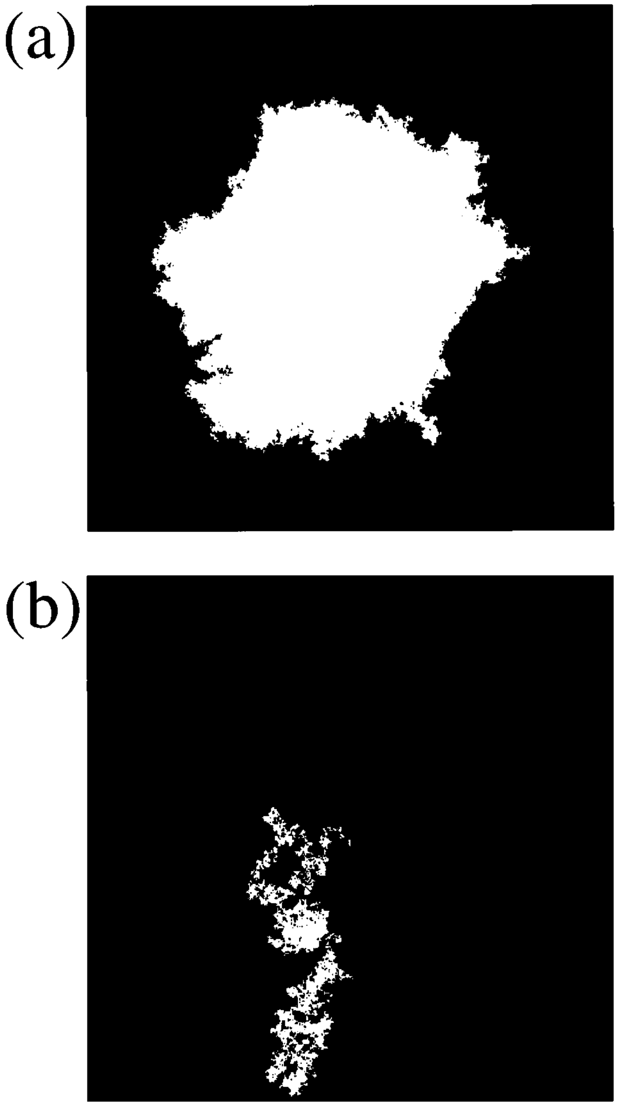

FIG. 1. The distribution of the visited (white) and unvisited (black) sites in a 22528×22528 square lattice for (a) the ballistic random walker and (b) the standard random walker (Brownian motion), after $10^{9.75}$ and $10^{7.75}$ time steps, respectively. In both cases, the walker started from the geometrical center of the figure.

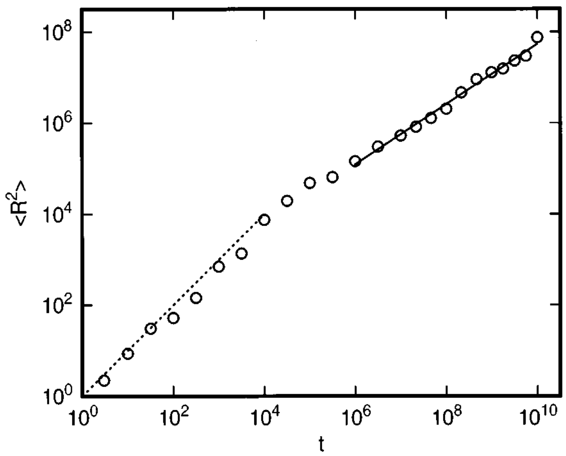

FIG. 2. Mean-square displacement, $\langle R^2(t)\rangle$, as a function of time for the ballistic random walker. The short time behavior is diffusive, $[\langle R^2(t)\rangle \sim t$, dashed line], followed by a crossover to a subdiffusive regime $[\langle R^2(t)\rangle \sim t^{0.66\pm0.02}$, continuous line]. Averages over 20 runs were taken.

find that, for early times, the diffusion follows Einstein's law ($\nu = 1/2$) [2]. This behavior dominates the scaling up to 10^2 time steps. However, the BRW is asymptotically subdiffusive: for time scales larger than $10^{5.5}$, we observe a crossover to the subdiffusive regime: $\langle R^2(t)\rangle \sim t^{0.66\pm0.02}$.

In order to understand the crossover behavior, we first discuss qualitatively the motion of the walker. At the early stages of the diffusion process, the density of A particles, $\rho(L,t)$, is very close to 1. Accordingly, the probability that the walker B hits an A particle (and consequently is scattered) is very high, and therefore its trajectory is very similar to that of BM. However, $\rho(L,t)$ decreases with time and the probability that the walker reaches an empty site in its evolution increases. Thus, between two scattering events, the walker has longer and longer distances to go ballistically. The set of visited sites is connected, and a closed contour of nondesorbed A particles defines the border of the cluster of visited sites. The asymptotic properties of the model depend essentially on the topology of this cluster. At this point we need to make two observations, which form the basis of our theoretical arguments: (1) For large times the cluster of visited sites is approximately circular. (2) Deviations from circularity generate only (asymptotically negligible) corrections. Next we derive the asymptotic scaling behavior of the cluster of empty sites based on these two properties.

Let us assume that, at a particular time, a circular cluster with radius R and area $S = \pi R^2$ has been formed. Whenever the walker reaches the circular border, an A particle is desorbed. In the next time step, the walker can either (i) bounce back, inverting its direction and traveling across the cluster without scattering until it reaches the opposite wall, (ii) be scattered in a direction perpendicular to the border normal, or (iii) keep the same direction and move one site deeper in the region of occupied sites. The time required to generate a change dS in the circle area obeys [11] $dt/dS = \alpha(R) + \beta R$, where β is a proportionality constant $(0 < \beta \leqslant 1/2)$. The contributions to $\alpha(R)$ depend on powers of R smaller than 1 and, therefore, are negligible in the large R limit. After integrating dt/dS, we obtain $t \sim R^3$, or $R^2 \sim t^{2/3}$, corresponding to subdiffusive behavior with $\nu = 1/3$. This agrees well with the numerical results $\nu = 0.33 \pm 0.01$ [12], shown in Fig. 2. This good coincidence supports our starting observation that the walker spends most of its time traveling across the empty central region. Consequently, there is a change in the dynamics of the system, corresponding to a crossover from a diffusive regime with $\nu \sim 1/2$, in the early stages of the evolution, induced by the Brownian-like motion, to an asymptotic subdiffusive behavior with $\nu = 1/3$.

III. DENSITY OF SURVIVING PARTICLES

We define $\rho_s(L)$ as the final density of unvisited sites, i.e., the density of A particles when the walker, starting at the geometrical center at $t = 0$, reaches the boundary of the

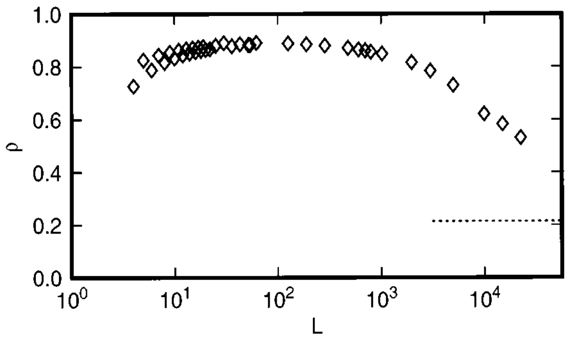

FIG. 3. Density of unvisited sites (surviving A particles) for the ballistic random walker. The dashed line shows the asymptotic density $1-\pi/4$ predicted by the mean-field theory as $L\to\infty$. Statistical averaging in the simulations ranges from 10^5 runs for the smallest lattice sizes to 64 runs for the largest ($L=22528$).

$L\times L$ square lattice. As shown in Fig. 3, for the BRW, $\rho_s(L)$ exhibits a broad plateau centered at $L=10^2$, after which it decreases.

To clarify this behavior, we again have to return to our earlier picture, that in the asymptotic regime the border forms a circle of radius R. However, R increases with time. In the model, the simulation is stopped, and thus $\rho_s(L)$ is calculated when the particle first reaches the wall of the square lattice. In the mean-field description described above, this corresponds to the circle reaching the boundary of the lattice. At this point the circle has a radius $L/2$, and an area $\pi L^2/4$. Since we assume that all particles inside the circle were removed, the number of surviving sites is given by $L^2-\pi L^2/4$, giving the asymptotic density as $\rho_s^*=1-\pi/4$. However, this limit is approached very slowly by $\rho_s(L)$; ρ_s^* is reached only when the border width is negligible compared with the cluster radius. Unfortunately, system size limitations do not allow us to observe the asymptotic behavior of the density (the largest system size, 22528×22528, is already large compared to sizes studied for similar problems in computational physics). However, as Fig. 3 indicates, the density indeed shows a tendency to decrease towards the predicted asymptotic value, ρ_s^*.

It is interesting to compare the observed dynamics with that of the BM in 2D. In the latter, the number of distinct sites visited behaves asymptotically as $t/\ln(t)$ [8]. Therefore, the density of remaining particles in a circle of radius $R\sim\sqrt{t}$ goes as $1-\gamma/\ln(t)$, with γ constant. Thus, $\rho_s(L)$ for the BM approaches 1 for large L. It is remarkable that a simple change in the dynamical rule, i.e., that there is only scattering on the (previously) unvisited sites, changes enormously the density of visited places for $L\to\infty$, going from 0 for the BM case to a finite constant for the BRW. Another difference when comparing with BM in 2D is the formation of a compact, almost circular cluster of visited sites.

IV. BORDER WIDTH

In the previous arguments, we assumed that the walker generated a perfect circle with a smooth boundary. In fact, the border width has some non-negligible roughness as can be seen in Fig. 1(a). This roughness increases with time, and if this increase is fast enough, it may invalidate our mean-field assumption that asymptotically the border is well approximated with a smooth circle. To validate our mean-field calculation, it is necessary to show that asymptotically the border width is negligible compared to R. For this, we study the radial distribution of unvisited sites, $\rho_R(r,L,t)$, which is obtained from radially averaging time snapshots of the 2D density distribution of unvisited sites, as the one shown in Fig. 1(a). Then we compute the partial derivative of $\rho_R(r,L,t)$, as a function of the radial coordinate r, with the origin at the geometrical center (starting point). This derivative is only different from 0 at the boundary between visited and unvisited sites, and has a maximum at the radial distance for which the variation in the density of unvisited sites is the largest. To characterize the size of the interval with nonvanishing $\partial\rho_R/\partial r$, we calculate the full width at half maximum (FWHM) of this derivative. A relevant quantity for our problem is the ratio between the FWHM and the distance of the boundary between visited and unvisited sites to the origin, $r_b(L,t)$, defined by $\rho_R(r_b,L,t)=0.5$. At a distance $r_b(L,t)$, the radial densities of visited and unvisited sites are equal, i.e., 0.5. We find that the ratio FWHM/r_b decreases in time. Therefore, for long times, the thickness of the boundary becomes negligible in comparison with r_b, as we assumed in the mean-field theory developed above.

Note that the region of nonvanishing $\partial\rho_R/\partial r$ corresponds to two different sorts of borders: those of small clusters of unvisited sites trapped inside the connected cluster of visited sites, and the single border between the cluster of visited sites and the outside 2D bulk of unvisited sites. To determine numerically and/or analytically the statistical properties of this single border would be an interesting task for future work. In particular, it would be worthwhile to investigate if the roughening of the boundary can be described by continuum theories normally used to describe the roughening of various interfaces, and to identify the particular universality class to which it belongs [13].

V. CONCLUSIONS

We have introduced and investigated a random-walk model in which the walker is scattered only when a site is visited by the walker for the first time. Subsequent visits to these sites have no effect on the walker. As a result, the walker follows straight (ballistic) trajectories between random changes in its direction. Extensive numerical simulations on a 2D square lattice have been carried out to show that the motion is subdiffusive. A mean-field theory is developed that can account for the subdiffusive behavior and for the asymptotic density of unvisited sites.

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[9] The general model, including an arbitrary initial distribution of both types of particles, can be studied in the context of interacting-particle systems, which have attracted considerable attention recently. Some of the models in this field are catalytic reactions mediated by a surface [R.M. Ziff *et al.*, Phys. Rev. Lett. **56**, 2553 (1986); P. Grassberger, Z. Phys. B **47**, 255 (1982)], contact processes, and related models with absorbing states [see, e.g., *Percolation Structures and Processes*, edited by G. Deutsher *et al.*, *Annals of the Israel Physical Society*, (Hiler, Bristol, 1980), Vol. 5; J. Marro and R. Dickman, *Nonequilibrium Phase Transitions and Critical Phenomena* (Cambridge University Press, Cambridge, 1996)], branching annihilating random walks [P. Grassberger *et al.*, J. Phys. A **17**, L105 (1984); P. Grassberger, *ibid.* **22**, L1103 (1989); I. Jensen, *ibid.* **26**, 3921 (1993)], $A+A\rightarrow 0$ (diffusive annihilation of particles of one type) [L. Peliti, J. Phys. A **19**, L365 (1986); K. Kang and S. Redner, Phys. Rev. A **30**, 2833 (1984)], $A+B\rightarrow 0$ (diffusive annihilation of particles of different species) [D. Toussaint and F. Wilcsek, J. Chem. Phys. **78**, 2642 (1983); K. Kang and S. Redner, Phys. Rev. Lett. **52**, 955 (1984); F. Leyvraz and S. Redner, Phys. Rev. A **46**, 3132 (1992); Phys. Rev. Lett. **66**, 2168 (1991); H. Larralde *et al.*, Phys. Rev. A **46**, 855 (1992); **46**, R6121 (1992); M. Araujo *et al.*, Phys. Rev. Lett. **68**, 1791 (1992); **71**, 3592 (1993)], models of ballistic annihilation (i.e., the particles move with a given velocity distribution instead of randomly hopping at each time, and annihilating each other when they collide) [E. Ben-Naim *et al.*, Phys. Rev. Lett. **70**, 1890 (1993); P. L. Krapivsky *et al.*, Phys. Rev. E **51**, 3977 (1995); J. Piasecki, *ibid.* **51**, 5535 (1995), and references therein], and models with traps [P. Grassberger and I. Procaccia, J. Chem. Phys. **77**, 6281 (1982); A. Szabo *et al.*, Phys. Rev. Lett. **61**, 2496 (1988)]. A study of our model in that framework will be addressed elsewhere [M.A. Muñoz, D.O. Martínez, P. Molinàs-Mata, and A.-L. Barabási (unpublished)].

[10] We define time step as the time spent in reaching a nearest neighbor site at constant speed.

[11] We derive this expression by calculating the mean free path (or time) between scattering events or time required to reduce the density of A particles by 1. With a probability 1/4, the B particle travels large distances (of order of the circle diameter, $4\beta R, 0<\beta\leqslant 1/2$) through the empty bulk until desorbing an A particle again (i). The product gives the βR term. Scattering perpendicular to the border normal (ii), with probability 1/2, results in a term proportional to $\sqrt{R}$, whereas a constant term, 1/4, arises from the B particle desorbing the neighboring A particle when moving one step towards the 2D bulk.

[12] While the radius of the circle is not equal to the mean-square displacement, we expect that the two quantities scale with the same exponent, since the motion of the walker is bounded by the perimeter formed by the unvisited sites, which in the mean-field description corresponds to the circle.

[13] For a review, see A.-L. Barabási and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, Cambridge, 1995); *Dynamics of Fractal Surfaces*, edited by F. Family and T. Vicsek (World Scientific, Singapore, 1991).