Weak subordination breaking for the quenched trap model

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We map the problem of diffusion in the quenched trap model onto a different stochastic process: Brownian motion that is terminated at the coverage time $\mathcal{S}_\alpha = \sum_{x=-\infty}^{\infty}(n_x)^\alpha$, with n_x being the number of visits to site x. Here $0 < \alpha = T/T_g < 1$ is a measure of the disorder in the original model. This mapping allows us to treat the intricate correlations in the underlying random walk in the random environment. The operational time $\mathcal{S}_\alpha$ is changed to laboratory time t with a Lévy time transformation. Investigation of Brownian motion stopped at time $\mathcal{S}_\alpha$ yields the diffusion front of the quenched trap model, which is favorably compared with numerical simulations. In the zero-temperature limit of $\alpha \to 0$ we recover the renormalization group solution obtained by Monthus [Phys. Rev. E **68**, 036114 (2003)]. Our theory surmounts the critical slowing down that is found when $\alpha \to 1$. Above the critical dimension 2, mapping the problem to a continuous time random walk becomes feasible, though still not trivial.

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I. INTRODUCTION

Random walks in disordered systems with a diverging expected waiting time have attracted vast interest over many decades. Two approaches in this field are the annealed continuous time random walk (CTRW) model and the quenched trap model (QTM). Starting in the 1970s, the Scher-Montroll CTRW approach was used to model subdiffusive photocurrents in amorphous materials [1–4] and for contaminant transport in hydrology [5]. Bouchaud and co-workers showed that the trap model is a useful tool for the description of aging phenomena in glasses [6–10]. Then fractional kinetic equations that describe the CTRW dynamics became a popular tool [11]. More recently these models were used to describe non-self-averaging [12,13] and weak ergodicity breaking [6,14], which is important for the statistical description of dynamics of single quantum dots [15] and single molecules in living cells [16,17].

This paper presents a different approach for random walks in a quenched random environment, i.e., site disorder at each lattice point is fixed in time. Because of its generality, this topic has attracted tremendous interest in terms of physics [11,18–24] and mathematics [25–27]. For the QTM the critical dimension is 2 [19,28–31]. Above two dimensions the Scher-Montroll CTRW, which is a mean field theory, qualitatively describes the type of subdiffusive process that originates from an anomalous waiting time distribution. According to Polya's theorem [32,33] on a simple lattice and in dimension 3, a random walk is nonrecurrent. Hence, in a disordered system the particle (roughly speaking) tends to visit new lattice points along its path. In contrast, in one dimension the random walk is recurrent and a particle visits the same lattice point many times. Thus, above the critical dimension the CTRW approach works well, but fails in one dimension due to correlations of the random walk with the disorder. In other words, the renewal theory used within the annealed CTRW framework is not a valid description of the QTM [19]. Beyond the mean field renormalization group methods are used to tackle the problem of random walks in quenched environments [22,28,34,35]. For example, Machta [28] found the scaling exponents of the QTM and Monthus [34] investigated its diffusion front in the limit of zero temperature (see details below). While the renormalization group method is powerful, it has its limitations: A simple approach that can predict the diffusion front of random walkers in the QTM is still missing.

We provide an alternative approach for random walks in the QTM, which we call weak subordination breaking. For the CTRW it is well known that one may decompose the process into ordinary Brownian motion and a Lévy time process, an approach called subordination [36–40]. In this scheme normal Brownian motion takes place in an operational time s. The disorder is effectively described by a Lévy time transformation from operational time s to laboratory time t (see details below). This method is not intended for random walks in fixed random environments since it is based on the renewal assumption. The latter implies the neglect of correlations in the sense that waiting times are not specific to a lattice site. So a different approach capable of dealing with quenched disorder is now investigated. A brief summary of our results was published in Ref. [41].

This paper is organized as follows. After presenting the QTM in Sec. II, we briefly review the standard subordination scheme in Sec. III. The concept of random time in the QTM is presented in Sec. IV, which leads to weak subordination breaking in Sec V. General properties of the diffusion front $\langle P(x,t)\rangle$ are found in Sec. VI, while Secs. VII and VIII deal with the limits of strong and weak disorder, respectively. Section IX discusses critical slowing down. Throughout the work we compare theory with numerical simulations.

II. QUENCHED TRAP MODEL

We consider a random walk on a one-dimensional lattice with lattice spacing equal to one. For each lattice site x there is a quenched random variable τ_x, which is the waiting time between jump events for a particle situated on x. After time τ_x has elapsed the particle jumps to one of its two nearest neighbors with equal probability. The particle starts on the origin $x = 0$ at time $t = 0$, waits for time τ_0, then jumps (with probability 1/2) to $x = 1$, waits there for τ_1, etc. Note that if the particle returns to $x = 0$ it will wait there again for a time interval τ_0. The $\{\tau_x\}$ are positive independent identically distributed random variables with a common probability density function (PDF) $\psi(\tau_x)$. The goal of this paper is to find the long-time behavior of $\langle P(x,t)\rangle$, the probability of finding the particle on x at time t averaged over the disorder. For details on QTM see [19,31,42,43].

In the literature two related models are usually considered. The first model, which we use in simulations presented below, assumes that for a given lattice site x a particle will wait for a fixed waiting time τ_x. A slightly more physical approach is to assume that waiting times on lattice point x are exponentially distributed with a mean τ_x. Bertin and Bouchaud [42] showed that the two approaches yield the same asymptotic results in the limit of long measurement times.

In this paper our main interest is with power law waiting times

$$\psi(\tau_x) \sim \frac{A}{|\Gamma(-\alpha)|}(\tau_x)^{-(1+\alpha)} \tag{1}$$

for $\tau \to \infty$ and $0 < \alpha < 1$. The mean waiting time $\langle \tau_x\rangle = \infty$ and in this sense the diffusion is scale free. According to the Tauberian theorem [32], the Laplace transform of the waiting time PDF is

$$\hat{\psi}(u) \sim 1 - Au^{\alpha} + \cdots \tag{2}$$

for $u \to 0$. In the QTM the physical mechanism leading to these power laws is based on trapping dynamics [19]. On a lattice points x we randomly assign traps. The energy depth of the trap on x is E_x and the process of activation from a trap is thermal. According to the Arrhenius law, $\tau_x \propto \exp(E_x/T)$, where T is the temperature. Then assume that the PDF of $E_x > 0$ is exponential $f(E_x) = \exp(-E_x/T_g)/T_g$, where T_g is a measure of the energy disorder. One easily finds

$$\alpha = \frac{T}{T_g}, \quad A = |\Gamma(-\alpha)|\alpha. \tag{3}$$

Due to the Boltzmann factor $\tau_x \propto \exp(E/T)$, small changes in energy lead to exponential changes in waiting times, thus it is enough to have an exponential distribution of energy traps to obtain power law waiting times. Experimental observation of the linear dependence of α on temperature, in photocurrent spectroscopy in As_2Se_3 can be found in Fig. 3 in Ref. [44]. We note that the stochastic dynamics under investigation describes several other mechanisms of anomalous diffusion (caused by effective waiting times that are anomalously distributed) beyond the QTM [12]. For example, random walks on comb structures with power law distributed lengths of the comb's teeth mimic a random walk on the percolation cluster. Thus the trap model describes both energetic disorder and spatial disorder.

In what follows we will also consider the limit $\alpha \to 1$. This limit is meant in the sense that $\hat{\psi}(u) \sim 1 - Au\ldots$, which means that the average waiting time is finite (a Gaussian diffusion front). The very special border case $\psi(\tau_x) \propto \tau^{-2}$ was treated by Bertin and Bouchaud [42]. It yields Gaussian diffusion with logarithmic corrections and is not treated here.

III. SUBORDINATION IN THE ANNEALED TRAP MODEL, CTRW APPROACH

We now briefly review the annealed version of the model: For the well investigated Scher-Montroll-Weiss CTRW [11,19,32] in particular we discuss the concept of time subordination [36–40]. Later we contrast the CTRW approach with the intricate problem of the quenched type. The CTRW model considered here is for a one-dimensional random walk on a lattice with lattice spacing equal to unity. Starting on the origin $x = 0$ at time $t = 0$, the particle waits for a time t_1 and then jumps to one of its nearest neighbors (lattice points $x = 1$ or -1) with equal probability. The process is then renewed, namely, the particle waits on lattice point 1 (for example) for time t_2 until it jumps back to 0 or 2, etc. The waiting times $\{t_1,t_2,\ldots,t_n,\ldots\}$ are independent, identically distributed random variables with a common PDF $\phi_\alpha(t)$. Here t_n is the nth waiting time, which is not correlated with a specific lattice point x and hence clearly the CTRW model is very different from the quenched case. Similar to the quenched case, we consider waiting time PDFs with a diverging averaged waiting time $\int_0^\infty t\phi_\alpha(t)dt = \infty$, namely,

$$\phi_\alpha(t) \sim \frac{A_\alpha}{|\Gamma(-\alpha)|}t^{-(1+\alpha)}, \tag{4}$$

with $0 < \alpha < 1$ and $A_\alpha > 0$. The corresponding Laplace transform of the waiting time PDF behaves like

$$\hat{\phi}_\alpha(u) \sim 1 - A_\alpha u^\alpha + \cdots \tag{5}$$

when u is small. It is well known that the diffusion is anomalous $\langle x^2\rangle \propto t^\alpha$ [11,19].

Let $P(x,t)$ be the probability of finding the particle on x at time t. By conditioning the number of jumps s performed until time t,

$$P(x,t) = \sum_{s=0}^{\infty} n_t(s)q(x,s), \tag{6}$$

where $n_t(s)$ is the probability of performing s jumps in the time interval $(0,t)$ and $q(x,s)$ is the probability that after s steps the particle is located on x. In the limit of large t the number of jumps s is also large. Following Ref. [19], we apply the Gaussian central limit theorem

$$q(x,s) \sim \frac{1}{\sqrt{2\pi s}}e^{-x^2/2s}, \tag{7}$$

which is valid when $s \to \infty$. Here we used the model assumption that the variance of the jump lengths is unity, i.e., the lattice spacing is equal to 1.

To find $n_t(s)$ we consider the random time

$$t = \sum_{i=1}^{s} t_i. \tag{8}$$

In the limit of large s the time is a sum of many independent identically distributed random variables with a diverging mean waiting time (since $0 < \alpha < 1$). Hence Lévy's limit theorem applies. Let

$$\eta = \frac{t}{s^{1/\alpha}}; \tag{9}$$

then in the $s \to \infty$ limit

$$\langle e^{-u\eta}\rangle = \hat{\phi}_\alpha^s\left(\frac{u}{s^{1/\alpha}}\right) = \left(1 - \frac{A_\alpha u^\alpha}{s} + \cdots\right)^s \to e^{-A_\alpha u^\alpha}. \quad (10)$$

Namely, the PDF of $\eta > 0$ is a one-sided Lévy function denoted by $l_{\alpha,A_\alpha,1}(\eta)$, which is defined via its Laplace pair

$$\int_0^\infty e^{-u\eta} l_{\alpha,A_\alpha,1}(\eta)d\eta = e^{-A_\alpha u^\alpha}. \quad (11)$$

These Lévy PDFs are well investigated: Their series expansion, asymptotic behaviors, and graphic presentations can be found in Refs. [45–47]. Information on these PDFs essential for our work are summarized in Appendix A. From the PDF of η we find the PDF of s. Since both s and t are increasing along the process the transformation is straightforward. Using Eq. (10) and $\eta^{-\alpha} = s/t^\alpha$ we find the well known PDF of s [19],

$$n_t(s) \sim \frac{t}{\alpha} s^{-1/\alpha - 1} l_{\alpha,A_\alpha,1}\left(\frac{t}{s^{1/\alpha}}\right). \quad (12)$$

In the long-time limit the Green's function of the CTRW process is thus given by [19,36]

$$P(x,t) \sim \int_0^\infty n_t(s) e^{-x^2/2s}/\sqrt{2\pi s}\, ds, \quad (13)$$

where we switched from a summation in Eq. (6) to integration.

The time transformation (13) maps normal Gaussian diffusion to anomalous diffusion. In Ref. [37] $P(x,t)$ was obtained in d dimensions by solving the integral transformation, which applies more generally to solutions of the fractional time Fokker-Planck equation [48]. More importantly, we may think of s as an operational time in which usual Brownian motion is performed. The operational time s is a random variable whose statistics is determined by the PDF $n_t(s)$, where t is a laboratory time. In other words, the annealed disorder turns the operational time to a random variable. We note that subordination scheme can be formulated for the trajectories of the corresponding paths, in a continuum limit of the walk, and has been the topic of extensive research [49–56].

Not surprisingly, subordination of this type does not work for the QTM in one dimension. As mentioned in the Introduction, the process of a random walk in a QTM is clearly not a simple renewal process. The particle returning to a lattice point already visited "remembers" its waiting time there. Mathematicians have rigorously shown that in dimensions higher than one [30] or in the presence of a bias [57] (see also Refs. [58–60]) the CTRW approach describes well the quenched dynamics since the particle does not tend to revisit the same lattice points many times, thus confirming physical insight in Refs. [18,19,28] (for dimension $d = 2$ logarithmic corrections are also important). Nevertheless, some specific quantities are still different for the annealed and the quenched type of behavior even for dimension higher than one (see, for example, Refs. [8,9]). While the diffusion front for the three-dimensional QTM belongs to the domain of attraction of the CTRW, the calculation of the anomalous diffusion constant is not trivial (see the discussion in the summary). Here we focus our attention on the unsolved case, i.e., the QTM in one dimension, since there the Scher-Montroll CTRW picture [11,19,32] breaks down.

IV. TIME IN THE QUENCHED TRAP MODEL

The time t in the QTM is

$$t = \sum_{x=-\infty}^{\infty} n_x \tau_x, \quad (14)$$

where n_x is the number of visits to lattice point x, which we call the visitation number of site x. Since we are interested in $\langle P(x,t)\rangle$, where the angular brackets are for an average over the disorder, we will consider ensembles of paths on a large ensemble of realizations of disorder. As mentioned, the $\{\tau_x\}$ are independent identically distributed random variables with a common PDF $\psi(\tau_x)$ and the $\{n_x\}$ are also random variables.

Let us consider the random variable

$$\eta = \frac{t}{(\mathcal{S}_\alpha)^{1/\alpha}}, \quad (15)$$

where

$$\mathcal{S}_\alpha = \sum_{x=-\infty}^{\infty} (n_x)^\alpha \quad (16)$$

and we call $\mathcal{S}_\alpha$ the α coverage time. At this stage it is convenient to consider paths where $\mathcal{S}_\alpha$ is fixed and t is random and later we will switch to the opposite situation (similar to the arguments for s and t in the CTRW model). When $\alpha = 1$, $\mathcal{S}_\alpha$ is the total number of jumps made $\sum_{x=-\infty}^{\infty} n_x = s$. In the opposite limit $\alpha \to 0$, the α coverage time $\mathcal{S}_0$ is the distinct number of sites visited by the random walker, which is called the span of the random walk. Notice that t in Eq. (14) is a sum of nonindependent and nonidentical random variables.

We show that the PDF of η, $\eta_{\rm PDF}$, in the limit $\mathcal{S}_\alpha \to \infty$, is a one-sided Lévy stable function

$$\eta_{\rm PDF} \equiv l_{\alpha,A,1}(\eta). \quad (17)$$

Namely, the heavy tailed distribution of the waiting times τ_x determines the statistics of η through the characteristic exponent α, while the visitation numbers $\{n_x\}$ determine the scaling through $\mathcal{S}_\alpha$. By definition the Laplace $\eta \to u$ transform of the PDF of η is

$$\langle e^{-\eta u}\rangle = \left\langle \exp\left[-\sum_{i=-\infty}^{\infty} \frac{n_i \tau_i}{(\mathcal{S}_\alpha)^{1/\alpha}} u\right]\right\rangle. \quad (18)$$

We average with respect to the disorder, namely, with respect to the independent and identically distributed random waiting times τ_x, and obtain

$$\langle e^{-u\eta}\rangle = \prod_{x=-\infty}^{\infty} \hat{\psi}\left[\frac{n_x u}{(\mathcal{S}_\alpha)^{1/\alpha}}\right], \quad (19)$$

where $\hat{\psi}(u)$ is the Laplace transform of the PDF of waiting times $\psi(\tau_x)$. Now assume $\hat{\psi}(u) = \exp(-Au^\alpha) \sim 1 - Au^\alpha + \cdots$. Then, using Eq. (19) we have

$$\langle e^{-u\eta}\rangle = \prod_{x=-\infty}^{\infty} \exp\left[-\frac{A(n_x)^\alpha u^\alpha}{\mathcal{S}_\alpha}\right] = e^{-Au^\alpha}. \quad (20)$$

Hence, if the waiting PDF is a one-sided Lévy PDF, i.e., $\hat{\psi}(u) = \exp(-Au^\alpha)$, so is the PDF of η. In Appendix B we consider the general case where $\psi(\tau_x)$ belongs to the domain of attraction Lévy PDFs [i.e., families of PDFs satisfying the equation $\hat{\psi}(u) \sim 1 - Au^\alpha + \cdots$]. We prove there that the statement in Eq. (17) is still valid.

From Eq. (17) we learn that the CTRW operational time s, that is, the number of jumps made in the random walk, loses its importance in the quenched model. In the QTM the operational time is the α coverage time $\mathcal{S}_\alpha$. We now invert the process fixing time t to find the PDF of $\mathcal{S}_\alpha$,

$$n_t(\mathcal{S}_\alpha) \sim \frac{t}{\alpha}(\mathcal{S}_\alpha)^{-1/\alpha-1} l_{\alpha,A,1}\left[\frac{t}{(\mathcal{S}_\alpha)^{1/\alpha}}\right]. \qquad (21)$$

In the following section we explain how to use the operational time $\mathcal{S}_\alpha$ to obtain the desired diffusion front of the QTM.

V. WEAK SUBORDINATION BREAKING

To find the solution of the problem, namely, to find $\langle P(x,t)\rangle$ for the QTM, we follow the following steps.

(i) Choose the laboratory time t, which is a fixed parameter.

(ii) Use a random number generator and draw the stable random variable η from the one-sided Lévy law $l_{\alpha,A,1}(\eta)$.

(iii) With η and t determine the hitting target $\mathcal{S}_\alpha$, which according to Eq. (15) is $\mathcal{S}_\alpha = (t/\eta)^\alpha$.

(iv) Generate a binomial random walk on a lattice, with probability 1/2 for jumping left and right. Stop the process once its $\mathcal{S}_\alpha$ crosses the hitting target set in step (iii).

(v) Record the position x of the particle at the end of the previous step.

(vi) Go to step (ii). After this loop is repeated many times, we generate a histogram of x.

The histogram once normalized yields $\langle P(x,t)\rangle$ when t is large. Notice that in this scheme there is no disorder. The second step is implemented with a simple algorithm provided by Chambers *et al.* [61]. These authors show how to generate stable random variables such as η using two independent uniformly distributed random variables and for convenience their formula is provided in Appendix A.

More importantly, we can now start treating the problem analytically and find the diffusion front. So far we have replaced the problem of random walks in the QTM with a different stochastic process: Brownian motion, which is stopped when the hitting target $\mathcal{S}_\alpha$ is crossed. In other words, we got rid of the disorder. Notice that the CTRW process and standard subordination [36–40] are reached once we replace $\mathcal{S}_\alpha$ with s. In this sense the QTM exhibits what we call weak subordination breaking: The operational time is now $\mathcal{S}_\alpha$, although the Lévy time transformation used already in the usual subordination scheme of Eq. (13) remains a useful tool.

VI. DIFFUSION FRONT OF THE QUENCHED TRAP MODEL

Let $P_B(x,\mathcal{S}_\alpha)$ be the PDF of x for a binomial random walk on a lattice at operational time $\mathcal{S}_\alpha$. The subscript B indicates that the underlying motion is Brownian. The corresponding paths are generated from a random walk on a one-dimensional lattice, with equal probability of jumping left and right, which is stopped when $\mathcal{S}_\alpha$ is reached (or crossed for the first time). The averaged over disorder propagator of the QTM is found by using Eq. (21) and the scheme presented in the preceding section:

$$\langle P(x,t)\rangle \sim \int_0^\infty P_B(x,\mathcal{S}_\alpha) n_t(\mathcal{S}_\alpha) d\mathcal{S}_\alpha, \qquad (22)$$

which is valid in the long-time limit. Equation (22) is a generalization of the subordination equation (13). Namely, it transforms Brownian motion stopped at the coverage time $\mathcal{S}_\alpha$ to the QTM dynamics in laboratory time t.

From Eq. (22) we may find general properties of the Green's function $\langle P(x,t)\rangle$ in terms of its corresponding Brownian partner $P_B(x,\mathcal{S}_\alpha)$. For example, the Laplace $t \to u$ transform

$$\langle \hat{P}(x,u)\rangle = Au^{\alpha-1}\hat{P}_B(x,Au^\alpha). \qquad (23)$$

Less formal relations are found if we exploit the scaling behavior of Brownian motion, as we now explain.

A. Scaling arguments

Brownian motion follows the usual diffusive scaling $x^2 \propto s$, where s is the number of steps. In Appendix A we show that $s \propto (\mathcal{S}_\alpha)^{2/(1+\alpha)}$, which is now explained using simple arguments. For Brownian motion the particle explores a region that scales like $s^{1/2}$. The visitation number n_x within this region (i.e., roughly $|x| < s^{1/2}$) is the number of jumps made s divided by the number of sites in the explored region $s^{1/2}$, so $n_x \propto s/s^{1/2} = s^{1/2}$. Since particles typically visit $|x| \gg s^{1/2}$ rarely, we have in that region $n_x \propto 0$. Hence $\mathcal{S}_\alpha \propto \sqrt{s}(n_x)^\alpha \propto s^{(1+\alpha)/2}$. Indeed, in Appendix C we show that

$$\langle \mathcal{S}_\alpha\rangle = \mathcal{C}_\alpha s^{(1+\alpha)/2} \qquad (24)$$

with

$$\mathcal{C}_\alpha = \frac{2^{(\alpha+3)/2}\Gamma\left(1+\frac{\alpha}{2}\right)}{\sqrt{\pi}(1+\alpha)}. \qquad (25)$$

When $\alpha = 1$ we have $\mathcal{C}_1 = 1$ since $\mathcal{S}_1 = \sum_{x=-\infty}^{\infty} n_x = s$. In the opposite limit $\alpha = 0$ we find a well known result obtained by Dvoretzky and Erdös [62],

$$\langle \mathcal{S}_0\rangle = \sqrt{\frac{8s}{\pi}}. \qquad (26)$$

By definition $\langle \mathcal{S}_0\rangle$ is the averaged number of distinct sites visited by an unbiased random walker [32].

Using $x \propto s^{1/2}$ and $\mathcal{S}_\alpha \propto s^{(1+\alpha)/2}$ scalings, we have $x \propto (\mathcal{S}_\alpha)^{1/(1+\alpha)}$. We emphasize that this is a property of simple binomial random walks, which we can now exploit to investigate the solution of the QTM. More specifically this scaling implies

$$P_B(x,\mathcal{S}_\alpha) = \frac{1}{(\mathcal{S}_\alpha)^{1/(1+\alpha)}} B_\alpha\left[\frac{x}{(\mathcal{S}_\alpha)^{1/(1+\alpha)}}\right]. \qquad (27)$$

Here $B_\alpha(z)$ is a non-negative function normalized according to $\int_{-\infty}^{\infty} B_\alpha(z)dz = 1$. Further from the symmetry of the walk $B_\alpha(z) = B_\alpha(-z)$. As shown in Fig. 1, the PDF $B_\alpha(z)$ exhibits an interesting transition between a V shape for $\alpha \to 0$ and a Gaussian shape when $\alpha \to 1$. In the following sections we will investigate $B_\alpha(z)$ in detail.

With $B_\alpha(z)$ we obtain useful relations between the diffusion front of the trap model and Brownian motion. Define the

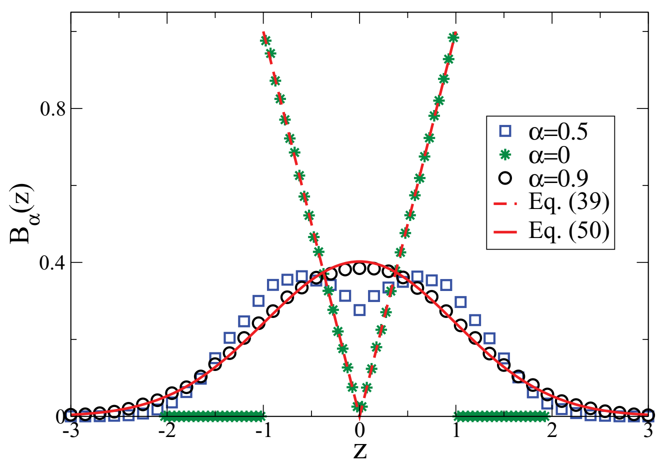

FIG. 1. (Color online) Presented behavior of the PDF $B_\alpha(z)$ as obtained by simulations of Brownian motion on a lattice (symbols) and compared to theoretical predictions [Eqs. (39) and (50)] without fitting. Here $B_\alpha(z)$ exhibits a transition between a Gaussian shape when $\alpha \to 1$ to a V shape when $\alpha \to 0$.

dimensionless time $\tilde{t} = t/A^{1/\alpha}$ and the scaling variable

$$\xi = \frac{x}{(\tilde{t})^{\alpha/(1+\alpha)}}. \tag{28}$$

Then it is easy to show that

$$\langle P(x,t)\rangle \sim \frac{g_\alpha(\xi)}{(\tilde{t})^{\alpha/(1+\alpha)}} \tag{29}$$

and using Eq. (22)

$$g_\alpha(\xi) = \int_0^\infty dy\, y^{\alpha/(1+\alpha)} B_\alpha(\xi y^{\alpha/(1+\alpha)}) l_{\alpha,1,1}(y). \tag{30}$$

For the behavior of $\langle P(x,t)\rangle$ on the origin we use

$$\int_0^\infty dy\, y^q l_{\alpha,1,1}(y) = \begin{cases} \infty & \text{for } q/\alpha > 1 \\ \frac{\Gamma(1-q/\alpha)}{\Gamma(1-q)} & \text{for } q/\alpha < 1 \end{cases} \tag{31}$$

and then find

$$\langle P(x=0,t)\rangle \sim B_\alpha(0)\frac{\Gamma\left(\frac{\alpha}{1+\alpha}\right)}{\Gamma\left(\frac{1}{1+\alpha}\right)(\tilde{t})^{\alpha/(1+\alpha)}}. \tag{32}$$

This is a useful result since the behavior of $B_\alpha(z)$ on the origin $z = 0$ gives the corresponding behavior of $\langle P(x=0,t)\rangle$ without the need to solve any integral. Further, Eq. (32) hints at an interesting behavior when $\alpha \to 0$. The ratio of the Γ functions diverges in that limit, hence, as shown in Fig. 1, $B_\alpha(z=0)$ must go to zero when $\alpha \to 0$ for $\langle P(x=0,t)\rangle$ to remain finite. Such a behavior is analytically investigated in the following section.

Another useful relation is found between the moments $\langle |x|^q\rangle = \langle \int_{-\infty}^{\infty} |x|^q P(x,t)dx\rangle$ of the original QTM and the moments $\langle |z|^q\rangle = \int_{-\infty}^{\infty} |z|^q B_\alpha(z)dz$. Using Eqs. (30) and (31) we find

$$\langle |x|^q\rangle = \langle |z|^q\rangle \frac{\Gamma\left(\frac{q}{1+\alpha}\right)}{\alpha\Gamma\left(\frac{q\alpha}{1+\alpha}\right)}(\tilde{t})^{\alpha q/(1+\alpha)}. \tag{33}$$

The scaling $x^2 \propto (\tilde{t})^{2\alpha/(1+\alpha)}$ was obtained long ago in Refs. [19,29] using elegant scaling arguments and in Ref. [28] using a renormalization group approach. The important content of Eqs. (30), (32), and (33) is that once we obtain $B_\alpha(z)$ from either theory or simulations of Brownian trajectories, we have a useful method to obtain exact statistical properties of the diffusion front.

TABLE I. Values of $\langle z^2\rangle$ and $B_\alpha(z=0)$, obtained from Brownian simulations on a lattice.

α	$\langle z^2\rangle$	$B_\alpha(z=0)$
0	0.5	0
0.1	0.592	0.08
0.2	0.673	0.15
0.3	0.746	0.2
0.4	0.808	0.24
0.5	0.859	0.28
0.6	0.907	0.3
0.7	0.929	0.33
0.8	0.961	0.35
0.9	0.986	0.38
1	1	$1/\sqrt{2\pi}$

On a computer our approach is very useful. For example, we have numerically generated Brownian trajectories on a lattice and obtained $B_\alpha(z)$ in Fig. 1 while $\langle z^2\rangle$ and $B_\alpha(0)$ are reported in Table I. With $\langle z^2\rangle$ given in Table I and Eq. (33) we get the mean square displacement of the QTM $\langle x^2\rangle$. Direct simulations of the QTM are favorably compared with the predictions of our theory in Fig. 2.

Finally, the cumulative distribution function $G_\alpha(\xi < \Xi) = \int_{-\infty}^{\Xi} g_\alpha(\xi)d\xi$, the probability that the random variable ξ attains a value less than Ξ, is found using Eq. (27):

$$G_\alpha(\xi < |\Xi|) = 1 - \int_0^\infty dz\, B_\alpha(z) L_\alpha\left[\left(\frac{z}{|\Xi|}\right)^{(1+\alpha)/\alpha}\right]. \tag{34}$$

Here $L_\alpha(y) = \int_0^y l_{\alpha,1,1}(y)dy$ is the cumulative distribution of a one-sided stable random variable. From symmetry

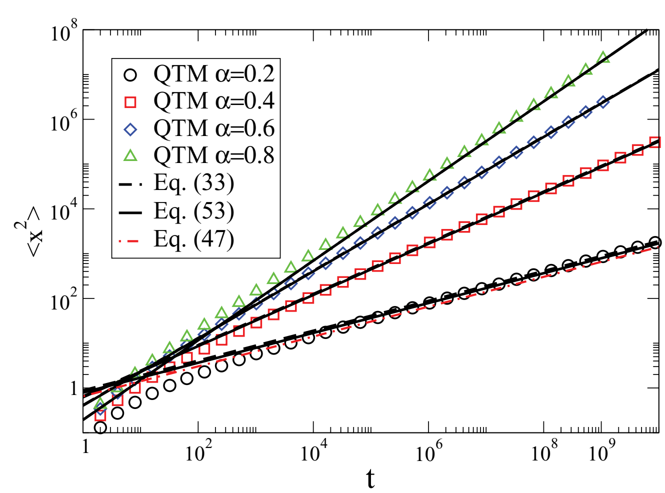

FIG. 2. (Color online) Mean square displacement versus time as obtained from QTM simulations (symbols), compared to the theory (lines) based on weak subordination breaking. Equation (53) is used for analytical predictions for $\alpha = 0.4,0.6,0.8$ and Eq. (47) is used for $\alpha = 0.2$.

$G_\alpha(\xi, -|\Xi|) = 1 - G_\alpha(\xi < |\Xi|)$. The integral representation of the distribution $L_\alpha(y)$ can be found in Ref. [61].

VII. LIMIT $\alpha \to 0$

As mentioned in the Introduction, the diffusion front $\langle P(x,t)\rangle$ was treated using a renormalization group method by Monthus [34]. We will now investigate this interesting limit using our approach. For that we must first find $B_\alpha(z)$ in the limit $\alpha \to 0$.

A. $\lim_{\alpha\to 0} B_\alpha(z)$ has a V shape

We consider Brownian motion on a lattice that is stopped once the distinct number of sites visited by the walker reaches the threshold $\mathcal{S}_0$ and as a reminder $\mathcal{S}_0$ is called the span. The position of the particle is then x and we are interested in the probability $P(x,\mathcal{S}_0)$ of finding the particle on x.

The particle starts on the origin, hence clearly we have $|x| \leqslant \mathcal{S}_0$. Further, $P(x=0,\mathcal{S}_0)=0$ since a particle starting on the origin cannot reach the threshold $\mathcal{S}_0$ when it is on the origin, i.e., a particle returning to the origin is not increasing $\mathcal{S}_0$ since the origin is not a new site visited by the walker. From symmetry $P(-x,\mathcal{S}_0)=P(x,\mathcal{S}_0)$.

Consider first $P(x=\mathcal{S}_0,\mathcal{S}_0)$. After the first step the particle can be either on $x=1$ with probability $1/2$ or on $x=-1$ with the same probability. Clearly a trajectory going through $x=-1$ cannot contribute to $P(x=\mathcal{S}_0,\mathcal{S}_0)$ since to reach $x=\mathcal{S}_0$ through $x=-1$ the span must be at least of length $\mathcal{S}_0+1$. So we consider only trajectories going through $x=1$. Trajectories going through $x=1$ are divided into three nonintersecting categories: (i) trajectories that never reach the origin $x=0$ along their path, (ii) trajectories that reach the origin but never cross it [see Fig. 3(a)], and (iii) trajectories that go below $x=0$. The latter will have a total span greater than $\mathcal{S}_0$ and hence do not contribute. For class (i) the span (after stepping into $x=1$ in the first step) is $\mathcal{S}_0-1$. Similarly for class (ii), the span is $\mathcal{S}_0$. For both cases the displacement (from $x=1$ to $\mathcal{S}_0$) is clearly $\mathcal{S}_0-1$. Hence we have

$$P(x=\mathcal{S}_0,\mathcal{S}_0) = \tfrac{1}{2}[P(x=\mathcal{S}_0-1,\mathcal{S}_0) + P(x=\mathcal{S}_0-1,\mathcal{S}_0-1)], \qquad (35)$$

where the first (second) term on the right-hand side describes trajectories returning (never returning) to the origin. The half in front of the square brackets is due to the displacement in the first jump event.

Continuing with similar reasoning, consider $P(x=\mathcal{S}_0-1,\mathcal{S}_0)$. The particle after the first step can be on either $x=1$ or -1. As shown in Fig. 3(b), if it is on $x=-1$ it must travel a distance $\mathcal{S}_0$ to reach its destination $\mathcal{S}_0-1$ while keeping the span $\mathcal{S}_0$. In contrast, if it jumps to $x=1$ the distance the particle must travel is $\mathcal{S}_0-2$ and the span is $\mathcal{S}_0$. Hence we have

$$P(x=\mathcal{S}_0-1,\mathcal{S}_0) = \tfrac{1}{2}P(x=\mathcal{S}_0,\mathcal{S}_0) + \tfrac{1}{2}P(x=\mathcal{S}_0-2,\mathcal{S}_0), \qquad (36)$$

where the first (second) term on the right-hand side describes trajectories starting on the origin and in the first step jumping to $x=-1$ ($x=1$). Similarly, for $\mathcal{S}_0-n>0$ with $n>0$ being an integer we have

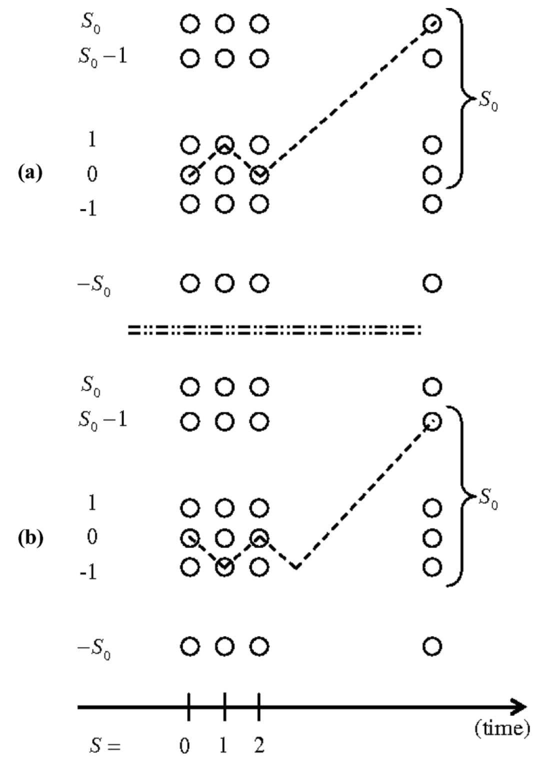

FIG. 3. (a) Trajectory with a span $\mathcal{S}_0$. The particle returns to the origin along its path [category (ii) in text]; hence, in the time interval $s>1$ (excluding the first step) the displacement is $\mathcal{S}_0-1$ and the span is $\mathcal{S}_0$. (b) A random walker with span $\mathcal{S}_0$ reaching $x=\mathcal{S}_0-1$ must pass through $x=-1$. Here the first jump event brings the particle to $x=-1$ and hence the span in $s>1$ is $\mathcal{S}_0$ and the displacement is $\mathcal{S}_0$.

$$P(x=\mathcal{S}_0-n,\mathcal{S}_0) = \tfrac{1}{2}P(x=\mathcal{S}_0-n-1,\mathcal{S}_0) + \tfrac{1}{2}P(x=\mathcal{S}_0-n+1,\mathcal{S}_0). \qquad (37)$$

Equations (35) and (37) are easily solved

$$P(x,\mathcal{S}_0) = \frac{|x|}{\mathcal{S}_0(\mathcal{S}_0+1)} \quad \text{for} \quad -\mathcal{S}_0 \leqslant x \leqslant \mathcal{S}_0 \qquad (38)$$

and $x \in \mathbf{Z}$. In the limit $\mathcal{S}_0 \gg 1$ we have, for the scaled variable $z = x/\mathcal{S}_0$, the PDF

$$\lim_{\alpha\to 0} B_\alpha(z) = \begin{cases} |z| & \text{for } |z|<1 \\ 0 & \text{otherwise.} \end{cases} \qquad (39)$$

We see that $B_{\alpha=0}(z)$ has a V shape. This reflects the observation that the particle reaching a large span $\mathcal{S}_0$ is most likely far from the origin and the probability of reaching the span $\mathcal{S}_0$ for the first time while the particle is on the origin is zero. We now use this property of Brownian motion to solve the quenched trap model in the limit $\alpha \to 0$.

B. Diffusion front in the $\alpha \to 0$ limit

Define the Fourier transform of the scaling function $g_\alpha(\xi)$ [Eq. (29)]

$$g_\alpha(k_\xi) = \int_{-\infty}^{\infty} e^{ik_\xi \xi} g_\alpha(\xi) d\xi, \qquad (40)$$

which as usual is also the moment generating function

$$g_\alpha(k_\xi) = \sum_{q=0}^{\infty} \frac{(ik_\xi)^{2q} \langle \xi^{2q} \rangle}{(2q)!}. \tag{41}$$

According to our theory, the moments $\langle (\xi)^{2q} \rangle = \int_{-\infty}^{\infty} g_\alpha(\xi) \xi^{2q} d\xi$ and similarly $\langle x^{2q} \rangle$ for the QTM are determined by Brownian motion with the help of the PDF $B_\alpha(z)$ [Eq. (33)]. In the limit $\alpha \to 0$ we find, using Eq. (39),

$$\langle z^{2q} \rangle = 2 \int_0^1 z^{2q} z \, dz = \frac{1}{1+q} \tag{42}$$

and hence for $\alpha \to 0$ Eqs. (28) and (33) give

$$\langle \xi^{2q} \rangle = \frac{(2q)!}{q+1}. \tag{43}$$

Therefore

$$\lim_{\alpha \to 0} g_\alpha(k_\xi) = \sum_{q=0}^{\infty} (-1)^q \left(\frac{1}{q+1} \right) (k_\xi)^{2q}. \tag{44}$$

Summing this series we find

$$\lim_{\alpha \to 0} g_\alpha(k_\xi) = \frac{\ln[1 + (k_\xi)^2]}{(k_\xi)^2}. \tag{45}$$

An inverse Fourier transform yields

$$\lim_{\alpha \to 0} g_\alpha(\xi) = e^{-|\xi|} - |\xi| E_1(|\xi|), \tag{46}$$

where $E_1(\xi) = \int_\xi^\infty (e^{-t}/t) dt$ is the tabulated exponential integral [63]. This result (written in a different but equivalent form) was obtained by Monthus [34] using the renormalization group method, which is exact in the limit $\alpha \to 0$. In Fig. 4 we show $g_\alpha(\xi)$ for simulations of the QTM ($\alpha = 0.1$), Brownian simulations using weak subordination breaking outlined in Sec. V, and an analytical curve [Eq. (46)]. We see that the theory that is exact when $\alpha \to 0$ works well also as an approximation for small values of α.

When α is small we find a useful approximation for the moments. Inserting $\langle |z|^q \rangle$ [Eq. (42)] in Eq. (33) we have

$$\langle |x|^q \rangle \simeq \frac{2}{2+q} \frac{\Gamma\left(\frac{q}{1+\alpha}\right)}{\alpha \Gamma\left(\frac{\alpha q}{1+\alpha}\right)} \left(\frac{t}{A^{1/\alpha}} \right)^{\alpha q/(1+\alpha)}. \tag{47}$$

Notice that in this limit $\Gamma[q/(1+\alpha)]/\{\alpha \Gamma[\alpha q/(1+\alpha)]\} \simeq \Gamma(1+q)$; hence for $q = 0$ we have $\langle |x|^0 \rangle = 1$, as expected from normalization. In Fig. 2 we show $\langle x^2 \rangle$ versus time for $\alpha = 0.2$. Numerical simulation of the QTM perfectly matches Eq. (47). Note that the theory based on Table I and Eq. (33) does a slightly better job since that approach is not limited to the $\alpha \ll 1$ regime.

VIII. APPROACHING THE GAUSSIAN LIMIT $\alpha = 1$

In this section we consider the case $\alpha \to 1$ from below. We now find an approximation for $B_\alpha(z)$ that yields the solution of the QTM in this limit.

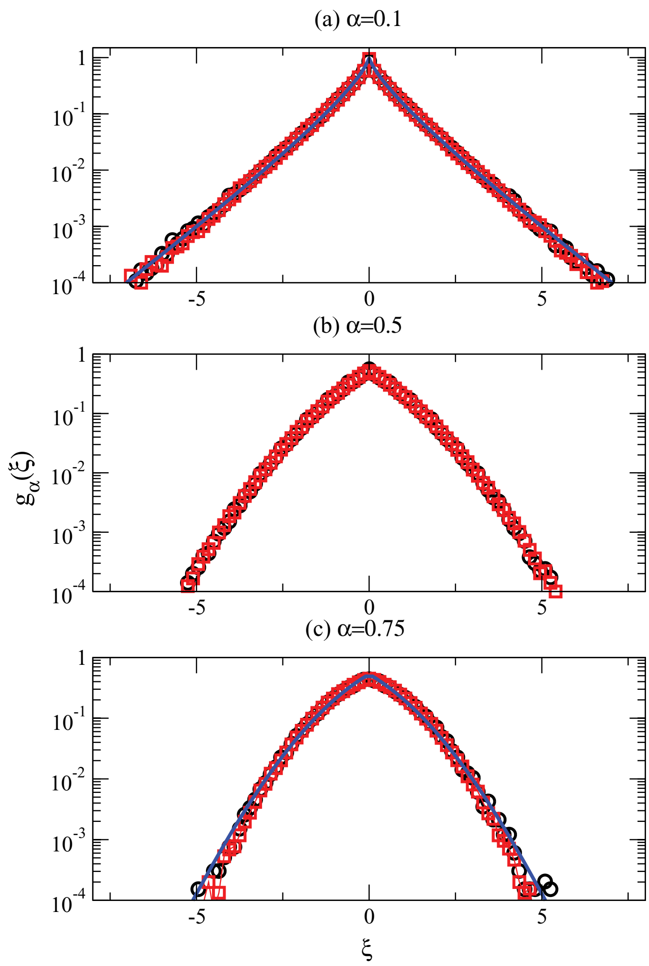

FIG. 4. (Color online) Diffusion front of the QTM [simulations (squares)] compared to the theory based on weak subordination breaking [the algorithm in Sec. V (circles)] and analytical predictions [Eqs. (46) and (52) (solid lines)] for $\alpha = 0.1$and0.75, respectively.

A. $B_\alpha(z)$ is Gaussian when $\alpha \to 1$

As before, to find $B_\alpha(z)$ we consider Brownian motion. The probability of finding the particle on x at time s is a Gaussian

$$P(x,s) = \frac{\exp\left(-\frac{x^2}{2s}\right)}{\sqrt{2\pi s}}, \tag{48}$$

as is well known. For $\alpha = 1$ we have $\mathcal{S}_1 = \sum_{x=-\infty}^{\infty} n_x = s$, namely, $\mathcal{S}_1$ is not a random variable at all since it is equal to the number of steps made in the underlying random walk. In other words, the PDF of $\mathcal{S}_1$ is a δ function centered on s. Therefore, when α is close enough to 1 we may neglect fluctuations. This means that we omit the average in Eq. (25) and use $\mathcal{S}_\alpha = \mathcal{C}_\alpha s^{(1+\alpha)/2}$. This approach together with Eq. (48) gives the PDF of finding the particle on x for a random walk stopped at the α coverage time $\mathcal{S}_\alpha$,

$$P_B(x,\mathcal{S}_\alpha) \simeq \frac{\exp\left[-\frac{x^2}{2(\mathcal{S}_\alpha/\mathcal{C}_\alpha)^{2/(1+\alpha)}}\right]}{[2\pi(\mathcal{S}_\alpha/\mathcal{C}_\alpha)^{2/(1+\alpha)}]^{1/2}}. \tag{49}$$

Hence

$$B_\alpha(z) \simeq \frac{\exp\left[-\frac{(\mathcal{C}_\alpha)^{2/(1+\alpha)} z^2}{2}\right]}{[2\pi/(\mathcal{C}_\alpha)^{2/(1+\alpha)}]^{1/2}} \tag{50}$$

and it follows that

$$\langle z^2\rangle = (\mathcal{C}_\alpha)^{-2/(1+\alpha)}. \quad (51)$$

In Fig. 1 $B_\alpha(z)$ obtained from Brownian simulations is compared with the analytical prediction [Eq. (50)] for $\alpha = 0.9$.

B. $\langle P(x,t)\rangle$ when $\alpha \simeq 1$

From Eqs. (22) and (49) we have

$$\langle P(x,t)\rangle \simeq \int_0^\infty d\mathcal{S}_\alpha \frac{\exp\left[-\frac{x^2}{2(\mathcal{S}_\alpha/\mathcal{C}_\alpha)^{2/(1+\alpha)}}\right]}{[2\pi(\mathcal{S}_\alpha/\mathcal{C}_\alpha)^{2/(1+\alpha)}]^{1/2}} n(\mathcal{S}_\alpha,t). \quad (52)$$

From Eq. (52) it is easy to get $g_\alpha(\xi)$, which is given in Eq. (D1) in Appendix D. In Fig. 4 we compare the scaling function obtained analytically and numerical simulations of the QTM with Brownian simulations according to the disorder-free algorithm in Sec. V. The approximate theory works reasonably well even for $\alpha = 0.75$.

Using Eqs. (33) and (51) we find the mean square displacement of the QTM

$$\langle x^2\rangle \simeq (\mathcal{C}_\alpha)^{-2/(1+\alpha)} \frac{\Gamma\left(\frac{2}{1+\alpha}\right)}{\alpha\Gamma\left(\frac{2\alpha}{1+\alpha}\right)} \left(\frac{t}{A^{1/\alpha}}\right)^{2\alpha/(1+\alpha)}. \quad (53)$$

Calculation of other moments is as simple since the reader may easily obtain $\langle |z|^q\rangle$ from the Gaussian PDF [Eq. (50)] and then apply Eq. (33). The behavior on the origin is found using Eqs. (32) and (50):

$$\langle P(x=0,t)\rangle \simeq \frac{(\mathcal{C}_\alpha)^{1/(1+\alpha)}}{\sqrt{2\pi}} \frac{\Gamma\left(\frac{\alpha}{1+\alpha}\right)}{\Gamma\left(\frac{1}{1+\alpha}\right)} (\tilde{t})^{-\alpha/(1+\alpha)}. \quad (54)$$

When $\alpha = 1$ we get the expected behavior $\langle P(x=0,t)\rangle = (2\pi\tilde{t})^{-1/2}$, which is normal diffusion.

The scaling function $g_\alpha(\xi)$ is analyzed in Appendix D. Using properties of stable PDFs, we show that when $\xi \ll 1$

$$g_\alpha(\xi) \sim g_\alpha(0) - 2^{(\alpha-1)/2}\left(\frac{1+\alpha}{\alpha}\right)\frac{\mathcal{C}_\alpha}{\Gamma\left(\frac{1-\alpha}{2}\right)}\xi^\alpha + \cdots, \quad (55)$$

with

$$g_\alpha(0) = \frac{(\mathcal{C}_\alpha)^{1/(1+\alpha)}}{\sqrt{2\pi}} \frac{\Gamma\left(\frac{\alpha}{1+\alpha}\right)}{\Gamma\left(\frac{1}{1+\alpha}\right)}. \quad (56)$$

In the limit $\alpha \to 1$ we use $\lim_{\alpha\to1}\mathcal{C}_\alpha = 1$ and Eq. (55) gives

$$\lim_{\alpha\to1} g_\alpha(\xi) \sim \frac{1}{\sqrt{2\pi}} - \lim_{\alpha\to1}\frac{2}{\Gamma\left(\frac{1-\alpha}{2}\right)}\xi^\alpha + \cdots. \quad (57)$$

The first term clearly reflects an ordinary Gaussian diffusion front. The second term vanishes in the limit $\alpha = 1$ since $\Gamma(0) = \infty$. This is because $g_1(\xi)$ is Gaussian and hence the second term in the expansion must be a ξ^2 term. So the $1/\Gamma(0)$ eliminates the ξ^α in Eq. (57) as $\alpha \to 1$. In the opposite limit of $\xi \gg 1$ a steepest descent method gives

$$g_\alpha(\xi) \sim b_1\xi^{-2[(1-\alpha)/(3-\alpha)]}e^{-b_2\xi^{2[(1+\alpha)/(3-\alpha)]}}, \quad (58)$$

where b_1 and b_2 are found in Appendix D. In the limit we find

$$\lim_{\alpha\to1} g_\alpha(\xi) = \frac{1}{\sqrt{2\pi}}e^{-\xi^2/2}, \quad (59)$$

the expected Gaussian behavior.

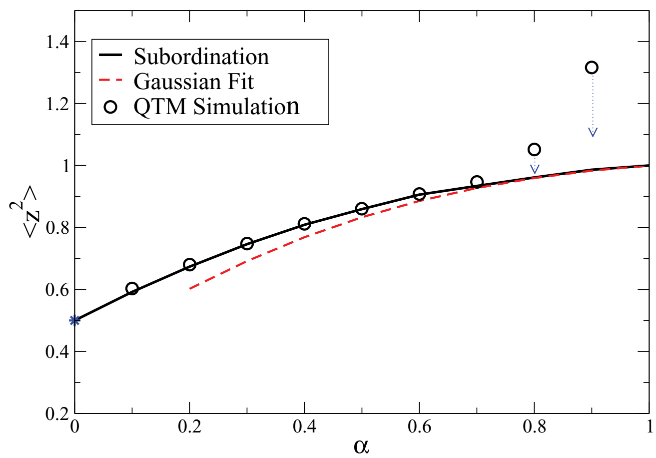

FIG. 5. (Color online) Behavior of $\langle z^2\rangle$ versus α as obtained using Brownian simulations as in Table I (solid curve), direct QTM simulations (circles), and a Gaussian fit (dashed line). According to theory $\langle z^2\rangle = 1/2$ for $\alpha \to 0$ and $\langle z^2\rangle = 1$ for $\alpha \to 1$. For $\alpha = 0.8$ and 0.9 the convergence of direct QTM simulations to theoretical results is very slow (see Fig. 6) and is achieved only by extrapolating the data in Fig. 6.

IX. CRITICAL SLOWDOWN $\alpha \to 1$

As discussed in Ref. [42], close to the critical point $\alpha = 1$ convergence of direct simulations of the QTM is extremely slow. In contrast, simulations of Brownian trajectories using a weak subordination scheme converges in reasonable time, at least on our computer. In this sense our approach is much more efficient compared with direct simulation of the QTM because our scheme, among other things, is a numerical tool that is able to investigate the limit $\alpha \to 1$, using reasonable amount of computational time.

In Fig. 5 we show $\langle z^2\rangle$ versus α. Here $\langle z^2\rangle$ was obtained by several means: (i) simulation of the QTM, which gives $\langle x^2\rangle$, and then with Eq. (33) we extract $\langle z^2\rangle$; (ii) Brownian simulations on a lattice (results in Table I); and (iii) analytical theory [Eqs. (42) and (51)]. For $\alpha > 0.8$ our simulations of the QTM did not converge even for $t = 10^9$. To check this issue better we define the deviation

$$\Delta(t) \equiv \left|\frac{\langle x^2\rangle\alpha\Gamma\left(\frac{2\alpha}{1+\alpha}\right)}{\Gamma\left(\frac{2}{1+\alpha}\right)(t/A^{1/\alpha})^{2\alpha/(1+\alpha)}} - \langle z^2\rangle\right|. \quad (60)$$

According to Eq. (33), $\lim_{t\to\infty}\Delta(t) = 0$. In Fig. 6 we present $\Delta(t)$ versus time. Here $\langle x^2\rangle$ is obtained from QTM simulations and $\langle z^2\rangle$ from Brownian trajectories (see Table I). In Fig. 6 we show that $\Delta(t) \sim t^{\alpha-1}$ for $\alpha = 0.9$ and observe a very slow decay towards the asymptotic value $\Delta(t) \to 0$. Simulations of the QTM did not converge (even for $t = 10^9$); however, by extrapolating the data (assuming that nothing dramatic happens for times larger than 10^9) we can conclude that $\Delta(t) \to 0$ and in that sense our theory is consistent with the simulations.

To overcome a critical slowdown in the region $\alpha \to 1$ we use the weak subordination scheme in Sec. V instead of direct numerical simulations of the QTM. In Fig. 7 we show the diffusion front. Good agreement between analytical predictions (valid for $\alpha \to 1$) [Eqs. (52), (55), and (58)] and

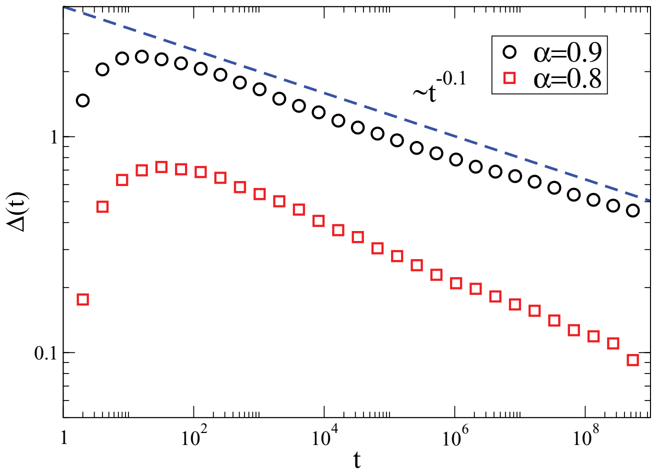

FIG. 6. (Color online) Behavior of Δ [Eq. (60)] as a function of t for $\alpha = 0.8$ and 0.9. A very slow convergence of Δ toward 0 for α close to 1 (a transition point between anomalous and normal types of diffusion) suggests a critical slowdown for $\alpha \to 1$ as noticed previously by Bertin and Bouchaud. The dashed line is a guide to the eye with a $t^{-0.1}$ behavior. The theoretical value of 0 for Δ hence can be achieved only by extrapolation.

the weak subordination breaking algorithm is presented for $\alpha = 0.9$.

X. DISCUSSION

The main focus of this paper has been on the diffusion front $\langle P(x,t)\rangle$ of random walkers in the quenched trap model in one dimension. We have shown that $\langle P(x,t)\rangle$ is found with a Lévy time transformation acting on Brownian motion stopped at the operational time $\mathcal{S}_\alpha$. Thus we mapped the random walk in a disordered environment to a Brownian motion that is stopped at the α coverage time $\mathcal{S}_\alpha$. This type of Brownian motion is interesting in its own right. For example, we have found a transition from a V shape to a Gaussian behavior for the scaling function $B_\alpha(z)$ describing this motion. Properties of this function determine the statistics of diffusion in the QTM. For α close to 1 and 0 we obtained analytical expressions for $B_\alpha(z)$ and $\langle P(x,t)\rangle$, while numerical information easily obtained from Brownian simulations provide a detailed description of the diffusion front in the range $0 < \alpha < 1$.

For $\alpha \to 0$ our formulas reduce to the renormalization group results obtained by Monthus [34]. The approach presented here is an alternative to the renormalization group method. Its advantage is that it is capable of dealing with the whole spectrum of α, at least numerically, including the critically slowed down regime of $\alpha \to 1$.

Is our method general or is it limited to the one-dimensional quenched trap model? Clearly our approach can be extended to higher dimensions or for random walks with biases. As mentioned in the Introduction, beyond the critical dimension, the QTM belongs to the domain of attraction of the CTRW. Hence, for an ordinary random walk on a lattice in dimension 3 we expect that $\mathcal{S}_\alpha$ is nonrandom and is equal to $c_\alpha s$ when time s is large and that c_α is a constant not yet determined. In that case the usual subordination method works for the corresponding trap model. Hence, once the constant c_α and the diffusion coefficient of the corresponding discrete time random walk are determined, we have the statistical information needed for the determination of the diffusion front of the QTM. A detailed analysis of the QTM for dimensions higher than one and for biased processes, using methods developed here, are left for future work.

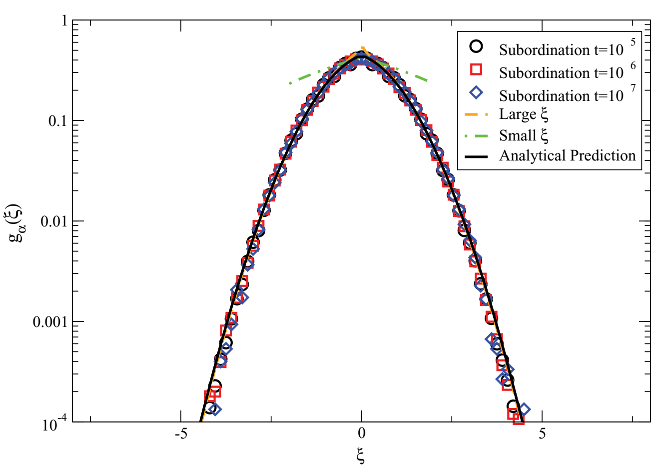

FIG. 7. (Color online) Scaling PDF $g_\alpha(\xi)$ for $\alpha = 0.9$ obtained by using the weak subordination scheme of Sec. V for $t = 10^5, 10^6, 10^7$ and compared to the analytical prediction [Eq. (52)] and large- and small-ξ expansions [Eqs. (55) and (58)]. A convergence of the weak subordination scheme is achieved already for $t = 10^5$ and thus overcomes the issue of a critical slowdown for direct simulations of the QTM that do not converge even for $t = 10^9$ (see Figs. 5 and 6).

ACKNOWLEDGMENTS

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APPENDIX A

Here we summarize some known results on one-sided Lévy stable random variables, which are used throughout this work. By definition $l_{\alpha,1,1}(t)$ is the inverse Laplace transform of $\exp(-u^\alpha)$. The large-t series expansion

$$l_{\alpha,1,1}(t) = \frac{1}{\pi}\sum_{n=1}^{\infty}\frac{\Gamma(1+n\alpha)}{n!}(-1)^{n-1}\sin(\pi n\alpha)t^{-(\alpha n+1)}. \quad \text{(A1)}$$

The asymptotic small-t behavior is [45]

$$l_{\alpha,1,1}(t) \sim Bt^{-\sigma}e^{-\kappa t^{-\tau}}, \quad \text{(A2)}$$

where

$$\tau = \frac{\alpha}{1-\alpha}, \quad \kappa = (1-\alpha)\alpha^{\alpha/(1-\alpha)}, \quad \sigma = \frac{2-\alpha}{2(1-\alpha)}, \quad B = \{[2\pi(1-\alpha)]^{-1}\alpha^{1/(1-\alpha)}\}^{1/2}. \quad \text{(A3)}$$

Closed form PDFs are found by summing the series of equations (A1) for specific choices of α [37,47]. For example, we insert the series (A1) in MATHEMATICA and use the command "Simplify" to get Lévy PDFs in terms of a combination of hypergeometric functions (e.g., for $\alpha = 1/4$). Similarly, Lévy's PDFS with $\alpha = 1/4, 1/3, 1/2, 2/3, 9/10$ can be expressed in terms of special functions. In this way we construct stable distributions. Some care must be practiced since on some occasions we found that for extremely small t MATHEMATICA yields wrong results [37]. This problem is easily fixed since we can use Eq. (A2) in that regime. Further, the problem is not crucial in the sense that it is found for so small t that practically the PDF there is zero, though not being aware of this issue solving integral transformations such as Eq. (49) can lead to wrong results. A useful special case is $\alpha = 1/2$ since

$$l_{1/2,1,1}(t) = \frac{1}{2\sqrt{\pi}} t^{-3/2} \exp\left(-\frac{1}{4t}\right). \tag{A4}$$

Chambers *et al.* [61] showed how to generate the stable random variable we call η from a one-sided Lévy PDF $l_{\alpha,1,1}(\eta)$. Let

$$a(\theta) = \frac{\sin[(1-\alpha)\theta][\sin(\alpha\theta)]^{\alpha/(1-\alpha)}}{(\sin\theta)^{1/(1-\alpha)}}, \quad 0 < \theta < \pi. \tag{A5}$$

Then $\eta = [a(\theta)/W]^{(1-\alpha)/\alpha}$, where θ is a uniform random number on $(0,\pi)$ and W is a random variable drawn from a standard exponential distribution $W = -\ln(x)$, where x is uniform on $(0,1)$.

APPENDIX B

In this appendix we obtain the distribution of η defined in Eq. (15). We are interested in random walks with fixed $\mathcal{S}_\alpha$ and in the limit $\mathcal{S}_\alpha \to \infty$. A large $\mathcal{S}_\alpha$ implies also a large number of steps (denoted with s); however, since $\mathcal{S}_\alpha$ is fixed s remains random. Our starting point is Eq. (19),

$$\langle e^{-u\eta} \rangle = \prod_{x=-\infty}^{\infty} \hat{\psi}\left[\frac{n_x u}{(\mathcal{S}_\alpha)^{1/\alpha}}\right]. \tag{B1}$$

It is important to note that the visitation numbers $\{n_x\}$ are determined by the probabilities of jumping left and right (equal to $1/2$ in our model) and that these random numbers do not depend on the waiting times since here $\mathcal{S}_\alpha$ is fixed. Hence the statistics of these visitation numbers are determined by simple binomial random walks.

The Laplace $\tau \to u$ transform of a rather general waiting time PDF is in the small-u limit

$$\hat{\psi}(u) = 1 - Au^\alpha + Bu^\beta + \cdots, \tag{B2}$$

where as mentioned $0 < \alpha < 1$, $A > 0$, and $\beta > \alpha$. The goal is to show that when $\mathcal{S}_\alpha \to \infty$ parameters such as B and β are not important. To see this insert Eq. (B2) in Eq. (B1) and find

$$\langle e^{-u\eta} \rangle = \prod_{x=-\infty}^{\infty} \left[1 - A\frac{(n_x)^\alpha}{(\mathcal{S}_\alpha)} u^\alpha + B\frac{(n_x)^\beta}{(\mathcal{S}_\alpha)^{\beta/\alpha}} u^\beta + \cdots\right]. \tag{B3}$$

This can be rewritten as

$$\langle e^{-u\eta} \rangle = 1 - Au^\alpha + \sum_{x=-\infty}^{\infty} \sum_{y=-\infty, y\neq x}^{\infty} \frac{A^2}{2} \frac{(n_x)^\alpha (n_y)^\alpha}{(\mathcal{S}_\alpha)^2} u^{2\alpha} + B\frac{\sum_{x=-\infty}^{\infty} (n_x)^\beta}{(\mathcal{S}_\alpha)^{\beta/\alpha}} u^\beta + \cdots. \tag{B4}$$

We note that

$$\sum_{x=-\infty}^{\infty} \sum_{y=-\infty, y\neq x}^{\infty} (n_x)^\alpha (n_y)^\alpha = \sum_{x=-\infty}^{\infty} \sum_{y=-\infty}^{\infty} (n_x)^\alpha (n_y)^\alpha - \sum_{x=-\infty}^{\infty} (n_x)^{2\alpha} = (\mathcal{S}_\alpha)^2 - \mathcal{S}_{2\alpha}; \tag{B5}$$

hence

$$\langle e^{-u\eta} \rangle = 1 - Au^\alpha + \frac{A^2}{2} \frac{(\mathcal{S}_\alpha)^2 - \mathcal{S}_{2\alpha}}{(\mathcal{S}_\alpha)^2} u^{2\alpha} + B\frac{\mathcal{S}_\beta}{(\mathcal{S}_\alpha)^{\beta/\alpha}} u^\beta + \cdots. \tag{B6}$$

We use $\mathcal{S}_{2\alpha}/(\mathcal{S}_\alpha)^2 \to 0$, which is justified at the end of this appendix, and hence

$$\frac{(\mathcal{S}_\alpha)^2 - \mathcal{S}_{2\alpha}}{(\mathcal{S}_\alpha)^2} \to 1 \tag{B7}$$

when $\mathcal{S}_\alpha \to \infty$. Similarly, $\mathcal{S}_\beta/(\mathcal{S}_\alpha)^{\beta/\alpha} \to 0$ for $\alpha < \beta$. Summarizing we find

$$\langle e^{-\eta u} \rangle \sim 1 - Au^\alpha + \frac{A^2 u^{2\alpha}}{2} + \cdots = e^{-Au^\alpha}. \tag{B8}$$

The parameters B and β are unimportant. Further, for a typical path there is no trace of the random variables $\{n_x\}$ in the final expression (B8). The latter equation implies that the PDF of η is a one-sided Lévy PDF as stated in Eq. (17).

To better estimate the convergence to this law we use a result obtained in Appendix C. There we show that for a binomial random walk with s steps we have

$$\langle \mathcal{S}_\alpha \rangle = \mathcal{C}_\alpha s^{(1+\alpha)/2}, \tag{B9}$$

where $\mathcal{C}_\alpha$ is a constant [Eq. (C15)]. We then assume the following relation to hold:

$$\mathcal{S}_\alpha = r s^{(1+\alpha)/2}, \tag{B10}$$

where r is a random variable that is independent of the number of steps s. Since in the QTM jumps to nearest neighbors have probability $1/2$ like the binomial random walk and since the statistics of the visitations numbers $\{n_x\}$ are independent of the waiting times (for fixed $\mathcal{S}_\alpha$), we may use Eq. (B9), derived for the binomial random walk, to analyze the QTM. We have $\mathcal{S}_{2\alpha} \propto s^{(1+2\alpha)/2}$ and hence $\mathcal{S}_{2\alpha} \propto (\mathcal{S}_\alpha)^{(1+2\alpha)/(1+\alpha)}$, so $\mathcal{S}_{2\alpha}/(\mathcal{S}_\alpha)^2 \propto (\mathcal{S}_\alpha)^{-1/(1+\alpha)}$, which goes to zero in the scaling limit $\mathcal{S}_\alpha \to \infty$, as we stated. Similarly, $\mathcal{S}_\beta/(\mathcal{S}_\alpha)^{\beta/\alpha} \propto s^{(1+\beta)/2}/s^{\beta(1+\alpha)/2\alpha} = s^{(\alpha-\beta)/(2\alpha)}$, which approaches zero since $\alpha < \beta$.

APPENDIX C

We consider a binomial random walk on a one-dimensional lattice. Time s is discrete $s = 0,1,2,\ldots$ and the particle has probability $1/2$ to jump to its nearest neighbors on its left or right. The walk starts on the origin $x = 0$. We now calculate the average $\langle \mathcal{S}_\alpha \rangle$ for an s step random walk. For that aim we obtain $\langle (n_x)^\alpha \rangle$ and then sum over x,

$$\langle \mathcal{S}_\alpha \rangle = \sum_{x=-\infty}^{\infty} \langle (n_x)^\alpha \rangle. \tag{C1}$$

We consider this problem in the continuum limit of the model, namely, we consider Brownian motion (see details below). Thus our final expression for $\langle \mathcal{S}_\alpha \rangle$ describes the limit of large s.

Let $P_{s,x}(n_x)$ be the probability of making n_x visits on lattice point x in the time interval $(0,s)$. As usual in these problems the Laplace transform

$$\hat{P}_{u,x}(n_x) = \int_0^\infty e^{-us} P_{s,x}(n_x) ds \tag{C2}$$

is useful. Here we already started taking the continuum limit since in the discrete time random walk s is not a continuous variable. We avoid a formal transition from a discrete random walk to the continuum limit to save space and time.

For a random walk starting on the origin let τ be the first time the particle reaches lattice point x and $f_x(\tau)$ be its PDF. Here τ is a first passage time for an unbiased random walk and it distribution is well known [33]. From symmetry $f_{-x}(\tau) = f_x(\tau)$. The number of visits on lattice point x, n_x, is determined by a first passage time from the origin to point x and then by the probability to revisit point x. Due to translation symmetry of the random walk the probability of $n_x - 1$ revisits to a lattice point x in a time interval $s - \tau$ (once reaching that point at τ) is identical to the probability of $n_x - 1$ visits on the origin (starting on the origin) within the same time interval. Hence translational symmetry gives

$$P_{s,x}(n_x) = \int_0^s f_x(\tau) P_{s-\tau,0}(n_x - 1) d\tau. \tag{C3}$$

Using the convolution theorem, $\hat{P}_{u,x}(n_x) = f_x(u)\hat{P}_{u,0}(n_x - 1)$. Here $P_{s,0}(n_0)$ is the probability to visit the origin n_0 times in the time interval $(0,s)$.

For the origin $x = 0$ we have

$$\hat{P}_{u,x=0}(n_0) = \begin{cases} \frac{1-\hat{f}_1(u)}{u} & n_0 = 0 \\ \hat{f}_1(u)^{n_0} \frac{1-\hat{f}_1(u)}{u} & n_0 \neq 0. \end{cases} \tag{C4}$$

Here $\hat{f}_1(u)$ is the Laplace transform of $f_1(\tau)$. To get a better insight about Eq. (C4) note that if $n_0 = 0$ we have $P_{s,x=0}(n_0 = 0) = 1 - \int_0^s f_1(\tau)d\tau$, which is the probability of not returning to the origin. To see this note that after one jump the particle is on either $x = 1$ or -1 and hence for n_0 to remain zero the particle must not return to the origin [of course $f_1(\tau)$ is the PDF of first passage times from $x = 1$ or -1 to the origin]. Applying the convolution theorem of the Laplace transform to $P_{s,x=0}(n_0 = 0) = 1 - \int_0^s f_1(\tau)d\tau$, we get the first line in Eq. (C4). Note that the original stay on the origin, at time $s = 0$, is not counted, so we may have $n_0 = 0$ once the particle never returns to the origin. The probability that $n_0 = 1$ is given by

$$P_{s,1}(n_0 = 1) = \int_0^s f_1(\tau) P_{s-\tau,0}(n_0 = 0) d\tau. \tag{C5}$$

Again using the convolution theorem, we find Eq. (C4) for $n_0 = 1$ and similarly for $n_0 > 1$. Using Eq. (C3) it is easily shown that for $x \neq 0$

$$\hat{P}_{u,x}(n_x) = \begin{cases} \frac{1-\hat{f}_x(u)}{u,} & n_x = 0 \\ \hat{f}_x(u)\hat{f}_1(u)^{n_x-1} \frac{1-\hat{f}_1(u)}{u}, & n_x \neq 0. \end{cases} \tag{C6}$$

The Laplace transform of the first passage time PDF is

$$\hat{f}_x(u) = \exp(-\sqrt{2}xu^{1/2}). \tag{C7}$$

The $\sqrt{2}$ comes from the fact that the diffusion constant is equal to $1/2$ since the variance of jump lengths is unity. In time τ, $f_x(\tau)$ is the one-sided Lévy PDF with index $1/2$ [see Eq. (A4)] and $f_x(\tau) \sim \tau^{-3/2}$ as is well known [33].

We now calculate $\langle (n_0)^\alpha \rangle_u$: The Laplace transform of $\langle (n_0)^\alpha \rangle_s$

$$\langle (n_0)^\alpha \rangle_u = \int_0^\infty (n_0)^\alpha \hat{P}_{u,0}(n_0) dn_0, \tag{C8}$$

where the integration (instead of summation) implies that we are considering the continuum limit of the random walk (i.e., Brownian motion). Inserting in Eqs. (C8), (C4), and (C7) we find

$$\langle (n_0)^\alpha \rangle_u \sim \left(\frac{1}{\sqrt{2}}\right)^\alpha \Gamma(1+\alpha) u^{-1-\alpha/2}, \tag{C9}$$

which is valid for small u corresponding to large s. Using Eqs. (C6) and (C7) we get the α moment of the visitation number for lattice point x,

$$\langle (n_x)^\alpha \rangle_u = e^{-x\sqrt{2}u^{1/2}} \Gamma(1+\alpha) \left(\frac{1}{\sqrt{2}}\right)^\alpha u^{-1-\alpha/2}. \tag{C10}$$

Notice that $\langle (n_x)^\alpha \rangle_u \sim \hat{f}_x(u) \langle (n_0)^\alpha \rangle_u$, reflecting the first arrival at x and the translation symmetry of the lattice.

Denote $\langle \mathcal{S}_\alpha \rangle_u$ as the Laplace $s \to u$ transform of $\langle \mathcal{S}_\alpha \rangle_s$. In the Brownian limit we replace the summation in Eq. (C1) with integration

$$\langle \mathcal{S}_\alpha \rangle_u = 2 \int_0^\infty \langle (n_x)^\alpha \rangle_u dx \tag{C11}$$

and with the help of Eq. (C10)

$$\langle \mathcal{S}_\alpha \rangle_u \sim \sqrt{2}^{1-\alpha} \Gamma(1+\alpha) u^{-3/2-\alpha/2}. \tag{C12}$$

Using the Laplace pair

$$u^{-(3+\alpha)/2} \to \frac{s^{(\alpha+1)/2}}{\Gamma\left(\frac{\alpha+3}{2}\right)}, \tag{C13}$$

we find with simple identities for the Γ function [63] the main result of this appendix:

$$\langle \mathcal{S}_\alpha \rangle = \mathcal{C}_\alpha s^{(1+\alpha)/2,} \tag{C14}$$

with

$$\mathcal{C}_\alpha = \frac{2^{(\alpha+3)/2} \Gamma\left(1 + \frac{\alpha}{2}\right)}{\sqrt{\pi}(1+\alpha)}. \tag{C15}$$

For $\alpha = 1$ we have $\mathcal{S}_1 = \sum_{x=-\infty}^{\infty} n_x = s$, a result that is retrieved from Eq. (C14) since $\mathcal{C}_1 = 1$. In the limit $\alpha = 0$ we have $\mathcal{S}_0$ equal to the span of the random walk, namely, to the number of distinct sites visited by the walker. As mentioned in the main text, in this limit we retrieve Eq. (26), which was found a long time ago in Ref. [62].

APPENDIX D

Here we investigate the function $g_\alpha(\xi)$ in the limit where $\alpha < 1$ is close to unity with the Gaussian approximation for $B_\alpha(z)$. Changing variables in Eq. (49) according to $\mathcal{S}_\alpha = t^\alpha \eta^{-(1+\alpha)/2}$, we find, using the definition in Eq. (29),

$$g_\alpha(\xi) = \frac{(\mathcal{C}_\alpha)^{1/(1+\alpha)}}{\sqrt{2\pi}} \frac{1+\alpha}{2\alpha} \times \int_0^\infty e^{-u\eta} \eta^{1/(2\alpha)} l_{\alpha,1,1}(\eta^{(1+\alpha)/(2\alpha)}) d\eta, \quad \text{(D1)}$$

where

$$u = \xi^2 (\mathcal{C}_\alpha)^{2/(1+\alpha)}/2. \quad \text{(D2)}$$

Equation (D1) is a Laplace transform. Inserting in Eq. (D1) $\xi = 0$, changing variables according to $y = \eta^{(1+\alpha)/(2\alpha)}$, and using Eq. (31), we get $g_\alpha(\xi = 0)$ [Eq. (56)]. The small-u limit (corresponding to small ξ) of Eq. (D1) is controlled by the large-η behavior of

$$\eta^{1/(2\alpha)} l_{\alpha,1,1}(\eta^{(1+\alpha)/(2\alpha)}) \sim \frac{\sin \pi\alpha}{\pi} \Gamma(1+\alpha) \eta^{-1-\alpha/2}, \quad \text{(D3)}$$

where we used the large-η expansion of stable PDFs [Eq. (A1)]. Using the Tauberian theorem, noting that $u^{\alpha/2}$ and $\eta^{-(1+\alpha/2)}/|\Gamma(-\alpha/2)|$ are Laplace pairs, Eqs. (D1) and (D3) together with some identities of the Γ function [63] give Eq. (55).

In the opposite limit of large ξ (i.e., large u) we use the small-η behavior of $\eta^{1/(2\alpha)} l_{\alpha,1,1}(\eta^{(1+\alpha)/(2\alpha)})$ in Eq. (D1). For that aim we use the small-η behavior of one-sided stable PDFs [Eq. (A2)]. We get

$$g_\alpha(\xi) = \bar{C} \int_0^\infty e^{-u\eta} \eta^{-\gamma} e^{-\kappa\eta^{-\delta}} d\eta, \quad \text{(D4)}$$

$$\gamma = \frac{3-\alpha}{4(1-\alpha)}, \quad \delta = \frac{1+\alpha}{2(1-\alpha)}, \quad \bar{C} = B \frac{(\mathcal{C}_\alpha)^{1/(1+\alpha)}}{\sqrt{2\pi}} \frac{1+\alpha}{2\alpha}. \quad \text{(D5)}$$

where κ and B are defined in Appendix A [Eq. (A3)].

We now use steepest descent method. Let $h(\eta) = u\eta + \kappa\eta^{-\delta}$. The extremum is on η_e, which is determined us usual from $\partial h/\partial\eta = 0$, so $\eta_e = (u/\kappa\delta)^{-1/(1+\delta)}$. Using the expansion

$$h(\eta) = h(\eta_e) + \tfrac{1}{2}\kappa\delta(\delta+1)(\eta_e)^{-\delta-2}\Delta^2 + \cdots, \quad \text{(D6)}$$

where $\Delta = \eta - \eta_e$ is small, we then have, after extending the domain of integration,

$$g_\alpha(\xi) \sim \bar{C}(\eta_e)^{-\gamma} e^{-h(\eta_e)} \times \int_{-\infty}^{\infty} \exp[-\delta(1+\delta)\kappa(\eta_e)^{-\delta-2}\Delta^2/2] d\Delta. \quad \text{(D7)}$$

Solving this Gaussian integral, we obtain

$$g_\alpha(\xi) = \tilde{\bar{C}} u^{-\mu} e^{-\bar{\kappa} u^{\delta/(1+\delta)}}, \quad \text{(D8)}$$

where $\tilde{\bar{C}} = \bar{C}\sqrt{2\pi}[\delta(1+\delta)\kappa]^{-1/2}(\kappa\delta)^\mu$, $\bar{\kappa} = (\kappa\delta)^{1/(1+\delta)} + \kappa(\kappa\delta)^{-\delta/(\delta+1)}$, and $\mu = (1-\alpha)/(3-\alpha)$. Reverting to the variable ξ (instead of u) using Eq. (D2), we get Eq. (58),

$$g_\alpha(\xi) = \tilde{\bar{C}} \left[\frac{\xi^2 (\mathcal{C}_\alpha)^{2/(1+\alpha)}}{2} \right]^{-\mu} \times \exp\left\{ -\bar{\kappa} \left[\frac{(\mathcal{C}_\alpha)^{2/(1+\alpha)} \xi^2}{2} \right]^{[(1+\alpha)/(3-\alpha)]} \right\}. \quad \text{(D9)}$$

To prepare for the limit $\alpha \to 1$ we rewrite

$$\tilde{\bar{C}} = (\mathcal{C}_\alpha)^{1/(1+\alpha)} \frac{1+\alpha}{2\alpha} \frac{B}{\sqrt{\delta(1+\delta)\kappa}}. \quad \text{(D10)}$$

Using $\lim_{\alpha\to 1} \mathcal{C}_\alpha = 1$,

$$\lim_{\alpha \to 1} \frac{B}{\sqrt{\delta(1+\delta)\kappa}} = \frac{1}{\sqrt{2\pi}}, \quad \text{(D11)}$$

and $\lim_{\alpha\to 1} \bar{\kappa} = 1$, we find the expected Gaussian behavior [Eq. (59)]. Rewriting we obtain

$$g_\alpha(\xi) \sim b_1 \xi^{-2[(1-\alpha)/(3-\alpha)]} e^{-b_2 \xi^{2[(1+\alpha)/(3-\alpha)]}} \quad \text{(D12)}$$

for $\xi \gg 1$ with $b_1 = \sqrt{(1+\alpha)/[2\pi\alpha(3-\alpha)]}D$, $b_2 = [(3-2\alpha)/2]D^2$, and $D = [(1+\alpha)^{1-\alpha}\alpha^\alpha \mathcal{C}_\alpha]^{1/(3-\alpha)}$.

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