Time transformation for random walks in the quenched trap model

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Diffusion in the quenched trap model is investigated with an approach we call weak subordination breaking. We map the problem onto Brownian motion and show that the operational time is

\[ S_x = \sum_{n_x}^{\infty} (n_x)^\alpha \]

where \( n_x \) is the visitation number at site \( x \). In the limit of zero temperature we recover the renormalization group (RG) solution found by Monthus. Our approach is an alternative to RG capable of dealing with any disorder strength.

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Random walks in disordered systems with diverging expected waiting times have attracted vast interest over many decades \([1,2]\). Two approaches in this field are the annealed continuous time random walk (CTRW) model and the by far more challenging quenched trap model (QTM). Starting in the seventies, the Scher-Montroll CTRW approach was used to model sub-diffusive photocurrents in amorphous materials \([3]\). Bouchaud showed that the trap model is a useful tool for the description of aging phenomena in glasses \([4,5]\). More recently these models were used to describe non self averaging \([6]\) and weak ergodicity breaking \([4,7]\) which are important for the statistical description of blinking quantum dots \([8]\) and diffusion of single molecules in living cells \([9]\).

This manuscript presents a new approach for random walks in a fixed random environment. With physical arguments \([1,10,11]\) and rigorous mathematics \([12,13]\) we know that the QTM in dimensions \( d > 2 \) is expected to qualitatively behave like its corresponding mean field CTRW, the latter being exact when \( d \rightarrow \infty \). For a random walk in a quenched disordered system intricate correlations induced by multiple visits to the same site make the problem non-trivial and interesting. For that reason RG methods \([10,14]\) were used to tackle this problem. With RG Machta \([10]\) found the scaling exponents of the QTM and Monthus \([14]\) investigated the diffusion front in the limit of zero temperature (see details below). While the RG is powerful it has its limitations: a simple approach which predicts the diffusion front is still missing.

We provide the long sought after breakthrough in the statistical analysis of sub-diffusion in the QTM. Our approach is based on a novel time transformation. It is well known that one may decompose the CTRW process into ordinary Brownian motion and a Lévy process, an approach called subordination \([13]\). In this scheme normal Brownian motion takes place in operational time \( s \). The disorder is effectively described by a Lévy time transformation from operational time \( s \) to laboratory time \( t \) (see some details below). This method is not generally suited for random walks in quenched environments since it uses the renewal assumption. In a quenched environment this very strong assumption implies that a given lattice site is visited only once along the path of the random walker, i.e. it neglects correlations. So a new approach capable of dealing with quenched disorder is now investigated. We focus on the one dimensional case since then the departure from mean field is the strongest. At the end of the Letter we explain how to extend our results to other interesting cases.

**Quenched trap model** \([1,14,16]\). We consider a random walk on a one dimensional lattice with lattice spacing equal one. For each lattice site \( x \) there is a quenched random variable \( \tau_x \) which is the waiting time between jump events for a particle situated on \( x \). After waiting for a period \( \tau_x \) 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 \( \tau_0 \), then with probability \( 1/2 \) jumps to \( x = 1 \) (or \( x = -1 \)), waits there for \( \tau_1 \) (or \( \tau_{-1} \)) then if the particle returns to \( x = 0 \) it waits for a time interval \( \tau_0 \) etc. The \( \{\tau_x\} \)s are positive independent identically distributed random variables with a common probability density function (PDF)

\[
\psi(\tau_x) \sim \frac{A}{\Gamma(-\alpha)} (\tau_x)^{-(1+\alpha)}
\]

for \( \tau_x \rightarrow \infty \) and \( 0 < \alpha < 1 \). Hence the Laplace transform of the waiting time PDF is \( \psi(u) \sim 1 - Au^\alpha + \cdots \) when \( u \rightarrow 0 \). As well known \([1]\) the QTM describes a random walk among traps whose energy depth \( E > 0 \) is exponentially distributed \( f(E) = \exp(-E/T_g)/T_g \) where \( T_g \) is a measure of the disorder. It is easy to show that \( \alpha = T/T_g \) and \( A = |\Gamma(-\alpha)|/\alpha \) where \( T \) is the thermal temperature. 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 a comprehensive mathematical review of the QTM see \([12]\).

| \( \alpha \) | 0 | 0.2 | 0.4 | 0.6 | 0.8 | 1 |
|---|---|---|---|---|---|---|
| \( \langle z \rangle \) | 0.5 | 0.67 | 0.81 | 0.91 | 0.96 | 1 |

**TABLE I:** Simple Brownian simulations on a lattice give \( \langle z \rangle \) which according to Eq. \([10]\) yield \( \langle x^2 \rangle \) for the QTM.

**Time in the quenched trap model** is \( t = \sum_{x=-\infty}^{\infty} n_x \tau_x \) where \( n_x \) is the number of visits to lattice point \( x \). Define
the random variable \( \eta = t/(S_\alpha)^{1/\alpha} \) where

\[
S_\alpha = \sum_{x=-\infty}^{\infty} (n_x)^\alpha.
\] (2)

When \( \alpha = 1 \), \( S_\alpha \) is the total number of jumps made \( \sum_{x=-\infty}^{\infty} n_x = s \). In the opposite limit \( \alpha \to 0 \), \( S_\alpha \) is the distinct number of sites visited by the random walker which is called the span of the random walk. We now show that in the scaling limit

the PDF of \( \eta \) is: \( l_{\alpha,1,1}(\eta) \),

where \( l_{\alpha,1,1}(\eta) \) is the one sided Lévy PDF whose Laplace \( \eta \to u \) pair is \( \exp(-\eta u^\alpha) \). Namely the heavy tailed distribution of the waiting times \( \tau_x \) determines the statistics of \( \eta \) through the characteristic exponent \( \alpha \), while the visitation numbers \( \{n_x\} \) provide the scaling through \( S_\alpha \). By definition the Laplace \( \eta \to u \) transform of the PDF of \( \eta \) is

\[
\langle e^{-\eta u} \rangle = \langle \exp \left[ -\sum_{i=-\infty}^{\infty} \frac{n_i \tau_i}{(S_\alpha)^{1/\alpha}} u \right] \rangle.
\] (4)

We average with respect to the disorder, namely with respect to the independent and identically distributed random waiting times \( \tau_x \), and obtain

\[
\langle e^{-\eta u} \rangle = \Pi_{x=-\infty}^{\infty} \hat{\psi} \left( \frac{n_x u^\alpha}{(S_\alpha)^{1/\alpha}} \right)
\]

where \( \hat{\psi}(u) \) is the Laplace transform of the PDF of waiting times \( \psi(\tau_x) \). We use \( \hat{\psi}(u) = \exp(-Au^\alpha) \sim 1-Au^\alpha + \cdots \)

\[
\langle e^{-\eta u} \rangle = \Pi_{x=-\infty}^{\infty} \exp \left[ -\frac{A(n_x)^\alpha u^\alpha}{S_\alpha} \right] = e^{-A u^\alpha}.
\] (5)

Hence the PDF of \( \eta \) is a one sided Lévy law Eq. 3.

In a longer publication we will complete the proof and consider the case where \( \psi(\tau_x) \) belongs to the domain of attraction Lévy PDFs (i.e. families of PDFs satisfying \( \psi(u) \sim 1-Au^\alpha + \cdots \)). We now invert the process fixing time \( t \) to find the PDF of \( S_\alpha \)

\[
n_t(S_\alpha) = \frac{t}{\alpha} (S_\alpha)^{-1/\alpha -1} l_{\alpha,1,1} \left[ \frac{t}{(S_\alpha)^{1/\alpha}} \right].
\] (6)

In the following we explain how to use the operational time \( S_\alpha \) to obtain the desired diffusion front of the QTM, in other words we explain how we get rid of the disorder and focus only on Brownian motion.

**Weak subordination breaking.** To find \( \langle P(x,t) \rangle \) we follow six steps: 1. Choose the laboratory time \( t \) which is a fixed parameter. 2. Use a random number generator and draw the stable random variable \( \eta \) from the one sided Lévy PDF \( l_{\alpha,1,1}(\eta) \). 3. With \( \eta \) and \( t \) determine the operational time \( S_\alpha = (t/\eta)^\alpha \). 4. Generate a simple symmetric random walk on a lattice (probability 1/2 for jumping left and right). Stop the process once its \( S_\alpha \) reaches the operational time set in step 3. 5. Record the position \( x \) of the particle at the end of the previous step. 6. Go to step 2. After this loop is repeated many times, we generate a histogram of \( x \). The histogram so created is identical to \( \langle P(x,t) \rangle \) when \( t \) is large. On a computer the second step is implemented with a simple algorithm provided by Chambers et al [17]. Notice that with this exact scheme we have mapped the random walk in a random environment to a Brownian motion problem. We see that for quenched disorder the operational time is \( S_\alpha \) and in this sense subordination is weakly broken: the Lévy transformation [12] is still maintained.

**The diffusion front of the QTM.** Let \( P_{S_\alpha}(x) \) be the PDF of \( x \) for the simple random walk on a lattice (Brownian motion) stopped at the operational time \( S_\alpha \). Since the QTM dynamics can be separated into two distinct processes: Brownian motion with operational time \( S_\alpha \) (step 4.) and the Lévy time transformation (steps 2. and 3.) we find

\[
\langle P(x,t) \rangle \sim \int_0^{\infty} P_{S_\alpha}(x) n_t(S_\alpha) \, dS_\alpha
\] (7)

where \( n_t(S_\alpha) \) is given in Eq. 6. For the mean field version of the model (i.e. CTRW) replace \( S_\alpha \) with the number of steps \( s \) of the Brownian motion, and then \( P_{S_\alpha}(x) \) is Gaussian as well known [15]. From normal Brownian motion we have the scaling behavior \( x \propto (S_\alpha)^{1/(1+\alpha)} \). To see this we use: (i) usual Brownian scaling \( x \propto s^{1/2} \) (ii) \( n_x \) within a region \( |x| < s^{1/2} \) is roughly the number of jumps made \( s \) divided by the number of sites in the explored region \( n_x \propto s/s^{1/2} = s^{1/2} \). Hence \( S_\alpha \propto \sqrt{s(n_x)^\alpha} \propto s^{1/(1+\alpha)} \) which gives \( x \propto (S_\alpha)^{1/(1+\alpha)} \). This scaling implies

\[
P_{S_\alpha}(x) = \frac{1}{(S_\alpha)^{1/(1+\alpha)}} B_\alpha \left[ \frac{x}{(S_\alpha)^{1/(1+\alpha)}} \right]
\] (8)
with \( B_\alpha(z) \) a normalized non negative function. Define the scaling variable \( \xi = x/ (t/A^{1/\alpha})^{\frac{1}{\alpha}} \) and \( g_\alpha (\xi) / (t/A^{1/\alpha})^{\frac{\alpha}{1+\alpha}} \) which according to Eq. (7) is

\[
g_\alpha (\xi) = \int_0^\infty dy y^{\frac{\alpha}{1+\alpha}} B_\alpha \left( \xi y^{\frac{\alpha}{1+\alpha}} \right) l_{\alpha,1,1} (y). \tag{9}\]

A general relation is found between the moments \( \langle |x|^q \rangle = \int_0^\infty |x|^q P(x,t) dx \) of the original QTM and the moments \( \langle |z|^q \rangle = \int_0^\infty |z|^q B_\alpha(z) dz \)

\[
\langle |x|^q \rangle = \langle |z|^q \rangle \left( \frac{\Gamma \left( \frac{q}{1+1/\alpha} \right)}{\alpha \Gamma \left( \frac{q+1}{1+1/\alpha} \right) \left( \frac{t}{A^{1/\alpha}} \right)^{q/\alpha}} \right). \tag{10}\]

The new content of Eqs. (9,10) is that once we obtain \( B_\alpha(z) \) either from theory or simulations of Brownian trajectories, we have a useful method to obtain exact statistical properties of the diffusion front.

Generating Brownian trajectories on a lattice we found \( B_\alpha(z) \) in Fig. 1 which shows an interesting transition from a V shape when \( \alpha \to 0 \) to a Gaussian shape, which we soon analyze analytically. With \( \langle z^2 \rangle \) given in Table I and Eq. (10) we get the mean square displacement of the QTM \( \langle z^2 \rangle \). We then favorably compare the predictions of our theory with simulations of the QTM in Fig. 2 (and analytical formulas soon developed). In Fig. 3 we show \( g_\alpha(\xi) \) and present excellent agreement between weak subordination breaking and direct simulation of the QTM. One advantage of our approach is that it is capable of dealing with the critical slowing down pointed out by Bertin and Bouchaud [16]. Briefly, QTM simulations do not converge on reasonable computer time scales for say \( \alpha > 0.8 \). In contrast weak subordination breaking scheme quickly converges since it is based on Brownian motion and there is no need to generate disordered systems. More importantly we now analyze Brownian motion analytically, obtain \( B_\alpha(z) \) in two important limits and then with Eqs. (9,10) provide solutions to the QTM.

The limit \( \alpha \to 0 \) corresponds to strong disorder. To find \( B_\alpha(z) \) we consider Brownian motion stopped at “time” \( S_0 \) where as mentioned \( S_0 \) is the span of the random walk. Consider \( P_{S_0} (S_0 \Delta n) \) where \( x = S_0 \Delta n > 0 \) and for simplicity we start with \( n = 1 \). The Brownian particle after the first step can be either on \( x = 1 \) or \( x = -1 \). If it is on \( x = -1 \) it must travel a distance \( S_0 \) to reach its destination \( x = S_0 - 1 \) and the span is \( S_0 \). On the other hand if it jumps to \( x = 1 \) the distance the particle must travel is \( S_0 - 2 \) and the span must still be \( S_0 \). Hence \( P_{S_0} (S_0 \Delta n) = |P_{S_0} (S_0) + P_{S_0} (S_0 - 2)|/2 \). More generally

\[
P_{S_0} (S_0 \Delta n) = \frac{1}{2} \left[ P_{S_0} (S_0 \Delta n - 1) + P_{S_0} (S_0 \Delta n + 1) \right], \tag{11}\]

and for the boundary term \( P_{S_0} (S_0) = |P_{S_0} (S_0 - 1) + P_{S_0 - 1} (S_0 - 1)|/2 \). Eq. (11) is easily solved \( P_{S_0} (x) = \frac{|x|}{S_0(S_0+1)} \) for \( -S_0 < x < S_0 \) and \( x \in \mathbb{Z} \). In the limit \( S_0 \gg 1 \) we have for the scaled

FIG. 2: The mean square displacement of the QTM versus time. Numerical data matches perfectly the theory based on weak subordination breaking (the lines plotted with \( \langle z^2 \rangle \) in Table I) and analytical formulas Eq. (13) for \( \alpha = 0.2 \) and Eq. (10) for \( \alpha = 0.4, 0.6, 0.8 \).

FIG. 3: The diffusion front of QTM (squares) perfectly matches theory based on weak sub-ordination breaking (circles) and analytical predictions (lines) Eqs. (9,14,15).
variable \( z = x/S_0 \) the V shape PDF (see Fig. 1)

\[
\lim_{\alpha \to 0} B_\alpha(z) = \begin{cases} |z| & \text{for } |z| < 1 \\ 0 & \text{otherwise.} \end{cases} \tag{12}
\]

This V shape reflects the tendency of a Brownian particle to reach a large span \( S_0 \) when it is far from the origin.

According to Eq. (10) the even moments \( \langle x^2 \rangle \) for the random walk in the QTM are given once we obtain \( \langle z^2 \rangle \). In the limit \( \alpha \to 0 \) we find using Eq. (12) \( \langle z^2 \rangle = 2 \int_0^1 z^2 dz = (1 + q)^{-1} \) hence with Eq. (10) we have for small \( \alpha \)

\[
\langle x^2 \rangle \simeq \frac{1}{2} \frac{\Gamma \left( \frac{2}{1+\alpha} \right)}{\alpha \Gamma \left( \frac{2\alpha}{1+\alpha} \right)} \frac{t}{A^{1/\alpha}} \tag{13}
\]

which is tested in Fig. 2. Inserting \( \langle z^2 \rangle = (1 + q)^{-1} \) in Eq. (10) we obtain the moments \( \langle x^2 \rangle \) of the QTM. Straight forward analysis then gives

\[
\lim_{\alpha \to 0} g_\alpha(\xi) = e^{-|\xi|} - |\xi|E_1(|\xi|) \tag{14}
\]

where \( E_1(\xi) = \int_\xi^\infty (e^{-t}/t)dt \) is the tabulated exponential integral. This scaling function was obtained by C. Monthus [14] using an RG method which is exact in the limit \( \alpha \to 0 \).

**Approaching the weak disorder limit \( \alpha \to 1 \).** For \( \alpha = 1 \) we have \( S_1 = \sum_{x=0}^\infty \alpha_x = s \), namely \( S_1 \) is non random since it is equal to the number of steps made. Therefore when \( \alpha \) is close enough to \( 1 \) we may neglect fluctuations and \( S_\alpha \approx \langle S_\alpha \rangle \). In a longer publication we will show that \( \langle S_\alpha \rangle = C_\alpha s^{1+\alpha} \), and \( C_\alpha = 2^{\alpha+3}/2 \Gamma (1+\alpha)2^{1/\alpha} \) [13] hence change of variables to \( S_\alpha \) gives

\[
B_\alpha(z) \sim \frac{\exp \left[ \frac{(C_\alpha)^{2-\alpha} z^2}{2} \right]}{(2\pi)^{1/2}(C_\alpha)^{2-\alpha} z^{2-\alpha}} \tag{15}
\]

It follows that \( \langle z^2 \rangle \sim (C_\alpha)^{2-\alpha} \) hence for the QTM

\[
\langle x^2 \rangle \simeq (C_\alpha)^{-2+\alpha} \frac{\Gamma \left( \frac{2}{1+\alpha} \right)}{\alpha \Gamma \left( \frac{2\alpha}{1+\alpha} \right)} \frac{t}{A^{1/\alpha}} \tag{16}
\]

In Fig. 1 \( B_\alpha(z) \) obtained from Brownian simulations is favorably compared with Eq. (15) for \( \alpha = 0.9 \). Surprisingly, as we show in Fig. 2 Eq. (10) works very well even for \( \alpha = 0.4 \). With Eqs. (10, 15) and steepest descent method we find for \( \xi >> 1 \)

\[
g_\alpha(\xi) \sim b_1 \xi^{-\frac{2-\alpha}{2-\alpha}} e^{-b_2 \xi^{\frac{2}{2-\alpha}}} \tag{17}
\]

with \( b_1 = \sqrt{(1+\alpha)/(2\alpha(3-\alpha))}D \), \( b_2 = [(3-2\alpha)/2]D^2 \) and \( D = [(1+\alpha)^{1-\alpha}\alpha \alpha \alpha C_\alpha]^{1/(3-\alpha)} \) which approach the expected normal Gaussian limit when \( \alpha \to 1 \). In the opposite limit \( \xi << 1 \) \( g_\alpha(\xi) \sim 1/\sqrt{2\pi} \xi^{-2(\alpha-1)/2}[(1+\alpha)/\alpha] \{C_\alpha/\Gamma [(1+\alpha)/2]\}^{\xi^2} \cdots \).

The method presented here is not limited to one dimension neither to unbiased motion. For example consider the QTM on a regular lattice in three dimensions. From ordinary Brownian motion we expect \( S_\alpha \sim c_\alpha s \), where now \( S_\alpha \) is non random and the (non trivial) parameter \( c_\alpha \) will depend on the lattice structure. In principle once \( c_\alpha \) is determined one can map the QTM with an equation like Eq. (17) to an ordinary Brownian motion. This will yield mean field CTRW dynamics which is still non trivial since the transformation depends on the parameter \( c_\alpha \). Note that the QTM dynamics describes also certain models of random walks on random geometries, e.g. fractal comb structures and naturally our approach captures also these cases.

Finally, weak subordination breaking scheme is not only a new approach which deals with anomalous diffusion in systems with quenched disorder. Our method can be used to solve other aspects of dynamics in disordered systems like aging and weak ergodicity breaking.

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