Time Transformation for Random Walks in the Quenched Trap Model

S. Burov and E. Barkai
Department of Physics, Institute of Nanotechnology and Advanced Materials, Bar Ilan University, Ramat-Gan 52900, Israel
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We investigate subdiffusion in the quenched trap model by mapping the problem onto a new stochastic process: Brownian motion stopped at the operational time $\mathcal{S}_\alpha = \sum_{x=-\infty}^{\infty} (n_x)^\alpha$ where n_x is the visitation number at site x and α is a measure of the disorder. In the limit of zero temperature we recover the renormalization group solution found by Monthus. Our approach is an alternative to the renormalization group and is 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. Such processes describe a wide variety of systems which exhibit diffusion slower than normal $\langle x^2 \rangle \sim t^\xi$ and $0 < \xi < 1$ [1,2]. Two approaches in this field are the annealed continuous time random walk (CTRW) model which is a mean field theory and by far the more challenging quenched trap model (QTM). Starting in the 1970s, the Scher-Montroll CTRW approach was used to model subdiffusive photocurrents in amorphous materials [3] and recently for subdiffusion of single molecules in living cells [4]. More generally, power law waiting times describe stochastic dynamics in a wide range of systems beyond the spatial random walk approach. Bouchaud showed that the trap model is a useful tool for the description of aging phenomena in glasses [5,6]. Supercooled liquids where jumps are performed between metabasins in configuration space [7] and even atomic-like systems such as blinking quantum dots [8] are analyzed with similar waiting time concepts.

Most of the theoretical works in the field use a mean field approach. This means that the waiting times in different states are assumed to be uncorrelated. Mathematically this implies the renewal assumption. For example, for a CTRW process on a lattice, waiting times between jump events are independent identically distributed random variables. In systems with fixed in time quenched disorder it is well known that such an assumption does not reflect reality, at least not below a critical dimension. Once a particle visits a given site more than once, the waiting times must be correlated and the disorder is not trivial.

This manuscript presents a new approach for random walks in a fixed random environment. With physical arguments [1,9,10] and rigorous mathematics [11,12] 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 $d \to \infty$. For a random walk in a quenched disordered system, intricate correlations induced by multiple visits to the same site make the problem interesting. For that reason renormalization group (RG) methods [9,13] were used to tackle this problem. With RG, Machta [9] found the scaling exponents of the QTM and Monthus [13] 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. Here we provide a statistical analysis of subdiffusion in the QTM with an approach based on a novel time transformation. Possible applications of our method to other nonequilibrium problems are mentioned at the end of the Letter.

Quenched trap model.—We consider a random walk on a one dimensional lattice with lattice spacing equal one [1,13,14]. 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 waiting for a period τ_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 τ_0, then with probability $1/2$ jumps to $x = 1$ (or $x = -1$), waits there for τ_1 (or τ_{-1}), then if the particle returns to $x = 0$ it waits for a time interval τ_0, etc. The $\{\tau_x\}$'s are positive independent identically distributed random variables with a common probability density function (PDF)

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

for $\tau_x \to \infty$ and $0 < \alpha < 1$. Hence, the Laplace transform of the waiting time PDF is $\hat{\psi}(u) \sim 1 - A u^\alpha + \cdots$ when $u \to 0$. As is 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 Letter 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].

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. We define the random variable $\eta = t/(\mathcal{S}_\alpha)^{1/\alpha}$ where

$$\mathcal{S}_\alpha = \sum_{x=-\infty}^{\infty} (n_x)^\alpha. \quad (2)$$

When $\alpha = 1$, $\mathcal{S}_\alpha$ is the total number of jumps made $\sum_{x=-\infty}^{\infty} n_x = s$. In the opposite limit $\alpha \to 0$, $\mathcal{S}_0$ 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

$$\text{the PDF of } \eta \text{ is } l_{\alpha,A,1}(\eta), \quad (3)$$

where $l_{\alpha,A,1}(\eta)$ is the one-sided Lévy PDF whose Laplace $\eta \to u$ pair is $\exp(-Au^\alpha)$. 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 $\{n_x\}$ provide the scaling through $\mathcal{S}_\alpha$. By definition, the Laplace $\eta \to u$ transform of the PDF of η is

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

We average with respect to the disorder, namely, with respect to the independent and identically distributed random waiting times τ_x, and obtain $\langle e^{-u\eta}\rangle = \Pi_{x=-\infty}^{\infty} \hat{\psi}[\frac{n_x u}{(\mathcal{S}_\alpha)^{1/\alpha}}]$ where $\hat{\psi}(u)$ is the Laplace transform of the PDF of waiting times $\psi(\tau_x)$. We use $\hat{\psi}(u) \sim \exp(-Au^\alpha) \sim 1 - Au^\alpha + \cdots$

$$\langle e^{-u\eta}\rangle \sim \Pi_{x=-\infty}^{\infty} \exp\left[-\frac{A(n_x)^\alpha u^\alpha}{\mathcal{S}_\alpha}\right] = e^{-Au^\alpha}. \quad (5)$$

Hence, the PDF of η is a one-sided Lévy law, Eq. (3). We now invert the process fixing time t to find the PDF of $\mathcal{S}_\alpha$

$$\mathcal{N}_t(\mathcal{S}_\alpha) \sim \frac{t}{\alpha}(\mathcal{S}_\alpha)^{-1/\alpha-1} l_{\alpha,A,1}\left[\frac{t}{(\mathcal{S}_\alpha)^{1/\alpha}}\right]. \quad (6)$$

We can now use the operational time $\mathcal{S}_\alpha$ to obtain the desired diffusion front of the QTM; in other words, we get rid of the disorder and focus only on Brownian motion. For an ensemble of paths on many realizations of disorder, the position of the particle is determined by the position of a Brownian particle stopped at the random operational time $\mathcal{S}_\alpha$. To see this, note that in the original model the probability to jump left and right is $1/2$ which implies Brownian scaling $x \sim \sqrt{s}$, and the laboratory time t enters through the random fluctuations of s. Similarly, visitation numbers are decoupled from waiting times since the duration of sticking times are not related to the probabilities of jumping left or right and, hence, statistical properties of x are determined by $\mathcal{S}_\alpha$ which as mentioned is itself a random variable influenced by the disorder through the time transformation Eq. (6). Next, we summarize the transformation to make it more precise.

Mapping the QTM onto Brownian motion.—We first define the new process (as an algorithm) and then return to analytical calculations. 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 η from the one-sided Lévy PDF $l_{\alpha,A,1}(\eta)$. 3. With η and t determine the operational time $\mathcal{S}_\alpha = (t/\eta)^\alpha$. 4. Generate a simple symmetric random walk on a lattice (probability $1/2$ for jumping left and right). Stop this Brownian process once its own $\mathcal{S}'_\alpha$ reaches the operational time $\mathcal{S}_\alpha$ set in step 3. 5. Record the position x of the particle at the end of the previous step. 6. Return 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.* [15]. Notice that with this exact scheme, we have mapped the random walk in a random environment to a Brownian motion problem.

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

$$\langle P(x,t)\rangle \sim \int_0^\infty P_{\mathcal{S}_\alpha}(x)\mathcal{N}_t(\mathcal{S}_\alpha)d\mathcal{S}_\alpha \quad (7)$$

where $\mathcal{N}_t(\mathcal{S}_\alpha)$ is given in Eq. (6). For the mean field version of the model (i.e., CTRW) replace $\mathcal{S}_\alpha$ with the number of steps s of the Brownian motion, and then $P_{\mathcal{S}_\alpha}(x)$ is Gaussian as is well known [16]. From normal Brownian motion we have the scaling behavior $x \propto (\mathcal{S}_\alpha)^{1/(1+\alpha)}$. To see this we use (i) usual Brownian scaling $x \propto s^{1/2}$ and (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 $\mathcal{S}_\alpha \propto \sqrt{s}(n_x)^\alpha \propto s^{(1+\alpha)/2}$ which gives $x \propto (\mathcal{S}_\alpha)^{1/(1+\alpha)}$. This scaling implies

$$P_{\mathcal{S}_\alpha}(x) = \frac{1}{(\mathcal{S}_\alpha)^{1/(1+\alpha)}} B_\alpha\left[\frac{x}{(\mathcal{S}_\alpha)^{1/(1+\alpha)}}\right] \quad (8)$$

with $B_\alpha(z)$ a normalized nonnegative function. Define the scaling variable $\xi = x/(t/A^{1/\alpha})^{\alpha/(1+\alpha)}$ and $\langle P(x,t)\rangle \sim g_\alpha(\xi)/(t/A^{1/\alpha})^{\alpha/(1+\alpha)}$ which according to Eq. (7) is

$$g_\alpha(\xi) = \int_0^\infty dy y^{\alpha/(1+\alpha)} B_\alpha(\xi y^{\alpha/(1+\alpha)}) l_{\alpha,1,1}(y). \quad (9)$$

A general 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 $\langle |z|^q\rangle = \int_{-\infty}^{\infty} |z|^q B_\alpha(z)dz$

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

The new content of Eqs. (9) and (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. Scaling in Eq. (10) is very different than the mean field prediction which gives $\langle |x|^q\rangle \propto t^{\alpha q/2}$ [1,2].

Generating Brownian trajectories on a lattice, we found $B_\alpha(z)$ in Fig. 1, which shows an interesting transition from

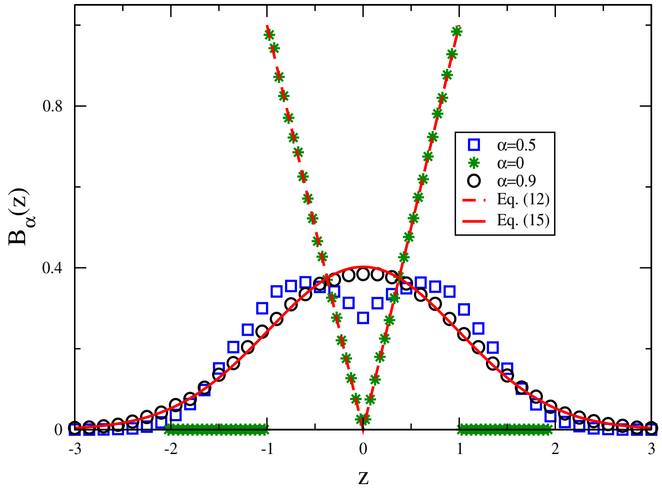

FIG. 1 (color online). The PDF $B_\alpha(z)$ exhibits a transition between a Gaussian shape when $\alpha \to 1$ to a V shape when $\alpha \to 0$. Simulations of Brownian motion on a lattice yield excellent agreement with theoretical predictions Eqs. (12) and (15) without fitting.

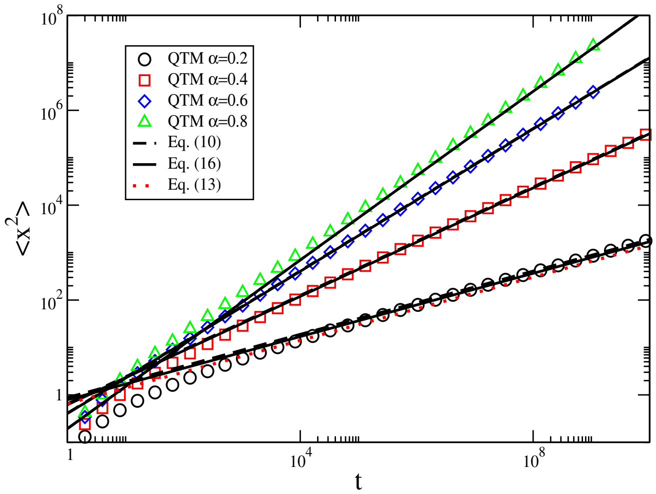

FIG. 2 (color online). The mean square displacement of the QTM versus time. Numerical data match perfectly our theory (the lines plotted with $\langle z^2 \rangle$ in Table I) and analytical formulas Eq. (13) for $\alpha = 0.2$ and Eq. (16) for $\alpha = 0.4, 0.6, 0.8$.

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 $\langle x^2 \rangle$. 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 our method 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 [14]. Briefly, QTM simulations do not converge on reasonable computer time scales for, say, $\alpha > 0.8$. In contrast, our 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) and (10) provide solutions to the QTM.

The limit $\alpha \to 0$ corresponds to strong disorder. To find $B_0(z)$ we consider Brownian motion stopped at "time" $\mathcal{S}_0$ where, as mentioned, $\mathcal{S}_0$ is the span of the random walk. Consider $P_{\mathcal{S}_0}(\mathcal{S}_0 - n)$ where $x = \mathcal{S}_0 - n > 0$ 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 $\mathcal{S}_0$ to reach its destination $x = \mathcal{S}_0 - 1$ and the span is $\mathcal{S}_0$. On the other hand if it jumps to $x = 1$ the distance the particle must travel is $\mathcal{S}_0 - 2$ and the span must still be $\mathcal{S}_0$. Hence $P_{\mathcal{S}_0}(\mathcal{S}_0 - 1) = [P_{\mathcal{S}_0}(\mathcal{S}_0) + P_{\mathcal{S}_0}(\mathcal{S}_0 - 2)]/2$. More generally

$$P_{\mathcal{S}_0}(\mathcal{S}_0 - n) = \frac{1}{2}[P_{\mathcal{S}_0}(\mathcal{S}_0 - n - 1) + P_{\mathcal{S}_0}(\mathcal{S}_0 - n + 1)], \tag{11}$$

and for the boundary term $P_{\mathcal{S}_0}(\mathcal{S}_0) = [P_{\mathcal{S}_0}(\mathcal{S}_0 - 1) + P_{\mathcal{S}_0 - 1}(\mathcal{S}_0 - 1)]/2$. Equation (11) is easily solved $P_{\mathcal{S}_0}(x) = \frac{|x|}{\mathcal{S}_0(\mathcal{S}_0+1)}$ for $-\mathcal{S}_0 \le x \le \mathcal{S}_0$ 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 V shape PDF [see Fig. 1]

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

α	0	0.2	0.4	0.6	0.8	1
$\langle z^2 \rangle$	0.5	0.67	0.81	0.91	0.96	1

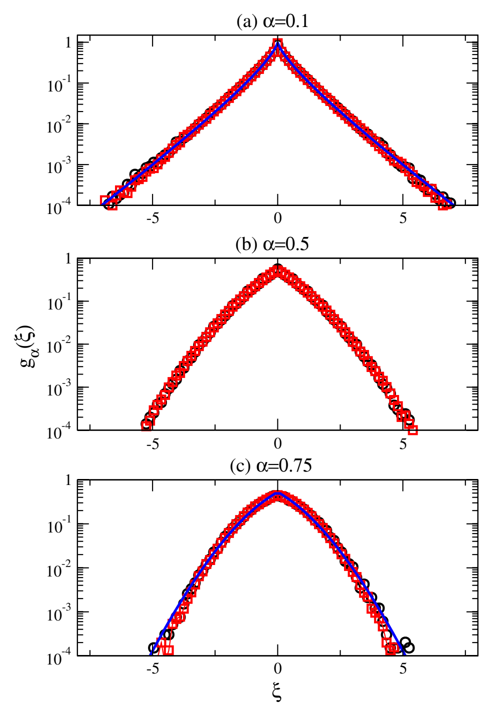

FIG. 3 (color online). The diffusion front of QTM (squares) match perfectly the presented theory (circles) and analytical predictions (lines) Eqs. (9), (14), and (15).

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

This V shape reflects the tendency of a Brownian particle to reach a large span $\mathcal{S}_0$ when it is far from the origin.

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

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

which is tested in Fig. 2. Inserting $\langle z^{2q}\rangle = (1+q)^{-1}$ in Eq. (10) we obtain the moments $\langle x^{2q}\rangle$ of the QTM. Straightforward 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 Monthus [13] 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 $\mathcal{S}_1 = \sum_{x=-\infty}^{\infty} n_x = s$; namely, $\mathcal{S}_1$ is nonrandom since it is equal to the number of steps made. Therefore, when α is close enough to 1 we may neglect fluctuations and $\mathcal{S}_\alpha = \langle \mathcal{S}_\alpha\rangle$. In a longer publication, we will show that $\langle \mathcal{S}_\alpha\rangle = \mathcal{C}_\alpha s^{(1+\alpha)/2}$ with $\mathcal{C}_\alpha = 2^{(\alpha+3)/2}\Gamma(1+\alpha/2)/[\sqrt{\pi}(1+\alpha)]$. As is well known, the PDF of finding the Brownian particle on x after s jumps is the Gaussian $P_s(x) = \exp(-x^2/2s)/\sqrt{2\pi s}$; hence, the change of variables to $\mathcal{S}_\alpha$ gives

$$B_\alpha(z) \sim [2\pi/(\mathcal{C}_\alpha)^{2/(1+\alpha)}]^{-1/2} \exp\left[-\frac{(\mathcal{C}_\alpha)^{2/(1+\alpha)} z^2}{2}\right]. \tag{15}$$

It follows that $\langle z^2\rangle \sim (\mathcal{C}_\alpha)^{-2/(1+\alpha)}$; hence, for the QTM

$$\langle x^2\rangle \simeq (\mathcal{C}_\alpha)^{-2/(1+\alpha)}\frac{\Gamma(\frac{2}{1+\alpha})}{\alpha\Gamma(\frac{2\alpha}{1+\alpha})}\left(\frac{t}{A^{1/\alpha}}\right)^{2\alpha/(1+\alpha)}. \tag{16}$$

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. (16) works very well even for $\alpha = 0.4$. With Eqs. (9) and (15) and the steepest descent method we find for $\xi \gg 1$

$$g_\alpha(\xi) \sim b_1 \xi^{-2(1-\alpha)/(3-\alpha)} e^{-b_2 \xi^{2(1+\alpha)/(3-\alpha)}} \tag{17}$$

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

The method presented in the Letter could be applied to many other situations. It is easily extended to higher dimensions, for transport in biased random walks and to the investigation of irreproducibility of time averages in single molecule experiments [4,17]. As mentioned, random walks in configuration space describe glassy dynamics and currently mean field theories are used for such systems [5,6], e.g., dynamics among metabasins describing supercooled liquids [7]. The mean field is expected to work only for a system with a very high connectivity, namely, a jump from one metabasin to any other is possible in principle. If this picture is abandoned, one has to take into account the connectivity of the energy landscape and the possibility of closed paths. More practically one may use our method to calculate measurable quantities like aging correlation functions which will differ from the mean field prediction. This might lead to a measurable classification of dynamics of many complex systems in terms of mean field or non-mean-field behaviors.

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