Random walks on random partitions in one dimension

Walter Nadler*
Institut für Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, D-72076 Tübingen, Germany

Tsongjy Huang† and D. L. Stein‡
Department of Physics, University of Arizona, Tucson, Arizona 85721

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Random walks on *state space partitions* provide an abstract generic picture for the description of macroscopic fluctuations in heterogeneous systems such as proteins. We determine the average residence probability and the average distribution of residence times in a particular macroscopic state for the ensemble of *random partitions* of a one-dimensional state space. In particular, the probability that a walker remains in an open-state cluster decays in a manner that is slower than exponential but faster than a power law. [S1063-651X(96)09809-1]

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I. INTRODUCTION

At physiological temperatures, proteins fluctuate strongly between different microscopic conformations [1–4]. On a macroscopic level, these microscopic fluctuations can manifest themselves as fluctuations between protein states of different functionality. One simple, well-known example is a protein acting as a passive ion channel that can be in either an open or a closed state [5,6]. Other examples are fluctuations of transport proteins between states of different binding activity for the ligand [7,8] or fluctuations of catalytic proteins between states of different catalytic effectivity. We will advocate here a generic, albeit abstract, view for the description of these macroscopic manifestations of microscopic conformational fluctuations.

Proteins are instances of systems with a high-dimensional state space [9]. This space of microscopic conformations can be partitioned into sets corresponding to the different macroscopic protein states. Usually, several microscopic conformations that are close to each other in state space will belong to the same macroscopic state and will form a more or less extended individual patch. All patches that belong to one particular macroscopic state then make up one partition set; see Fig. 1. There are several relevant topologies for the respective structures of the partition regions in that high-dimensional state space: one or several of them may percolate throughout the entire state space, but not the others, or all of them may percolate. Note that, due to the high dimensionality of the state space, independent percolation of different partitions is possible. However, having none percolate requires special geometries and is unlikely to be encountered [10].

Thermal fluctuations can, in general, be modeled successfully as a random walk in some state space [11–13]. Conformational fluctuations of proteins, particularly at physiological temperatures, are no exception to that. Fluctuations of the macroscopic state of a protein arise in this picture from the random walk leaving a patch corresponding to one macrostate and entering the patch of another macrostate. During the time the random walk stays in that patch the protein stays in that macrostate until it leaves the patch again either to enter the one it came from or to enter another; see Fig. 1. We will call this approach the random walk on state space partition (RWSSP) picture of macroscopic fluctuations.

Due to the complicated interactions involved in a strongly heterogeneous system such as a protein, the random walk in protein state space has to be viewed as one on a very rugged

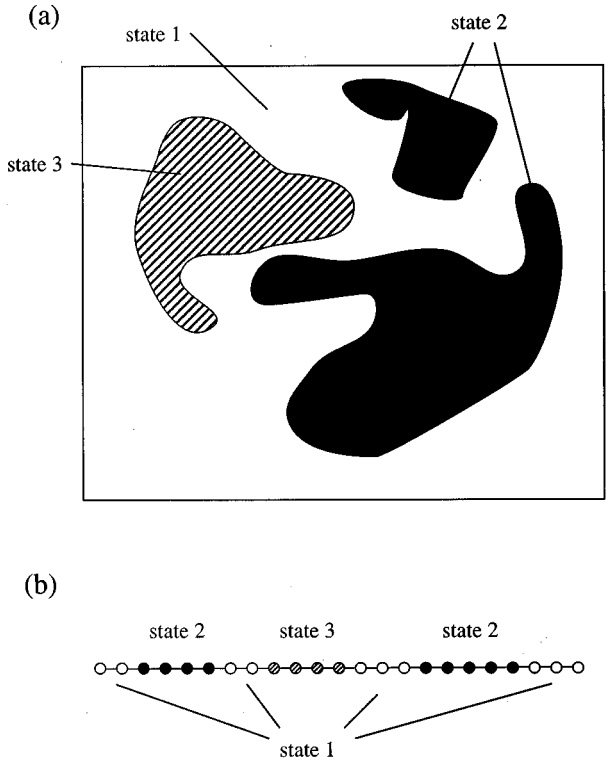

FIG. 1. Sketch of state space partitioning in (a) two dimensions and (b) one dimension.

*Electronic address: walter.nadler@uni-tuebingen.de
†Electronic address: thuang@physics.arizona.edu
‡Electronic address: dls@physics.arizona.edu

potential surface [14]. Particularly in the low-temperature regime, this ruggedness imposes strong limitations on the parts of state space that are accessible at all, a feature known as ''broken ergodicity'' [15,16]. Although there has been considerable work on stochastic processes on rugged potentials, the properties of macroscopic fluctuations due to rugged potential random walks on partitions are completely unknown up to now. Nevertheless, they could possibly give interesting insights into the low-temperature behavior of glasses and of proteins.

Here, however, we will be concerned with the high-temperature regime. In this regime, random walks on rugged potentials can be viewed on macroscopic length scales as free diffusion with some suitably renormalized diffusion coefficient [17–19]. It is also known that, e.g., Mössbauer data on protein fluctuations can be described successfully using an effective temperature-dependent diffusion coefficient in a smooth, slowly varying potential [20–22]. We will therefore assume in the following that the random walk in the protein conformational state space can be described in a first approximation as free diffusion.

The open-state–closed-state fluctuations of passive ion channel proteins are a very suitable candidate for illustrating the scheme that we sketched above. In this case there is a simple, natural partitioning of state space, namely, the open and closed states. In our approach, a channel that switches from the open to the closed state can be thought of as crossing the boundary from a region of open-state configurations to a region of closed-state configurations. On the other hand, there already exists a vast array of experimental literature on the fluctuation properties of these channel proteins; see, e.g., Ref. [23] and references therein. Since single-channel fluctuations can be monitored individually using the patch clamp technique [24], residence times in the open-state and closed-state partitions are readily accessible for a statistical analysis. In particular, the distribution of residence times in the closed state, usually called the closing time distribution $P_{\text{closed}}(t)$, is often observed to exhibit an algebraic regime with a $t^{-3/2}$ power law in many ion channel proteins [25–28].

We have discussed some preliminary results of an analysis of this model in other papers [29,30]. There we treated a particular form of state space partitioning, motivated by the ion channel situation—a single patch corresponding to an open state, surrounded by closed states—and we investigated the generic behavior of the closing time distribution and its dependence on state space dimension.

In this paper we begin a more detailed study of the RWSSP approach. Here we will not make any specific assumptions about the partitioning of state space but rather we will treat it as *random*: each state is assigned to one macroscopic partition with a probability p and to the other (or others) with a probability $1-p$. We will be interested in the behavior of the distribution of residence times in that particular partition, *averaged* over the defined ensemble of state space partitionings. In this way we will be able to distinguish whether any experimentally observed dynamics depends on a particular topology and geometry of state space partitioning or whether it can be explained simply as a generic property of a particular *state space volume fraction* of the macroscopic states in question.

We will confine our attention in this paper to the one-dimensional version of the model. We do not expect these results to apply to observations on closing time distributions in ion channel proteins, whose state space, as noted above, is high dimensional. However, the work here is a prerequisite to an understanding of the higher-dimensional behavior of the model and its analysis is interesting in its own right. In one dimension we can solve the model exactly in at least three different ways, two of which we discuss here. The third technique, not discussed below, uses generating functions and provides no additional insights. We find that in one dimension our model exhibits an interesting and nontrivial time evolution. In particular, the probability that a walker remains in an open-state cluster decays in a manner that is slower than exponential but faster than a power law.

II. MODEL

We consider a one-dimensional lattice with unit spacing. Each site is present with probability p and absent with probability $1-p$. At each time step, a random walker has an equal probability of stepping to the left or to the right. The question we seek to answer is this: Given that an ensemble of random walkers starts at time zero at the edge of a connected cluster of sites, what fraction still resides within the same cluster a time t later?

We frame the problem in this way because this quantity is equivalent to the fraction of proteins remaining in a particular macroscopic state, given that they switched to that state at $t=0$. That state could be, e.g., either the open state or the closed state of an ion channel protein. However, as noted above, the observable usually reported in measurements of ion channel fluctuations is the distribution of *closing* times. What is the connection between the distribution of residence times in a particular state $P(t)$ and the above defined fraction? Let $N(t)$ denote the fraction of proteins that remain in the macroscopic state at time t, given that all switched to that state at $t=0$. We will call it, in analogy to the terminology in reaction-diffusion systems, the *surviving fraction*. Since at time t only those proteins that have a residence time greater than t contribute to $N(t)$, we have

$$N(t)=\int_t^\infty dt' P(t') \tag{2.1}$$

and so the residence time distribution is given by

$$P(t)=-dN(t)/dt. \tag{2.2}$$

Therefore, by computing $N(t)$ we can deduce $P(t)$.

We will take the origin as a vacant site to the left of a cluster. The random walker starts at site 1 at $t=0$, thereby satisfying our formulation of the problem. We will denote the averages over all distributions of present and absent sites (with probability p) by $\langle\ \rangle_p$.

III. EIGENFUNCTION EXPANSION

In our first approach we calculate exactly the time evolution of the fraction of random walkers inside a cluster of size l and the corresponding residence time distribution by solving the eigenvalue problem of the corresponding transition rate matrix. The quantities $\langle N(t)\rangle_p$ and $\langle P(t)\rangle_p$ are then ob-

tained by averaging over the distribution of cluster sizes p_l in the ensemble. We first formulate the problem in continuous time. However, the problem can be solved equally well in a discrete time formulation, which is done later in this section. In Sec. IV we will present, as an alternative approach, a direct counting technique to solve the discrete time problem.

Let us consider a random walker that starts at an edge of a one-dimensional cluster of size l and is able to escape from that cluster at both ends. The probability distribution $\mathbf{p}_l(t)$ over the sites $1,\ldots,l$ is then the solution of the equation

$$\dot{\mathbf{p}}_l(t)=\mathbf{A}_l\mathbf{p}_l(t), \tag{3.1}$$

where the *transition rate* matrix $\mathbf{A}_l$ is given by

$$\mathbf{A}_l=\tau^{-1}\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ & & \vdots & & & \\ 0 & 0 & 0 & \cdots & 1 & -2 \end{pmatrix}, \tag{3.2}$$

with τ being the hopping time scale. Since the choice of the starting edge is arbitrary, we use the initial condition

$$\mathbf{p}_l(0)=\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{3.3}$$

It is a straightforward exercise to exploit the cyclic properties of $\mathbf{A}_l$ and determine the eigenvalues λ_j and eigenvectors $\mathbf{e}(j)$ by a Fourier transform ansatz. One finds

$$\lambda_j=-2[1-\cos(k_j)]/\tau=-4\sin^2(k_j/2)/\tau \tag{3.4}$$

and

$$e_i(j)=\sqrt{\frac{2}{l+1}}\sin(ik_j), \tag{3.5}$$

with

$$k_j=\frac{\pi}{l+1}j, \quad j=1,\ldots,l. \tag{3.6}$$

We note that the eigenvectors (3.5) are already normalized. With these eigenvectors and eigenvalues the solution of Eqs. (3.1)–(3.3) is given by

$$\mathbf{p}_l(t)=\sum_{j=1}^{1}\mathbf{e}(j)e_1(j)e^{\lambda_j t}. \tag{3.7}$$

From this result the fraction of random walkers still in the l cluster at time t is obtained by summing over all components of $\mathbf{p}_l(t)$,

$$N_l(t)=\sum_{j=1}^{l}\sum_{i=1}^{l}e_i(j)e_1(j)e^{\lambda_j t}=\sum_{j=1}^{l}a_j(l)e^{\lambda_j t}, \tag{3.8}$$

where the expansion coefficients are

$$a_j(l)=\frac{4}{l+1}\sin^2\left(\frac{j\pi}{2}\right)\cos^2\left(\frac{j\pi}{2(l+1)}\right). \tag{3.9}$$

Note that the term $\sin^2(j\pi/2)$ is one for odd values of j and zero for even j. Using Eq. (2.2), the residence time distribution $P_l(t)$ follows from Eq. (3.8):

$$P_l(t)=-\sum_{j=1}^{l}a_j(l)\lambda_j e^{\lambda_j t}. \tag{3.10}$$

In the corresponding discrete time problem, the distribution $\mathbf{p}_l(t)$ is defined only for discrete values of $t=0,1,\ldots$ and the differential equation (3.1) is replaced by

$$\mathbf{p}_l(t+1)=\mathbf{W}_l\mathbf{p}_l(t), \tag{3.11}$$

where the *transition probability* matrix $\mathbf{W}_l$ is given by

$$\mathbf{W}_l=\begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & & \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ & & & \vdots & & \\ 0 & 0 & 0 & \cdots & \frac{1}{2} & 0 \end{pmatrix}. \tag{3.12}$$

Eigenvalues and eigenvectors are determined analogously to the continuous time case. Now the eigenvalues are

$$\lambda_j=\cos(k_j) \tag{3.13}$$

and the eigenvectors are identical to Eq. (3.5). In the discrete time case the exponential is replaced by an appropriate power of the respective eigenvalue, i.e., we get for the fraction of random walkers still in the l cluster at time t

$$N_l(t)=\sum_{j=1}^{l}a_j(l)\lambda_j^t, \tag{3.14}$$

with the same expansion coefficients $a_j(l)$ as in the continuous time case. The residence time distribution has to be determined in this case by a discrete variant of Eq. (2.2), i.e.,

$$P_l(t)=N_l(t)-N_l(t+1)=\sum_{j=1}^{l}a_j(l)\lambda_j^t(1-\lambda_j). \tag{3.15}$$

Finally, we have to average our above results over the distribution of l clusters. The relative probability of a cluster of occupied sites of length l is given by $(1-p)^2p^l$, where the term $(1-p)^2$ arises from the two unoccupied sites at each end. Correct normalization then leads to

$$p_l=(1-p)p^{l-1}. \tag{3.16}$$

Calculating the average is again straightforward,

$$\langle N(t)\rangle_p=\sum_{l=1}^{\infty}N_l(t)p_l, \tag{3.17}$$

with a similar form for $\langle P(t)\rangle_p$. Finally, the solution for $\langle N(t)\rangle_p$ in the continuous time basis is

$$\langle N(t)\rangle_p=(1-p)\sum_{l=1}^{\infty}\frac{4p^{l-1}}{l+1}\sum_{j=1}^{l}\cos^2\left[\frac{j\pi}{2(l+1)}\right]\sin^2\left(\frac{j\pi}{2}\right)\times\exp\left[-4\sin^2\left(\frac{j\pi}{2(l+1)}\right)\frac{t}{\tau}\right],\tag{3.18}$$

whereas in a discrete time basis it is

$$\langle N(t)\rangle_p=(1-p)\sum_{l=1}^{\infty}\frac{4p^{l-1}}{l+1}\sum_{j=1}^{l}\cos^2\left[\frac{j\pi}{2(l+1)}\right]\sin^2\left(\frac{j\pi}{2}\right)\times\cos^t\left(\frac{j\pi}{l+1}\right).\tag{3.19}$$

A detailed numerical analysis of these results will be given in Sec. V. In Sec. IV we will present an alternative derivation of the discrete time results, based on a direct counting scheme for individual random walks, that will prove useful for higher-dimensional systems. However, before doing so we will give a discussion on how the time scales of the discrete time and continuous time results are related. For that purpose it is useful to analyze the surviving fraction $N_l(t)$ for a large l cluster. Asymptotically for large l, the sum in Eq. (3.8) can be replaced by an integral and the fast oscillating function $\sin^2(j\pi/2)$ can be replaced by $\frac{1}{2}$. This procedure leads eventually to

$$N_\infty(t)=\lim_{l\to\infty}N_l(t)=e^{-2t/\tau}[I_0(2t/\tau)+I_1(2t/\tau)]\tag{3.20}$$

in the continuous time case, where I_0 and I_1 are the modified Bessel functions of order zero and one, respectively [31]. [We note that this functional dependence appears often when reaction-diffusion processes in semi-infinite one-dimensional systems are considered; see, e.g., Ref. [27]; see also Ref. [32], for a case where a physically unrelated quantity, the time-dependent rate coefficient at a trap in the thermodynamic limit of a one-dimensional N-particle diffusion problem, obeys the same basic equations as our $N_l(t)$.] In the discrete time case the result is

$$N_\infty(t)=\frac{1}{\pi}\int_0^\pi dx[\cos^t(x)+\cos^{t+1}(x)].\tag{3.21}$$

Only the cosine term with an even exponent gives a nonzero contribution after integration. Therefore, we get eventually

$$N_\infty(t)=\frac{\left(2\left\lfloor\frac{t+1}{2}\right\rfloor-1\right)!!}{\left(2\left\lfloor\frac{t+1}{2}\right\rfloor\right)!!},\tag{3.22}$$

where the floor function $\lfloor x\rfloor$ gives the integer part of x and the double factorial is defined by $(2m)!!=2^m m!$ and $(2m-1)!!=2^m\Gamma(m+1/2)/\sqrt{\pi}$ [31]. For large values of t the functions (3.20) and (3.22) approach

$$N_\infty(t)\to\frac{1}{\sqrt{\pi t/\tau}}\tag{3.23}$$

and

$$N_\infty(t)\to\frac{1}{\sqrt{\pi\left\lfloor\frac{t+1}{2}\right\rfloor}},\tag{3.24}$$

respectively. The above results show that the choice $\tau=2$ is necessary for a comparison of the discrete and continuous time cases and that they become equivalent, at least for large t. However, as was to be expected from the choice of the model, the discrete time case exhibits the feature that $N_l(t)$ is constant for pairs of successive time points.

IV. DIRECT COUNTING PROCEDURE

The next method employs a direct counting technique. This method will prove to be particularly useful in examining our problem on higher-dimensional lattices. However, we defer discussion of that problem to a future paper. Here we will just introduce the technique and show its application.

We consider an n-step walk [corresponding to n time steps, i.e., we will relabel $\langle N(t)\rangle_p$ to $\langle N(n)\rangle_p$] and ask for the probability that the walker has not been absorbed, i.e., has not stepped onto a missing site. The basic idea in this approach is the observation that each time the walker steps on a previously *untested* site, there is a probability p that the walker remains in the starting cluster. Any step to a previously tested site, of course, will result in the walker remaining in its starting cluster with probability one. Let $C(n)$ denote all possible realizations of an n-step walk, subject to the constraint of never stepping to a negative level, and let $g(k)$ equal the number of sites touched *at least once* by the kth realization of such a walk. For unbiased walks it then follows that

$$\langle N(n)\rangle_p=(\tfrac{1}{2})^n\sum_{k=1}^{C(n)}p^{g(k)}.\tag{4.1}$$

However, although a good starting point for simulations, this formula is still impractical to deal with analytically. Rather, we classify each n-step walk by the site m it finally reaches and by the largest distance from level 0 it assumes during the walk; the latter we denote by $m+i$. Clearly, each such walk has visited exactly $m+i$ different sites. Let $C_{m+i}(n,m)$ be the number of walks in that class; Eq. (4.1) can then be rewritten as

$$\langle N(n)\rangle_p=(\tfrac{1}{2})^n\sum_{m=0}^{n}p^m\sum_{i=0}^{\lfloor(n-m)/2\rfloor}p^iC_{m+i}(n,m).\tag{4.2}$$

It turns out that it is helpful to use a somewhat different quantity, namely, the number of ways in which a walker, starting at site 0 and never stepping onto a negative site, can reach site m without going *beyond* level $m+i$. We will call this quantity $W_{m+i}(n,m)$.

It is easily seen that

$$C_{m+i}(n,m)=W_{m+i}(n,m)-W_{m+i-1}(n,m).\tag{4.3}$$

Using this relation, Eq. (4.2) can be rearranged as

$$\langle N(n)\rangle_p=(\tfrac{1}{2})^n\sum_{m=0}^{n}\left[\sum_{i=0}^{\lfloor (n-m)/2\rfloor}p^{m+i}(1-p)W_{m+i}(n,m)+p^{(n+m)/2+1}W_{(n+m)/2}(n,m)\right]. \tag{4.4}$$

The advantage of using the quantities $W_{m+i}(n,m)$ is that they can be determined by repeated application of the reflection principle for unbiased random walks [33]. The calculation is straightforward, though tedious, and the result is

$$\begin{aligned}W_{m+i}(n,m)=&\binom{n}{\frac{n+m}{2}}-\sum_{k=0}\left[\binom{n}{\frac{n+m}{2}+1+k(m+2+i)}-\binom{n}{\frac{n+m}{2}+2+i+k(m+2+i)}\right]\\&-\sum_{j=0}\left[\binom{n}{\frac{n+m}{2}+1+i+j(m+2+i)}-\binom{n}{\frac{n+m}{2}+(j+1)(m+2+i)}\right],\end{aligned} \tag{4.5}$$

where the upper limits of the sums over k and j are finite and depend on the condition that the value of the lower element of a binomial coefficient must be less than or equal to the value of the upper element. In Appendix A we show that

$$\left(\frac{1}{2}\right)^n W_l(n,m)=\frac{2}{l+2}\sum_{j=1}^{l+1}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\times\sin\left(\frac{(m+1)j\pi}{l+2}\right). \tag{4.6}$$

We now prove the equivalence of Eq. (3.19) and Eqs. (4.4) and (4.5). Since in an n-step walk the walker cannot reach a level higher than $\lfloor (n+m)/2\rfloor$ and a site m beyond level n, i.e., $C_i(n,m)=0$ for $i>\lfloor (n+m)/2\rfloor$ and $m\geqslant n$, the sums over i and m in Eq. (4.2) can be extended to infinity,

$$\langle N(n)\rangle_p=(\tfrac{1}{2})^n\sum_{m=0}^{\infty}\sum_{i=0}^{\infty}p^{m+i}C_{m+i}(n,m). \tag{4.7}$$

Combining Eq. (4.7) with Eqs. (4.3) and (4.4), we have

$$\langle N(n)\rangle_p=\sum_{m=0}^{\infty}\sum_{l=m}^{\infty}\frac{2p^l(1-p)}{l+2}\sum_{j=1}^{l+1}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\times\sin\left(\frac{(m+1)j\pi}{l+2}\right), \tag{4.8}$$

which can be rewritten as

$$\begin{aligned}\langle N(n)\rangle_p&=\sum_{l=0}^{\infty}\frac{2p^l(1-p)}{l+2}\sum_{j=1}^{l+1}\sum_{k=1}^{l+1}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\times\sin\left(\frac{kj\pi}{l+2}\right)\\&=\sum_{l=1}^{\infty}\frac{2p^{l-1}(1-p)}{l+1}\sum_{j=1}^{l}\sum_{k=1}^{l}\cos^n\left(\frac{j\pi}{l+1}\right)\sin\left(\frac{j\pi}{l+1}\right)\times\sin\left(\frac{kj\pi}{l+1}\right).\end{aligned} \tag{4.9}$$

The series $\Sigma_{k=1}^{l}\sin[kj\pi/(l+1)]$ is evaluated by rearranging the terms in the series

$$\begin{aligned}\sum_{k=1}^{l}\sin\left(\frac{kj\pi}{l+1}\right)=&\left[\sin\left(\frac{j\pi}{l+1}\right)+\sin\left(\frac{jl\pi}{l+1}\right)\right]+\left[\sin\left(\frac{2j\pi}{l+1}\right)+\sin\left(\frac{(l-1)j\pi}{l+1}\right)\right]+\left[\sin\left(\frac{3j\pi}{l+1}\right)\right.\\&\left.+\sin\left(\frac{(l-2)j\pi}{l+1}\right)\right]+\cdots,\end{aligned} \tag{4.10}$$

which after some straightforward but tedious manipulation yields

$$\sum_{k=1}^{l+1}\sin\left(\frac{kj\pi}{l+1}\right)=\sin\left(\frac{j\pi}{2}\right)\csc\left[\frac{j\pi}{2(l+1)}\right]\sin\left[\frac{j\pi(l+2)}{2(l+1)}\right]. \tag{4.11}$$

Plugging the above result back into Eq. (4.9), we finally have

$$\langle N(n)\rangle_p=(1-p)\sum_{l=1}^{\infty}\frac{4p^{l-1}}{l+1}\sum_{j=1}^{l}\cos^n\left(\frac{j\pi}{l+1}\right)\cos^2\left[\frac{j\pi}{2(l+1)}\right]\times\sin^2\left(\frac{j\pi}{2}\right), \tag{4.12}$$

which is identical to Eq. (3.19).

V. RESULTS

From a numerical point of view, the continuous time and discrete time cases differ fundamentally. While for the discrete time case the infinite sum eigenfunction expansion result Eq. (3.19) can be replaced by a finite sum, using Eqs. (4.4) and (4.6), this cannot be done in the continuous time case Eq. (3.18). In this paper we will follow traditional lines and take the result for the continuous time case as the starting point for a numerical analysis of the behavior of the quantities of interest. Details of an effective numerical evaluation of Eqs. (4.4) and (4.6) are deferred to a future paper. We note, however, that both approaches show excellent numerical agreement over many decades.

Since, for a particular value of t and p, $N_l(t)$ increases monotonically as l increases, whereas p^{l-1} decreases, it is necessary to find a good truncation criterion for the infinite sum. Fortunately, $N_l(t)$ is bounded from above by

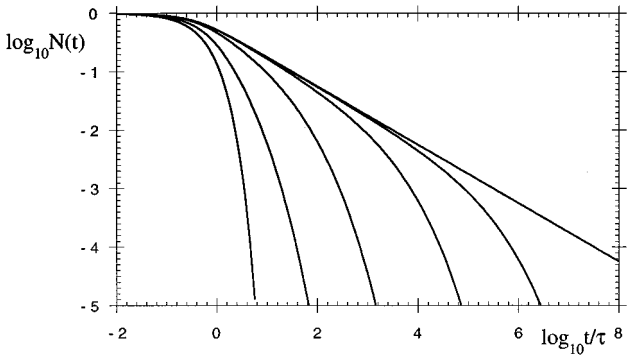

FIG. 2. $\langle N(t)\rangle$ vs t for $p=0,0.5,0.9,0.99,0.999,1$ (from left to right).

$$N_\infty(t)=e^{-2t/\tau}[I_0(2t/\tau)+I_1(2t/\tau)]; \tag{5.1}$$

see Sec. III. The Bessel functions in Eq. (5.1) can be evaluated to sufficient accuracy using standard techniques [31,34]. Utilizing $N_\infty(t)$ it is possible to give an approximation to $\langle N(t)\rangle_p$ that involves only the evaluation of a finite sum

$$\langle N(t)\rangle_{p,\text{approx}}=(1-p)\sum_{l=1}^{L} p^{l-1}N_l(t)+p^L N_\infty(t), \tag{5.2}$$

where L is determined from the condition

$$N_\infty(t)-N_L(t)<\frac{\epsilon}{1-\epsilon}\,p^{-L}\langle N(t)\rangle_{p,\text{approx}}, \tag{5.3}$$

where $0<\epsilon\ll 1$ was assumed. This condition guarantees that the relative error of $\langle N(t)\rangle_{p,\text{approx}}$ is smaller than ϵ.

Our numerical results for $\langle N(t)\rangle_p$ in Eq. (3.18) are shown in Figs. 2 and 3 for a wide range of values of p. For $p=0$ the state space partition of interest contains only a single site. Since an escape is possible to each neighboring site, this leads to a single-exponential decay $\exp(-2t/\tau)$. In the other extreme case, for $p=1$, we have a semi-infinite stretch of states, and $\langle N(t)\rangle_{p=1}$ is given by $N_\infty(t)$, defined in Eq. (5.1) above. The long-time behavior of $N_\infty(t)$ is then algebraic,

$$N_\infty(t)\to\frac{1}{\sqrt{\pi t/\tau}}. \tag{5.4}$$

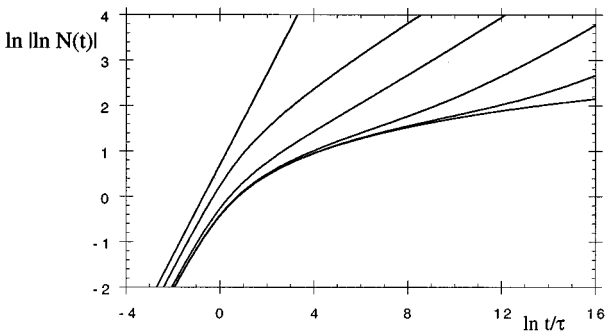

FIG. 3. $\langle N(t)\rangle$ vs t in a ln-ln vs ln plot for $p=0,0.5,0.9,0.99,0.999,1$ (from left to right).

For intermediate values of p it is clearly seen that $\langle N(t)\rangle_p$ is faster than algebraic but slower than exponential. In order to analyze the nonexponentiality of $\langle N(t)\rangle_p$ in more detail, we have replotted the data of Fig. 2 in a ln-ln vs ln plot in Fig. 3. The advantage of such a representation is that a Kohlrausch or Williams-Watts behavior $\exp[-(t/\tau_K)^\beta]$, used very often successfully as a nonexponential two-parameter fit function, shows up as a straight line with slope β. Figure 2 demonstrates that two to three different regimes can be distinguished. First, there is an initial exponential decay. For most values of p, this single-exponential decay turns eventually into a nonexponential decay that can be described approximately as Kohlrausch behavior with $\beta<1$, with β depending on p, as demonstrated by the approximately straight lines with slope smaller than 1 for large values of $\ln t$. For values of p close to one, however, there appears an intermediate regime where $\langle N(t)\rangle_p$ follows closely $N_\infty(t)$, until it also turns into a Kohlrausch decay.

The initial single-exponential decay can be easily analyzed. Using the fact that $\dot{N}_1(0)=-2/\tau$ and $\dot{N}_l(0)=-1/\tau$ for $l>1$, it follows immediately that

$$\left.\frac{d}{dt}\right|_{t=0}\langle N(t)\rangle_p=-(2-p)/\tau, \tag{5.5}$$

which determines the initial exponential to be $\exp[-(2-p)t/\tau]$.

There is always some arbitrariness involved when a nonexponential decay is fitted to a particular decay function, e.g., a Kohlrausch function. One of the main problems is the choice of the time range that is used for the fit. Since Fig. 3 suggests that it is particularly the long-time regime that exhibits a Kohlrausch behavior, a more systematic approach is possible. In the following, we will approximate the long-time behavior of $\langle N(t)\rangle_p$ by a Kohlrausch-like function

$$N_K(t)=q\exp[-(t/\tau_K)^\beta], \tag{5.6}$$

where the parameters β, τ_K, and q are determined by the requirement that Eq. (5.6) describes correctly the low-frequency behavior of the Laplace transform of the exact function $\langle N(t)\rangle_p$. This guarantees that Eq. (5.6) is the best possible Kohlrausch-like function to describe the long-time behavior of $\langle N(t)\rangle_p$. An advantage of the procedure we use is that the low-frequency moments of $\langle N(t)\rangle_p$ can be determined in closed form. How this is done in detail is discussed in Appendix B.

Figure 4 demonstrates the quality of the Kohlrausch fit by giving a comparison with the exact behavior for some values of p. Figures 5(a), 5(b), and 5(c) show the dependence of the parameters β, τ_K, and q, respectively, on p. It is clear that $\beta(0)=1$ for $p=0$. For $p\to 1$, β approaches a nonzero limit value $\beta(1)=0.271\,38$. However, in this limit the contribution of the Kohlrausch function (5.6), measured by q, vanishes linearly with $(1-p)$, while the time scale τ_K diverges with $(1-p)^{-1}$. This result is obvious since in that limit the long-time behavior becomes the algebraic decay obtained for a semi-infinite cluster Eq. (5.4). Still, we can expect that the Kohlrausch description gives a satisfactory picture of the long-time behavior for values of p from 0.5 up to 0.99, as Fig. 4 demonstrates.

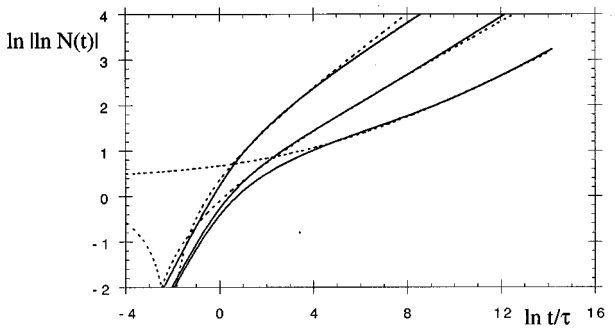

FIG. 4. Comparison of $\langle N(t)\rangle$ (solid line) and the Kohlrausch fit Eq. (5.6) (dashed line) for $p=0.5,0.9,0.99$ (from left to right).

VI. SUMMARY AND DISCUSSION

We have analyzed the average residence probability and the average distribution of residence times in a particular macroscopic state for the ensemble of *random partitions* of a one-dimensional state space. We find that our model exhibits an interesting and nontrivial anomalous time evolution. In particular, the probability that a walker remains in a particular cluster of states decays slower than an exponential but faster than a power law. The long-time behavior can be modeled satisfactorily as a stretched exponential.

Anomalous relaxation of correlation functions is a well-known feature of glasses and other heterogeneous systems; see Ref. [35] and references therein. Many theories that give rise to anomalous dynamical behavior fall into one of two classes. The first is essentially a static disorder picture. Here the system is assumed to be confined to some small patch of its state space, e.g., due to high barriers at low temperatures. These frozen-in state space patches differ between different instances of the system in a sample, which leads to an overall averaging for the observable in question. In its simplest form this approach leads to a distribution of relaxation times for single-exponential decay functions, but more sophisticated treatments also exist. The other approach can be thought of as a dynamic disorder picture. Simple local processes interact with one another, e.g., due to dense packing at low temperatures, thereby leading to strongly constrained overall dynamics, often modeled as a random walk on a rugged potential landscape.

In our approach the physical reason for the anomalous dynamical behavior is different from both of the above approaches. The microscopic dynamics of the system is not constrained; the system wanders freely through its state space. (This is appropriate for a system at relatively high temperatures, as described in the Introduction.) Here state space patches arise naturally because the macroscopic observable under study has only two states. The observed anomalous dynamical behavior then arises from the resulting partition of the state space. It would be interesting to see whether this framework can give also some insight into the description of relaxation processes in other glasslike systems.

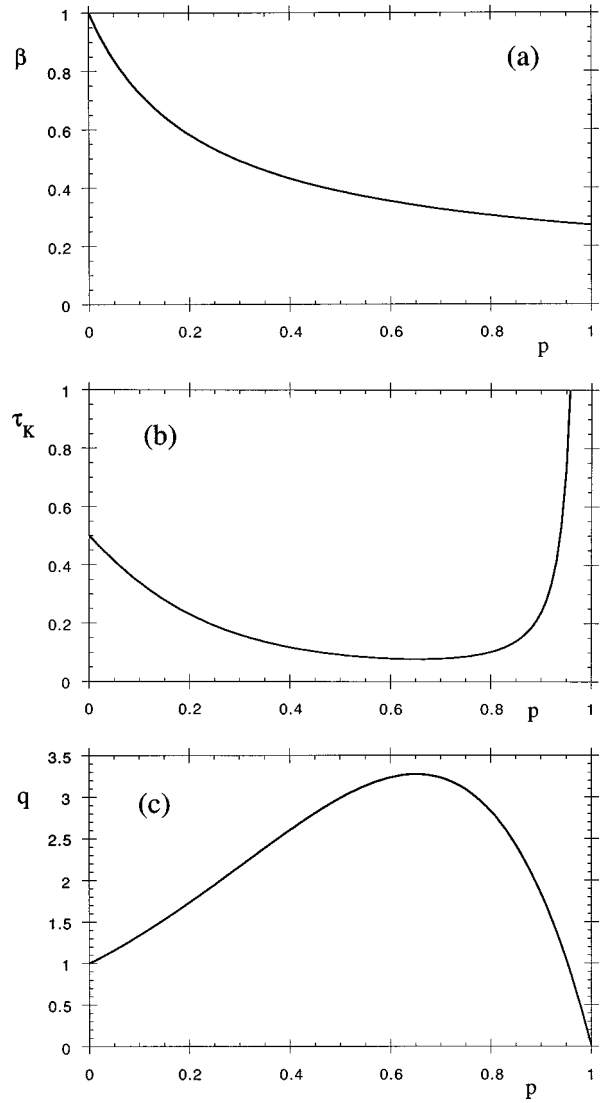

FIG. 5. Kohlrausch parameters vs p for the long-time behavior of $\langle N(t)\rangle$: (a) β, (b) τ_K, and (c) q vs p.

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APPENDIX A: DERIVATION OF EQ. (4.6)

In this appendix we derive Eq. (4.6), which is the probability that an n-step walk ending at site m never goes beyond level l, given that the walk starts from site 0. We first extend the sum over j to $l+2$ on the right-hand side of Eq. (4.6), which will not affect the result, since the term corresponding to $j=l+2$ is zero. The advantage of this change will be seen later when we do the summations. Therefore, we demonstrate that

$$\left(\frac{1}{2}\right)^n W_l(n,m)=\frac{2}{l+2}\sum_{j=1}^{l+2}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\times\sin\left(\frac{(m+1)j\pi}{l+2}\right). \tag{A1}$$

Rewriting the right-hand side of Eq. (A1), we find that

$$\frac{2}{l+2}\sum_{j=1}^{l+2}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{(m+1)j\pi}{l+2}\right)=\frac{2}{l+2}\sum_{j=1}^{l+2}\left[\frac{e^{i[j\pi/(l+2)]}+e^{-i[j\pi/(l+2)]}}{2}\right]^n$$
$$\times\left[\frac{e^{i[j\pi/(l+2)]}-e^{-i[j\pi/(l+2)]}}{2i}\right]\left[\frac{e^{i[(m+1)j\pi/(l+2)]}-e^{-i[(m+1)j\pi/(l+2)]}}{2i}\right]$$
$$=-\frac{2^{-n-1}}{l+2}\sum_{j=1}^{l+2}\sum_{k=0}^{n}\binom{n}{k}e^{i[j\pi/(l+2)](n-2k)}[e^{i[(m+2)j\pi/(l+2)]}$$
$$+e^{-i[(m+2)j\pi/(l+2)]}-e^{i[mj\pi/(l+2)]}-e^{-i[mj\pi/(l+2)]}]$$
$$=-\frac{2^{-n-1}}{l+2}\sum_{k=0}^{n}\binom{n}{k}\left[\sum_{j=1}^{l+2}e^{i[(n-2k+m+2)j\pi/(l+2)]}\right.$$
$$+\sum_{j=1}^{l+2}e^{i[(n-2k-m-2)j\pi/(l+2)]}-\sum_{j=1}^{l+2}e^{i[(n-2k+m)j\pi]/(l+2)}$$
$$\left.-\sum_{j=1}^{l+2}e^{i[(n-2k-m)j\pi/(l+2)]}\right]. \tag{A2}$$

Applying the formula

$$\sum_{j=1}^{l+2}e^{i[kj\pi/(l+2)]}=\frac{e^{i[k\pi/(l+2)]}(e^{i[(l+2)k\pi/(l+2)]}-1)}{e^{i[k\pi/(l+2)]}-1}, \tag{A3}$$

Eq. (A2) becomes

$$-\frac{2^{-n-1}}{l+2}\sum_{k=0}^{n}\binom{n}{k}\left[\frac{e^{i[(n-2k+m+2)\pi/(l+2)]}(e^{i[(n-2k+m+2)(l+2)\pi/(l+2)]}-1)}{e^{i[(n-2k+m+2)\pi/(l+2)]}-1}\right.$$
$$+\frac{e^{i[(n-2k-m-2)\pi/(l+2)]}(e^{i[(n-2k-m-2)(l+2)\pi/(l+2)]}-1)}{e^{i[(n-2k-m-2)\pi/(l+2)]}-1}-\frac{e^{i[(n-2k+m)\pi/(l+2)]}(e^{i[(n-2k+m)(l+2)\pi/(l+2)]}-1)}{e^{i[(n-2k+m)\pi/(l+2)]}-1}$$
$$\left.-\frac{e^{i[(n-2k-m)\pi/(l+2)]}(e^{i[(n-2k-m)(l+2)\pi/(l+2)]}-1)}{e^{i[(n-2k-m)\pi/(l+2)]}-1}\right]. \tag{A4}$$

Equation (A4) is always real. Furthermore, only some of the values of the k's lead to non-zero terms. Those terms that contribute to the sum in Eq. (A4) correspond to $k=(n+m)/2+1+k'(l+2)$, $(n-m)/2-1+k'(l+2)$, $(n+m)/2+k'(l+2)$, and $(n-m)/2+k'(l+2)$, where k' is any integer between $-\infty$ and ∞. We then apply l'Hôspital's rule to evaluate these terms. As an example, we compute the first term here.

In order to make the notation more compact, let $e^{i[(n-2k+m)\pi/(l+2)]}=s$. Therefore, we have $e^{i[(n-2k+m+2)(l+3)\pi/(l+2)]}=s^{l+3}$. The first term in Eq. (A4) is now

$$-\frac{2^{-n-1}}{l+2}\sum_{k=0}^{n}\binom{n}{k}\frac{e^{i[(n-2k+m+2)(l+3)\pi/(l+2)]}-e^{i[(n-2k+m+2)\pi/(l+2)]}}{e^{i[(n-2k+m+2)\pi/(l+2)]}-1}=-\frac{2^{-n-1}}{l+2}\sum_{k=0}^{n}\binom{n}{k}\frac{s^{l+3}-s}{s-1}. \tag{A5}$$

We apply l'Hôspital's rule to obtain the residues for Eq. (A5) at $s=1$, which yields

$$\lim_{s\to 1}\frac{s^{l+3}-s}{s-1}=\lim_{s\to 1}\frac{\dfrac{ds^{l+3}}{dk}-\dfrac{ds}{dk}}{\dfrac{ds}{dk}}, \tag{A6}$$

where

$$\frac{ds}{dk}=\frac{-2\pi i}{l+2}\,s. \tag{A7}$$

When $s=1$, we have $(n-2k+m+2)/(l+2)=2k'$, where $k'=-\infty,\ldots,-2,-1,0,1,2,\ldots,\infty$. Replacing k by k', we then have, at $s=1$,

$$-\frac{2^{-n-1}}{l+2}\sum_{k'=\infty}^{\infty}\binom{n}{\frac{n+m}{2}+1+k'(l+2)}\left[\frac{(l+3)\,\frac{-2\pi i}{l+2}-\frac{2\pi i}{l+2}}{\frac{-2\pi i}{l+2}}\right]$$

$$=-2^{-n-1}\sum_{k'=0}^{\infty}\left[\binom{n}{\frac{n+m}{2}+1+k'(l+2)}+\binom{n}{\frac{n-m}{2}-1+(k'+1)(l+2)}\right]. \tag{A8}$$

Doing the same to the other terms, we finally have

$$\frac{2}{l+2}\sum_{j=1}^{l+1}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{(m+1)j\pi}{l+2}\right)$$

$$=\left(\frac{1}{2}\right)^{n/2}\left\{-\sum_{k'=0}^{\infty}\left[\binom{n}{\frac{n+m}{2}+1+k'(l+2)}+\binom{n}{\frac{n+m}{2}+1+l-m+k'(l+2)}\right]\right.$$

$$\left.+\sum_{k'=0}^{\infty}\left[\binom{n}{\frac{n+m}{2}+k'(l+2)}+\binom{n}{\frac{n+m}{2}+2+l-m+k'(l+2)}\right]\right\}$$

$$=\left(\frac{1}{2}\right)^{n/2}\left\{\binom{n}{\frac{n+m}{2}}-\sum_{k=0}^{\infty}\left[\binom{n}{\frac{n+m}{2}+1+k(l+2)}-\binom{n}{\frac{n+m}{2}+2+l-m+k(l+2)}\right]\right.$$

$$\left.-\sum_{j=0}^{\infty}\left[\binom{n}{\frac{n+m}{2}+1+l-m+j(l+2)}-\binom{n}{\frac{n+m}{2}+(j+1)(l+2)}\right]\right\}$$

$$=\left(\frac{1}{2}\right)^{n/2}\left\{\frac{m+1}{\frac{n+m}{2}+1}\binom{n}{\frac{n+m}{2}}+\sum_{k=0}^{\infty}\left[\frac{m+1+2(k+1)(l+2)}{\frac{n+m}{2}+1+(k+1)(l+2)}\binom{n}{\frac{n+m}{2}+(k+1)(l+2)}\right.\right.$$

$$\left.\left.-\frac{2l-m+3+2k(l+2)}{\frac{n+m}{2}+2+l-m+k(l+2)}\binom{n}{\frac{n+m}{2}+1+l-m+k(l+2)}\right]\right\}$$

$$=\left(\frac{1}{2}\right)^{n}W_l(n,m). \tag{A9}$$

With $l=m+i$, $W_l(n,m)$ in Eq. (A9) is indeed the same as in Eq. (4.5). In fact, there are a finite number of terms in Eq. (A9) that have nonzero values for the binomial coefficients. In other words, the upper limit of the sum over k is finite unless the upper element n of those binomial coefficients is infinite. Therefore

$$\left(\frac{1}{2}\right)^{n}W_l(n,m)=\frac{2}{l+2}\sum_{j=1}^{l+1}\cos^n\left(\frac{j\pi}{l+2}\right)\sin\left(\frac{j\pi}{l+2}\right)\times\sin\left(\frac{(m+1)j\pi}{l+2}\right), \tag{A10}$$

which is the desired result.

APPENDIX B: GENERALIZED MOMENT KOHLRAUSCH FIT

The method of generalized moment expansion [36–40,21,41] allows a systematic analysis of the long-time behavior of observables. In particular, it provides a possibility to obtain the parameters of exponential and nonexponential approximations to the observable in question in a systematic way. In the following we will give a short review of the basic ideas and apply them to obtain a Kohlrausch-like description of the long-time behavior of $\langle N(t)\rangle$.

The Laplace transform of a dynamical observable, e.g., of $N_l(t)$, Eq. (3.14), defined by

$$\widetilde{N}_l(\omega)=\int_0^\infty e^{-\omega t}N_l(t)dt, \tag{B1}$$

can be expanded formally for small frequencies

$$\widetilde{N}_l(\omega)\sim\sum_{n=1}^{\infty}\mu_{-n}(-\omega)^{n-1}. \tag{B2}$$

The low-frequency expansion coefficients μ_{-n}, also called generalized moments, are given by

$$\mu_{-n}=\frac{1}{(n-1)!}\int_0^\infty t^{n-1}N(t)dt. \tag{B3}$$

Generalized moments can usually be represented as matrix elements of powers of the inverse stochastic operator that governs the time evolution of the observable. In our particular case of a random walk on a cluster of length l, Eq. (B3) can be represented alternatively using powers of the inverse of the transition matrix $\mathbf{A}^{(l)}$,

$$\mu_{-n}=(-1)^n\mathbf{1}^T[\mathbf{A}^{(l)}]^{-n}\mathbf{e}_1, \tag{B4}$$

where $\mathbf{1}^T$ denotes the constant row vector $(1,1,1,\dots)$ and the unit vector $\mathbf{e}_1=(1,0,0,\dots)^T$ arises from the initial condition Eq. (3.3). We note, in passing, that replacing $-n$ by n in Eq. (B4) gives the well-known high-frequency moments of the Mori-Zwanzig projection operator formalism [42,43].

An analytical evaluation of Eq. (B4) is, in our case, possible, e.g., using the techniques of Refs. [21] and [39]. In particular, one introduces the auxiliary vector

$$\mathbf{m}=[\mathbf{A}^{(l)}]^{-1}\mathbf{1}. \tag{B5}$$

This auxiliary vector is the solution of the equation

$$\mathbf{A}^{(l)}\mathbf{m}=-\mathbf{1}, \tag{B6}$$

which can be solved analytically since $\mathbf{A}^{(l)}$ is a tridiagonal matrix. Only the first component of that vector is of interest since μ_{-1} is given by

$$\mu_{-1}=\mathbf{e}_1^T\mathbf{m}. \tag{B7}$$

A generalization of this scheme to higher-order moments is straightforward. In particular, we obtain

$$\mu_{-1}=l/2, \tag{B8a}$$

$$\mu_{-2}=l(l+1)(l+2)/24, \tag{B8b}$$

$$\mu_{-3}=l(l+1)(l+2)(l^2+2l+2)/240. \tag{B8c}$$

For the ensemble-averaged observable $\langle N(t)\rangle_p$, however, we still have to average Eqs. (B8) over the cluster size distribution (see Sec. III) with the result

$$\langle\mu_{-1}\rangle_p=\frac{1}{2(1-p)}, \tag{B9a}$$

$$\langle\mu_{-2}\rangle_p=\frac{1}{4(1-p)^3}, \tag{B9b}$$

$$\langle\mu_{-3}\rangle_p=\frac{(1+p)^2}{8(1-p)^5}. \tag{B9c}$$

Based on the generalized moments of a dynamical observable, one can obtain approximations that exhibit the correct long-time behavior. This is done by the requirement that the approximations reproduce a specified number of these moments [39]. Specifically, an n-parameter approximation function of a particular functional form is required to reproduce the moments μ_{-1} to μ_{-n} of the exact observable. In this sense, the approximation obtained is the *best possible approximation* of that functional form.

Of particular interest in our case is a Kohlrausch-like function

$$N_K(t)=qe^{-(t/\tau_K)^\beta}, \tag{B10}$$

which reproduces the correct long-time behavior of $\langle N(t)\rangle_p$. We require therefore that the parameters q, τ_K, and β are chosen so that the moments of Eq. (B10),

$$\mu_{-\nu}=\frac{q}{(\nu-1)!}\frac{\tau_K^\nu}{\beta}\Gamma\left(\frac{\nu}{\beta}\right),\quad \nu=1,2,3, \tag{B11}$$

reproduce the moments of $\langle N(t)\rangle_p$ [Eq. (B9)]. This leads to the nonlinear equation

$$2\frac{\langle\mu_{-1}\rangle_p\langle\mu_{-3}\rangle_p}{\langle\mu_{-2}\rangle_p^2}=\frac{\Gamma(1/\beta)\Gamma(3/\beta)}{\Gamma(2/\beta)^2} \tag{B12}$$

for the (numerical) determination of β. With β given, the other parameters are obtained immediately by

$$\tau_K\frac{\langle\mu_{-2}\rangle_p}{\langle\mu_{-1}\rangle_p}\frac{\Gamma(1/\beta)}{\Gamma(2/\beta)} \tag{B13a}$$

and

$$q=\langle\mu_{-1}\rangle_p\left[\frac{\tau}{\beta}\Gamma\left(\frac{1}{\beta}\right)\right]^{-1}. \tag{B13b}$$

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