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Effective medium approximation for random walks with non-Markovian dynamical disorder

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We analyze a random walk, in which a walker makes transitions between sites in a lattice with rates whose values are determined by fluctuating medium variables. The values of these medium variables fluctuate between zero (blocked jump) and a nonzero value (permitted jump). The dynamics of the walker are determined by the fluctuations of these medium variables, but the medium variables are unaffected by the motion of the walker. The case in which the medium variables obey conventional rate equations (a Pauli master equation) has been analyzed by Harrison and Zwanzig [Phys. Rev. A **32**, 1072 (1985)] and by Sahimi [J. Phys. C **19**, 1311 (1986)], who developed an effective medium approximation (EMA) solution for this model. We consider here a generalization of this model, in which the medium variables are non-Markovian, with dynamics governed by a generalized master equation containing a memory kernel. A generalized EMA is developed for this case, whose accuracy is tested numerically for a "lattice" of two sites. Calculations based on this approach are then presented for a lattice of infinite extent.

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I. INTRODUCTION

A random walk with dynamical disorder is a process in which an entity makes transitions among states, with rates whose values fluctuate in time [1–12]. If these transition rates fluctuate between zero and a nonzero value, this stochastic process may be visualized as a random walk in which a walker executes hops on a lattice structure and encounters gates that randomly open and close [2–4]. Such models have been applied to electrical conductivity in microemulsions [1] and to charge carrier motion in polymer electrolytes [9], and have formed the mathematical basis for a theory of polymer dynamics in the melt [12]. These models describe the dynamics of two sets of degrees of freedom: those associated with the walker and those associated with the random variables whose values determine the transition rates of the walker. We refer to these latter variables as medium variables. In the class of models considered here, the motion of the walker is affected by the state of the medium variables that control its transition rates, but the dynamics of the medium variables are unaffected by the state of the walker [5]. If the dynamics of walker and of medium variables are governed by Markov processes, then the random walk with dynamical disorder falls into the class of problems denoted *composite Markov processes* by van Kampen [13]. These are stochastic processes in which the fluctuations of one set of variables control the dynamics of another set of variables [14,15]. Related models that have been studied previously include random walks in which the walker is characterized by internal states [16,17], diffusion processes with a fluctuating diffusion coefficient [13,18–23], and models of chemical reactions with fluctuating rate coefficients [24,25].

Druger, Ratner, and Nitzan [2] formulated and analyzed a model in which a walker takes nearest-neighbor jumps on a lattice with hopping rates that fluctuate between zero and a finite value. This model is characterized by *global dynamical disorder* [10] since the entire collection of random hopping rates is simultaneously renewed. A model characterized by *local dynamical disorder* [10] was treated by Harrison and Zwanzig [3] and by Sahimi [4]. The model is similar to that of Druger *et al.* [2], except that the hopping rates fluctuate independently of each other. Harrison and Zwanzig [3] and Sahimi [4] developed a dynamical mean-field theory, denoted the effective medium approximation (EMA), which is a generalization of the previously developed EMA for random walks on lattices with static disorder [26,27]. Granek and Nitzan have generalized this model and its EMA treatment to include the case in which the medium variables are characterized by more than two states, which allows consideration of random walks with correlated dynamical disorder [7]. The EMA strategy has been applied by Zwanzig [6] to a model of particle diffusion in a continuous medium, characterized by spatial regions of fluctuating diffusion coefficient. Exactly soluble random walk models with dynamical disorder have been treated by Hernandez-Garcia *et al.* [10]. Treatments of dynamically disordered random walks with the continuous-time random-walk formalism have been presented by Budde and co-workers [11].

In the present work, we consider a generalized version of the model treated by Harrison and Zwanzig [3] and by Sahimi [4]. In that model, the dynamics of the medium variables are Markovian, and the probabilities of finding these variables in a particular state obey a Pauli master equation with time-independent rate coefficients. The

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medium variables approach equilibrium with exponential decay. Here we treat the case in which the medium variables have dynamics that are characterized by more than one time scale. Our motivation arises from our model of polymer dynamics, in which the medium variables represent the obstacles posed to one macromolecule by another and which therefore should relax with a spectrum of time scales corresponding to the range of conformational relaxation times of a polymer molecule [12]. We replace the Pauli master equation governing the medium dynamics in the model of Harrison and Zwanzig [3] and of Sahimi [4], by a generalized master equation [17,28] in which multiplication by a time-independent rate constant is replaced by convolution with a memory function. Numerical calculations are performed for the case in which this memory kernel decays exponentially in time. In this case, the medium variables approach equilibrium with dynamics that are either biexponential or a damped oscillation. We demonstrate that the EMA procedure of Harrison and Zwanzig [3] and of Sahimi [4] is inapplicable to this case and propose a generalized EMA (GEMA), which preserves the form of the EMA, but may be applied to the case of non-Markovian medium dynamics. In the limit that the decay time of the memory kernel is small compared to the time integral of the kernel, the EMA is recovered.

Our model is specified in Sec. II, and the GEMA is developed in Sec. III. We assess the accuracy of the GEMA in Sec. IV by applying it to a simplified "random walk" with two sites whose exact numerical solution is feasible. The GEMA is shown to provide semiquantitative agreement with exact results over a wide range of time scales and parameter values. The GEMA is applied to a one-dimensional lattice of infinite extent in Sec. V, where we present calculations of the time dependence of the probability of the walker's remaining at the initial site and of the walker's mean-squared displacement. The dynamics of the medium variables for the case of an exponentially decaying memory function are examined in Appendix A and the origin of a plateau in the time dependence of the probability that the walker remains at its initial site is analyzed in Appendix B.

II. POSING THE PROBLEM

We consider the dynamics of a single random walker that executes transitions among the N sites of a lattice of arbitrary structure, according to a Pauli master equation

$$\frac{d\mathbf{p}}{dt}=\mathbf{W}(\boldsymbol{\sigma})\cdot\mathbf{p} \ . \tag{2.1}$$

The probability that the walker occupies site j at time t is denoted $p_j(t)$ and the vector of probabilities $(p_1,p_2,\ldots,p_N)$ is represented by $\mathbf{p}(t)$. The N-dimensional transition matrix $\mathbf{W}$ depends on a set of stochastic variables $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\ldots)$, one of which is associated with each pair of sites in the lattice between which the walker may jump. The rate at which the walker hops between sites j and k has the form $w_{jk}\sigma_m$, in which w_{jk} depends on the separation of sites j and k, but not on $\boldsymbol{\sigma}$. The variables $\boldsymbol{\sigma}$, which we denote the *medium variables*, have values that fluctuate in time between 0 and 1. These stochastic variables are taken to be uncorrelated, so that the time-dependent distribution of $\boldsymbol{\sigma}$, $\Phi(\boldsymbol{\sigma},t)$, factors into a product of distributions $\phi(\sigma_j,t)$ [3,4]:

$$\Phi(\boldsymbol{\sigma},t)=\prod_j \varphi(\sigma_j,t) \ . \tag{2.2}$$

The distribution of the medium variables is taken to obey an equation of motion that is nonlocal in time [17,28]:

$$\dot{\Phi}(\boldsymbol{\sigma},t)=\sum_{\boldsymbol{\sigma}'}\int_0^t d\tau\,\Omega_{\boldsymbol{\sigma}\boldsymbol{\sigma}'}(t-\tau)\Phi(\boldsymbol{\sigma}',\tau) \ . \tag{2.3}$$

The equation of motion of the single-variable distribution has the form

$$\dot{\phi}(\sigma,t)=\sum_{\sigma'}\int_0^t d\tau\,K(t-\tau)A_{\sigma\sigma'}\varphi(\sigma',\tau) \ , \tag{2.4a}$$

$$A_{00}=-A_{10}=-c \ , \tag{2.4b}$$

$$A_{11}=-A_{01}=-(1-c) \ . \tag{2.4c}$$

When the medium variables are in equilibrium, $\sigma=1$ with probability c and $\sigma=0$ with probability $1-c$. The goal of this problem is the determination of the dynamics of the random walker, averaged over the fluctuations of the medium.

A strategy for treating a limiting case of this problem was developed by Harrison and Zwanzig (HZ) [3] and by Sahimi [4]. In this limit, the medium variables have a memory that is infinitely short lived, so that $K(t)=\gamma\delta(t)$. Substitution of this form into Eq. (2.4a) yields conventional rate equations for the dynamics of the medium variables. In the present work, we develop a generalization of this strategy that is valid for $K(t)$ with a finite decay rate. Since this generalization builds on the work of HZ, we must briefly review their formalism for the case $K(t)\propto\delta(t)$. HZ define a joint probability distribution for the random variables $\mathbf{p}$ and $\boldsymbol{\sigma}$, $f(\mathbf{p},\boldsymbol{\sigma},t)$, which obeys the following continuity equation

$$\frac{\partial f(\mathbf{p},\boldsymbol{\sigma},t)}{\partial t}=-\nabla_{\mathbf{p}}\cdot[\mathbf{W}(\boldsymbol{\sigma})\cdot\mathbf{p}f(\mathbf{p},\boldsymbol{\sigma},t)] +\sum_{\boldsymbol{\sigma}'}\Theta_{\boldsymbol{\sigma}\boldsymbol{\sigma}'}f(\mathbf{p},\boldsymbol{\sigma}',t) \ , \tag{2.5a}$$

$$\Theta_{\boldsymbol{\sigma}\boldsymbol{\sigma}'}=\gamma\sum_j A_{\sigma_j\sigma_j'}\prod_{m\neq j}\delta_{\sigma_m\sigma_m'} \ . \tag{2.5b}$$

The first term on the right-hand side of Eq. (2.5a) describes changes in $f(\mathbf{p},\boldsymbol{\sigma},t)$ resulting from dynamics of the random walker for a fixed state of the medium variables and the second term reflects dynamics of $f(\mathbf{p},\boldsymbol{\sigma},t)$ from fluctuations of the medium variables for a fixed set of random walker probabilities $\mathbf{p}$.

HZ next define $P_j(\boldsymbol{\sigma},t)$ to be the probability that the walker occupies site j *and* that the medium variables have the values $\boldsymbol{\sigma}$ at time t. These probabilities are moments of the distribution $f(\mathbf{p},\boldsymbol{\sigma},t)$:

$$\mathbf{P}(\boldsymbol{\sigma},t)=\int d\mathbf{p}\,\mathbf{p}f(\mathbf{p},\boldsymbol{\sigma},t) \ . \tag{2.6}$$

Equations of motion for the $\mathbf{P}(\boldsymbol{\sigma},t)$ are obtained by differentiating (2.6) with respect to time, substituting the right-hand side of Eq. (2.5a) into the right-hand side of Eq. (2.6), and integrating by parts:

$$\dot{\mathbf{P}}(\sigma,t)=\mathbf{W}(\sigma)\cdot\mathbf{P}(\sigma,t)+\sum_{\sigma'}\Theta_{\sigma\sigma'}\mathbf{P}(\sigma',t) . \tag{2.7}$$

The quantity that is ultimately of interest is $\Pi_j(t)$, the probability that the walker is located at site j at time t, regardless of the values of the medium variables. This probability may be obtained by summing $\mathbf{P}(\sigma,t)$ over all states of the medium

$$\mathbf{\Pi}(t)=\sum_{\sigma}\mathbf{P}(\sigma,t) . \tag{2.8}$$

In order to adapt this formalism to the case in which the medium has a memory, we must generalize the continuity equation in (2.5a). To do so, we rewrite the equation of motion for the medium variable distribution in Eq. (2.3), which is nonlocal in time, in a form that is local in time [29]:

$$\dot{\Phi}(\sigma,t)=\sum_{\sigma'}L_{\sigma\sigma'}(t)\Phi(\sigma',t) , \tag{2.9a}$$

$$L_{\sigma\sigma'}(t)=\frac{\int_0^t d\tau\,\Omega_{\sigma\sigma'}(t-\tau)\Phi(\sigma',\tau)}{\Phi(\sigma',t)} . \tag{2.9b}$$

The transformation from (2.3) to (2.9) is trivial; we multiplied and divided each term in the sum of (2.3) by $\Phi(\sigma',t)$. In order to determine the explicit form of the operator $\mathbf{L}(t)$, we must know $\Phi(\sigma,t)$ and hence must already know the solution to Eq. (2.3). The significance of Eqs. (2.9) is that there exists an operator $\mathbf{L}(t)$, for which Eq. (2.9a) holds. We may then generalize the continuity equation in (2.5a) and the equation of motion for $\mathbf{P}(\sigma,t)$ in (2.7) to

$$\frac{\partial f(\mathbf{p},\sigma,t)}{\partial t}=-\nabla_{\mathbf{p}}\cdot[\mathbf{W}(\sigma)\cdot\mathbf{p}f(\mathbf{p},\sigma,t)]+\sum_{\sigma'}L_{\sigma\sigma'}(t)f(\mathbf{p},\sigma',t) , \tag{2.10a}$$

$$\dot{\mathbf{P}}(\sigma,t)=\mathbf{W}(\sigma)\cdot\mathbf{P}(\sigma,t)+\sum_{\sigma'}L_{\sigma\sigma'}(t)\mathbf{P}(\sigma',t) . \tag{2.10b}$$

Equations (2.10) are obtained from Eqs. (2.5a) and (2.7) by replacing the time-independent transition operator for the medium variables $\Theta_{\sigma\sigma'}$ by the time-dependent operator $L_{\sigma\sigma'}(t)$. The validity of this substitution rests on the fact that Eq. (2.9a) is local in time. A time-local equation of motion for the medium variables leads to the continuity equation in Eq. (2.10a), according to the same argument that led to Eq. (2.5a). In the limit in which the medium variables have no memory $\Omega_{\sigma\sigma'}(t)=\Theta_{\sigma\sigma'}\delta(t)$, Eqs. (2.10a) and (2.10b) reduce to the HZ results in Eqs. (2.5a) and (2.7). In Sec. III, we treat a special case of this model, in which the medium variables are assumed to be in equilibrium at all times: $\phi(1,t)=c$ and $\phi(0,t)=1-c$. This condition was also assumed by HZ [3]. In this case, the operator $L_{\sigma\sigma'}$ in Eq. (2.9b) takes on a simpler form, as $\Phi(\sigma,t)=\Phi(\sigma,\tau)$:

$$L_{\sigma\sigma'}(t)=\int_0^t d\tau\,\Omega_{\sigma\sigma'}(\tau) . \tag{2.11}$$

Having recast the general problem in which the medium variables have memory into a form that is analogous to that employed by HZ for the case of infinitely short memory, we proceed to the solution of Eq. (2.10b) within an effective medium approximation in Sec. III.

III. DEVELOPMENT OF A GENERALIZED EMA

In Sec. II, we analyzed a random walk on a lattice of arbitrary structure in which hopping rates are controlled by fluctuating medium variables, whose dynamics are governed by a memory function of arbitrary form. We now specialize to a random walk with nearest-neighbor steps on a one-dimensional lattice of N sites. For this random walk, the rate at which the walker hops between sites n and m has the form $w\sigma_n\delta_{m,n+1}+w\sigma_{n-1}\delta_{m,n-1}$. The value of the stochastic variable σ_n, which fluctuates between 0 and 1 according to Eqs. (2.4), determines the jump rate between sites n and $n+1$. We also specialize the discussion to a particular form of the memory function $K(t)$ in Eq. (2.4a):

$$K(t)=\gamma\alpha e^{-\alpha t} . \tag{3.1}$$

This memory kernel is characterized by two time scales: the decay time α^{-1} and the inverse of the time integral γ^{-1}. The solution of Eq. (2.4a) in this case is presented in Appendix A. For this choice of memory function, the relaxation of the single-variable distribution $\phi(\sigma,t)$ to equilibrium is biexponential. For $4\gamma<\alpha$, the system is overdamped and the relaxation is biexponential with real time constants. For $4\gamma>\alpha$, the time constants are complex and the relaxation has the form of a damped oscillation. As described in Appendix A, Eq. (2.4) with $K(t)$ given by (3.1) yields unphysical results for certain ranges of values of c, γ, and α, in the underdamped regime. We will avoid these regimes in the numerical calculations presented in Secs. IV and V. In the limit of infinitely short memory $\alpha\to\infty$, Eq. (2.4) takes the form of the Harrison-Zwanzig model [3].

The object of the present calculation is to determine $\Pi_j(t)$, which is defined in (2.8) to be the probability that the walker occupies site j at time t, averaged over the fluctuations of the medium. The EMA developed by Harrison and Zwanzig [3] and by Sahimi [4] accomplishes this goal for the case in which the medium variables have an infinitely short memory $\alpha\to\infty$. In this section, we begin by attempting to apply the EMA to the case in which the medium dynamics are determined by a memory function with a finite decay rate α. The EMA in the form developed by HZ [3] and by Sahimi [4] will be found to be inapplicable to this case. However, the manner in which it breaks down will provide motivation for our generalization of the EMA.

The vector of medium-averaged probabilities $\mathbf{\Pi}(t)$ is defined in Eq. (2.8). Since the EMA is most conveniently expressed in terms of Laplace transforms, we introduce the Laplace transform of $\mathbf{\Pi}(t)$ below:

$$\hat{\mathbf{\Pi}}(s)=\int_0^\infty dt\,e^{-st}\mathbf{\Pi}(t)=\hat{\mathbf{G}}(s)\cdot\mathbf{\Pi}(0) , \tag{3.2a}$$

$$\mathbf{P}(\sigma,0)=\Phi_{\text{eq}}(\sigma)\mathbf{\Pi}(0) . \tag{3.2b}$$

The second equality in Eq. (3.2a) defines the Green's function $\hat{\mathbf{G}}(s)$, whose element $\hat{G}_{nm}(s)$ is the Laplace transform of the conditional probability, averaged over the medium fluctuations, that the walker, initially located at site m, is located at site n at a later time. In Eq. (3.2b), we specify the same initial conditions for the walker and the medium as were chosen by HZ [3]. The walker's initial state is specified by a vector of probabilities $\mathbf{\Pi}(0)$ and the medium is assumed to be in equilibrium. Since the walker's dynamics do not affect the medium dynamics, the medium is therefore in equilibrium at all times.

In the EMA, the propagator $\hat{\mathbf{G}}(s)$ for the one-dimensional random walk with dynamical disorder is assumed to have the form of an effective propagator $\hat{\mathbf{G}}_e(s)$:

$$\hat{\mathbf{G}}(s)=\hat{\mathbf{G}}_e(s)=[s\mathbf{I}-\psi(s)\mathbf{W}]^{-1} , \tag{3.3a}$$

$$W_{mn}=w[\delta_{m,n+1}+\delta_{m,n-1}-2\delta_{mn}] . \tag{3.3b}$$

The N-dimensional unit matrix is denoted $\mathbf{I}$. The effects of the fluctuating medium variables are contained within the effective medium function $\psi(s)$, which may be viewed as the inverse of a frequency-dependent friction coefficient of the walker. If we set $\psi(s)=1$ in Eq. (3.3a), the result is the correct Green's function for the random walk in which the medium variables $\{\sigma_n\}$ are set equal to unity for all times.

The EMA strategy for computing $\psi(s)$ is based upon consideration of a system in which a single jump rate $w_{n,n+1}$ is allowed to fluctuate, but all others have the effective medium form $w\psi(s)$. For an infinite lattice ($N\rightarrow\infty$), the value of the index n is irrelevant because of the translational invariance of the lattice. For this system, the transition matrix of the random walk depends on a single fluctuating variable σ_n, which for convenience we call σ. We denote this transition matrix $\mathbf{W}^{(1)}(\sigma)$:

$$\mathbf{W}^{(1)}(\sigma)=\psi(s)\mathbf{W}+[\sigma-\psi(s)]\mathbf{V} , \tag{3.4a}$$

$$V_{jk}=w[\delta_{jn}\delta_{k,n+1}+\delta_{j,n+1}\delta_{kn}-\delta_{jn}\delta_{kn}-\delta_{j,n+1}\delta_{k,n+1}] . \tag{3.4b}$$

For this random walk with one fluctuating jump rate, the vector of probabilities $\mathbf{P}(\sigma,t)$, defined in Eq. (2.6), is denoted $\mathbf{P}^{(1)}(\sigma,t)$ and its Laplace transform is represented by $\hat{\mathbf{P}}^{(1)}(\sigma,s)$. An equation obeyed by $\hat{\mathbf{P}}^{(1)}(\sigma,s)$ is obtained as follows. The equation of motion for $\mathbf{P}(\sigma,t)$ in Eq. (2.10b) is specialized to the case of the memory function in (3.1). The Laplace transform of this equation for the case of a single fluctuating medium variable has the form

$$[s\mathbf{I}-\mathbf{W}^{(1)}(\sigma)]\cdot\hat{\mathbf{P}}^{(1)}(\sigma,s)-\gamma\sum_{\sigma'}A_{\sigma\sigma'}[\hat{\mathbf{P}}^{(1)}(\sigma',s)-\hat{\mathbf{P}}^{(1)}(\sigma',s+\alpha)]=\mathbf{P}^{(1)}(\sigma,0) . \tag{3.5}$$

The elements of the transition matrix $A_{\sigma\sigma'}$ for the medium variable are listed in Eqs. (2.4b) and (2.4c). $\hat{\mathbf{P}}^{(1)}(\sigma,s)$ is related to the initial walker distribution $\mathbf{\Pi}(0)$ through a propagator $\mathbf{R}_\sigma(s)$:

$$\hat{\mathbf{P}}^{(1)}(\sigma,s)=\mathbf{R}_\sigma(s)\cdot\mathbf{\Pi}(0) . \tag{3.6}$$

This propagator is an N-dimensional matrix whose element $[\mathbf{R}_\sigma(s)]_{mn}$ is the Laplace transform of the joint probability that the walker is located at site m at time t having begun at site n at time 0 and that the medium variable has the value σ at time t. This probability has been averaged over the initial state of the medium variable at time 0. The sum of $\mathbf{R}_\sigma(s)$ over all values of σ yields the fully averaged propagator $\hat{\mathbf{G}}(s)$, defined in Eq. (3.2a). Since within the EMA this propagator is assumed to have the form in Eq. (3.3a), we have

$$\mathbf{R}_0(s)+\mathbf{R}_1(s)=[s\mathbf{I}-\psi(s)\mathbf{W}]^{-1} . \tag{3.7}$$

The substitution of Eq. (3.6) into Eq. (3.5) yields the following pair of coupled equations for $\mathbf{R}_0(s)$ and $\mathbf{R}_1(s)$:

$$[s\mathbf{I}-\mathbf{W}\psi-(1-\psi)\mathbf{V}]\mathbf{R}_1(s)+\gamma(1-c)[\mathbf{R}_1(s)-\mathbf{R}_1(s+\alpha)]-\gamma c[\mathbf{R}_0(s)-\mathbf{R}_0(s+\alpha)]=c\mathbf{I} , \tag{3.8a}$$

$$[s\mathbf{I}-\mathbf{W}\psi+\psi\mathbf{V}]\mathbf{R}_0(s)+\gamma c[\mathbf{R}_0(s)-\mathbf{R}_0(s+\alpha)]-\gamma(1-c)[\mathbf{R}_1(s)-\mathbf{R}_1(s+\alpha)]=(1-c)\mathbf{I} . \tag{3.8b}$$

Equations (3.7), (3.8a), and (3.8b) constitute three independent relations connecting the matrices $\mathbf{R}_0$ and $\mathbf{R}_1$.

In the EMA, we seek a scalar function $\psi(s)$ with the property that Eqs. (3.7) and (3.8) are satisfied. Since these are relations among matrices, it is not obvious that such a function exists. We follow HZ [3] by taking linear combinations of these relations, which yield results of a convenient form:

$$\psi\mathbf{V}\mathbf{R}_0(s)=(1-\psi)\mathbf{V}\mathbf{R}_1(s) , \tag{3.9}$$

$$[(s+\gamma)\mathbf{I}-\psi\mathbf{W}+\psi\mathbf{V}]\times[c\mathbf{R}_0(s)-(1-c)\mathbf{R}_1(s)]+(1-c)\mathbf{V}\mathbf{R}_1(s)-\gamma[c\mathbf{R}_0(s+\alpha)-(1-c)\mathbf{R}_1(s+\alpha)]=0 . \tag{3.10}$$

Equation (3.9) follows from the addition of Eqs. (3.8a) and (3.8b), together with the application of Eq. (3.7). Equation (3.10) was obtained by multiplying Eq. (3.8a) by $1-c$, by multiplying Eq. (3.8b) by c, and by subtracting the results. These relations contain the matrix $\mathbf{V}$, which has the property that for any N-dimensional matrix $\mathbf{M}$, the product $\mathbf{VMV}$ is proportional to $\mathbf{V}$:

$$\mathbf{VMV}=m\mathbf{V} , \tag{3.11a}$$

$$m=w[M_{n+1,n}+M_{n,n+1}-M_{nn}-M_{n+1,n+1}] . \tag{3.11b}$$

We simplify Eq. (3.10) by left-multiplying both sides by $\mathbf{V}[(s+\gamma)\mathbf{I}-\psi(s)\mathbf{W}]^{-1}$. After this multiplication and application of Eq. (3.9), Eq. (3.10) becomes

$$\mathbf{V}\mathbf{R}_1(s)\left[\frac{c(1+\psi g)(1-\psi)}{\psi}-(1-c)[1-g(1-\psi)]\right]$$
$$-\gamma\mathbf{V}\hat{\mathbf{G}}_c^{(\gamma)}(s)[c\mathbf{R}_0(s+\alpha)-(1-c)\mathbf{R}_1(s+\alpha)]=0\ , \tag{3.12a}$$

$$\hat{\mathbf{G}}_e^{(\gamma)}(s)=[(s+\gamma)\mathbf{I}-\psi(s)\mathbf{W}]^{-1}\ , \tag{3.12b}$$

$$\mathbf{V}\hat{\mathbf{G}}_e^{(\gamma)}(s)\mathbf{V}=g\mathbf{V}\ . \tag{3.12c}$$

The matrix $\hat{\mathbf{G}}_e^{(\gamma)}(s)$ in (3.12b) is obtained from $\hat{\mathbf{G}}_e(s)$ by replacing $s\mathbf{I}$ in (3.3a) with $(s+\gamma)\mathbf{I}$. The form of the scalar g, defined in Eq. (3.12c), may be obtained from Eq. (3.11).

The case of infinitely short memory, treated by HZ [3], may be obtained from the present analysis in the limit $\alpha\rightarrow\infty$. In this limit, the left-hand side of Eq. (3.12a) simplifies considerably, since $\mathbf{R}_0(s+\alpha)$ and $\mathbf{R}_1(s+\alpha)$ both vanish for infinite Laplace frequency. In that case, Eq. (3.12a) can only be satisfied if the scalar in square brackets in the first term vanishes. Setting the scalar expression in square brackets in Eq. (3.12a) equal to zero yields the self-consistent equation derived by HZ. For finite α, Eq. (3.12a) suggests that no scalar function $\psi(s)$ can be found such that the equation is satisfied. Thus, if we wish to preserve the convenient form of the EMA, in which all effects of the fluctuating medium are represented by a scalar effective medium function $\psi(s)$, then we must impose additional approximations.

The breakdown of the EMA approach for finite α arises from the form of Eq. (3.5), which is nonlocal in Laplace frequency, as it contains $\hat{\mathbf{P}}^{(1)}(\sigma,s)$ evaluated at the frequencies s and $s+\alpha$. We therefore make a simplifying approximation that eliminates this property of Eq. (3.5). To do so, we return to the time domain and substitute Eq. (2.11) into Eq. (2.10b) to obtain an equation of motion for the probability that the walker occupies a certain site and that the medium variables have certain values:

$$\dot{\mathbf{P}}(\sigma,t)=\mathbf{W}(\sigma)\cdot\mathbf{P}(\sigma,t)+\sum_{\sigma'}\int_0^t d\tau\,\Omega_{\sigma\sigma'}(t-\tau)\mathbf{P}(\sigma',t)\ . \tag{3.13}$$

We simplify the second term by the following approximation:

$$\sum_{\sigma'}\int_0^t d\tau\,\Omega_{\sigma\sigma'}(t-\tau)\mathbf{P}(\sigma',t)$$
$$\rightarrow\sum_{\sigma'}\int_0^t d\tau\,\Omega_{\sigma\sigma'}(t-\tau)e^{\mathbf{W}(\sigma')(t-\tau)}\mathbf{P}(\sigma',\tau)\ . \tag{3.14}$$

Within the time integral in Eq. (3.13), we have assumed that the time evolution operator for $\mathbf{P}(\sigma,t)$ equals $\exp[\mathbf{W}(\sigma)t]$, where $\mathbf{W}(\sigma)$ is the random walk transition matrix of Eq. (2.1). This assumption is exactly correct in the trivial limit in which the random walker is uncoupled from the medium variables, i.e., $\mathbf{W}$ is independent of σ. For the model under consideration in which the transition matrix does depend on the medium variables, (3.14) represents a factorization approximation. The approximation in (3.14) replaces an integral, which does not have the form of a convolution, by a convolution integral. This approximation is motivated by the simplification that results, if the integral does have the form of a convolution. If the derivation of Eq. (3.5) is repeated within this approximation, the result is the replacement of the second term on the left-hand side by a term that depends on $\hat{\mathbf{P}}^{(1)}(\sigma,s)$ and does not include $\hat{\mathbf{P}}^{(1)}(\sigma,s+\alpha)$:

$$\sum_{\sigma'}A_{\sigma\sigma'}[\hat{\mathbf{P}}^{(1)}(\sigma',s)-\hat{\mathbf{P}}^{(1)}(\sigma',s+\alpha)]$$
$$\rightarrow\sum_{\sigma'}A_{\sigma\sigma'}\{\alpha[(s+\alpha)\mathbf{I}-\mathbf{W}^{(1)}(\sigma')]^{-1}\}\hat{\mathbf{P}}^{(1)}(\sigma',s)\ . \tag{3.15}$$

We then make a second simplifying approximation that is in the spirit of the original EMA by replacing the transition matrix with one fluctuating medium variable, $\mathbf{W}^{(1)}(\sigma')$, by the effective medium transition matrix $\psi(s)\mathbf{W}$:

$$\sum_{\sigma'}A_{\sigma\sigma'}\{\alpha[(s+\alpha)\mathbf{I}-\mathbf{W}^{(1)}(\sigma')]^{-1}\}\hat{\mathbf{P}}^{(1)}(\sigma',s)$$
$$\rightarrow\alpha\hat{\mathbf{G}}_e^{(\alpha)}(s)\sum_{\sigma'}A_{\sigma\sigma'}\hat{\mathbf{P}}^{(1)}(\sigma',s)\ , \tag{3.16a}$$

$$\hat{\mathbf{G}}_e^{(\alpha)}(s)\equiv[(s+\alpha)\mathbf{I}-\psi(s)\mathbf{W}]^{-1}\ . \tag{3.16b}$$

The consequence of these two approximations is to replace Eq. (3.5) by

$$[s\mathbf{I}-\mathbf{W}^{(1)}(\sigma)]\cdot\hat{\mathbf{P}}^{(1)}(\sigma,s)-\mathbf{Z}(s)\cdot\sum_{\sigma'}A_{\sigma\sigma'}\hat{\mathbf{P}}^{(1)}(\sigma',s)$$
$$=\mathbf{P}^{(1)}(\sigma,0)\ , \tag{3.17a}$$

$$\mathbf{Z}(s)=\alpha\gamma\hat{\mathbf{G}}_e^{(\alpha)}(s)\ . \tag{3.17b}$$

The accuracy of approximating (3.5) by (3.17a) will be assessed in Sec. IV.

We next repeat the analysis that led to the EMA equations in (3.9) and (3.10) within the approximation of (3.17a). The form of (3.9) is unchanged, but Eq. (3.10) is now local in Laplace frequency in that it depends on the propagators $\mathbf{R}_0$ and $\mathbf{R}_1$ evaluated at a single frequency:

$$[\mathbf{H}^{-1}+\psi\mathbf{V}][c\mathbf{R}_0(s)-(1-c)\mathbf{R}_1(s)]$$
$$+(1-c)\mathbf{V}\mathbf{R}_1(s)=0\ , \tag{3.18a}$$

$$\mathbf{H}=[s\mathbf{I}-\psi\mathbf{W}+\mathbf{Z}(s)]^{-1}\ . \tag{3.18b}$$

The approximate version of (3.10) is shown in (3.18a), with the N-dimensional matrix $\mathbf{H}$ defined in (3.18b). We seek the function $\psi(s)$ that satisfies Eqs. (3.9) and (3.18a). An explicit self-consistent equation for this quantity may be determined by left-multiplying Eq. (3.18a) by $\mathbf{VH}$, by applying Eq. (3.9), and the property of $\mathbf{V}$ given in Eq. (3.11):

$$\mathbf{V}\mathbf{R}_1(s)\left[\frac{c(1+\psi h)(1-\psi)}{\psi}-(1-c)\{1-h(1-\psi)\}\right]=0\ , \tag{3.19a}$$

$$h=w[H_{n+1,n}+H_{n,n+1}-H_{nn}-H_{n+1,n+1}]\ . \tag{3.19b}$$

Equation (3.19a) will be satisfied if the scalar expression in square brackets vanishes. Setting this quantity to zero yields our generalized EMA self-consistent equation

$$h\psi(1-\psi)-\psi+c=0 \ . \tag{3.20}$$

We denote by GEMA the approximation to the Green's function that results from solution of this equation and substitution of the resulting $\psi(s)$ into Eq. (3.3a). We reserve the term EMA for the strategy developed by Harrison and Zwanzig [3] and by Sahimi [4]. The dependence of (3.20) on the decay rate of the medium α is contained within h, which is defined in Eq. (3.19b) in terms of elements of the matrix **H**. **H** depends on α through the matrix $\mathbf{Z}(s)$ in Eq. (3.17b). In the limit of an infinitely short memory of the medium $\alpha\to\infty$, $\mathbf{Z}(s)$ approaches $\gamma\mathbf{I}$ and the self-consistent equation in (3.20) becomes the EMA equation of HZ and of Sahimi. The GEMA may thus be viewed as an extension of the EMA to a medium characterized by finite memory.

We have developed the GEMA for the particular memory kernel given in Eq. (3.1). Numerical calculations are given in Secs. IV and V for this case. We close this section by noting that the strategy can be generalized to any kernel $K(t)$ whose Laplace transform exists. Applying the analysis that led to Eqs. (3.17)–(3.20) to the case of arbitrary $K(t)$ results in replacing $\mathbf{Z}(s)$ in Eq. (3.17b) by

$$\mathbf{Z}(s)=\left[\int_0^\infty dt\, e^{-st}K(t)\exp(\mathbf{W}t)\right]_{w\to w\psi(s)} . \tag{3.21}$$

To determine $\mathbf{Z}(s)$, the Laplace transform in (3.21) is performed and subsequently the jump rate w is replaced by the effective frequency-dependent rate $w\psi(s)$. $\mathbf{Z}(s)$ may be written explicitly in terms of the eigenvectors $\{|q\rangle\}$ and eigenvalues $\{\lambda_q\}$ of **W** and the Laplace transform of the memory kernel $\hat{K}(s)$:

$$\mathbf{Z}(s)=\sum_q |q\rangle\hat{K}[s-\lambda_q\psi(s)]\langle q| \ . \tag{3.22}$$

For the exponentially decaying memory kernel of (3.1), (3.22) yields the expression in (3.17b). In principle, the GEMA may be implemented for an arbitrary memory kernel by application of Eq. (3.22). In practice, determination of the explicit form of the matrix **H** in Eq. (3.18b) for a matrix $\mathbf{Z}(s)$ of arbitrary form may prove challenging.

IV. THE TWO-SITE PROBLEM

In Sec. III, we developed a generalized effective medium approximation for a random walk on a lattice of infinite extent, in which the jump rates are controlled by stochastic medium variables. We assess the accuracy of this approximation by applying it to a simplified version of the problem, whose exact numerical solution is tractable. We consider a "random walk" with just two sites, in which the jump rate fluctuates between the values of 0 and w. The equation of motion for $\mathbf{P}(\sigma,t)$ is given in Eq. (2.10b). For the case of two sites with the exponential memory function in Eq. (3.1), Eq. (2.10b) becomes

$$\begin{aligned}
\dot{P}_1(0,t)&=-\gamma(1-e^{-\alpha t})[cP_1(0,t)-(1-c)P_1(1,t)] \ ,\\
\dot{P}_2(0,t)&=-\gamma(1-e^{-\alpha t})[cP_2(0,t)-(1-c)P_2(1,t)] \ ,\\
\dot{P}_1(1,t)&=-w[P_1(1,t)-P_2(1,t)]\\
&\quad+\gamma(1-e^{-\alpha t})[cP_1(0,t)-(1-c)P_1(1,t)] \ ,\\
\dot{P}_2(1,t)&=-w[P_2(1,t)-P_1(1,t)]\\
&\quad+\gamma(1-e^{-\alpha t})[cP_2(0,t)-(1-c)P_2(1,t)] \ .
\end{aligned} \tag{4.1}$$

In (4.1), $P_j(\sigma,t)$ is the probability that the walker occupies site j with the medium variable in state σ. Our model reduces to that treated by HZ in the limit $\alpha\to\infty$ [3]. Since the HZ method treats exactly the fluctuations of a single medium variable, and since the two-site problem is characterized by a single medium variable, the EMA of HZ is *exactly correct* for the $\alpha\to\infty$ limit of the two-site problem. The GEMA is therefore exactly correct for this model in the limit $\alpha\to\infty$, but gives an approximate solution for finite α. In the $\alpha\to\infty$ limit, (4.1) becomes a set of four coupled linear, first-order differential equations with constant coefficients, whose solution may be found in closed form. For finite α, these coupled linear equations have time-dependent coefficients and their solution may be found by numerical integration. In this section, we compare the GEMA solution of Eqs. (4.1) to the exact numerical solution.

The GEMA self-consistent equation in (3.20) depends on the number of sites in the lattice only through the parameter h, which is expressed in terms of elements of the matrix **H** in Eq. (3.19b). The form of **H** may be seen from Eqs. (3.17b) and (3.18b) to depend on the form of the effective medium propagator $\hat{\mathbf{G}}_e(s)$, defined in Eq. (3.3a). For the two-site model, $\hat{\mathbf{G}}_e(s)$ is the two-dimensional matrix with elements

$$\begin{aligned}
[\hat{\mathbf{G}}_e(s)]_{11}=[\hat{\mathbf{G}}_e(s)]_{22}&=\frac{s+w\psi(s)}{s^2+2ws\psi(s)} \ ,\\
[\hat{\mathbf{G}}_e(s)]_{12}=[\hat{\mathbf{G}}_e(s)]_{21}&=\frac{w\psi(s)}{s^2+2ws\psi(s)} \ .
\end{aligned} \tag{4.2}$$

The elements of the two-dimensional matrix **H** may be obtained by using Eq. (3.16b) to convert the elements of $\hat{\mathbf{G}}_e(s)$ in Eq. (4.2) to elements of $\hat{\mathbf{G}}_e^{(\alpha)}(s)$, by calculating the elements of $\mathbf{Z}(s)$ from Eq. (3.17b), and by performing the matrix inversion in Eq. (3.18b). The self-consistent equation in (3.20) is a quadratic equation in ψ for the two-site problem:

$$\begin{aligned}
&2w[s+2(1-c)w]\psi^2\\
&\quad+[s^2+2(s+\alpha)(1-c)w+\alpha s-2wcs+\alpha\gamma]\psi\\
&\qquad-c[\alpha\gamma+s(s+\alpha)]=0 \ .
\end{aligned} \tag{4.3}$$

Our goal is the calculation of $G_{jj}(t)$, the probability that the walker resides at site j at time t, given that it was located at site j at $t=0$, averaged over the states of the medium. This probability may be obtained for the two-site problem within the GEMA by substituting the physically reasonable solution of Eq. (4.3) for $\psi(s)$ into the expression for $[\hat{G}_e(s)]_{11}$ in Eq. (4.2) and then inverting the

Laplace transform.

Figures 1–6 show the time dependence of $G_{jj}(t)$, calculated as just described, with the Laplace transform in Eqs. (4.2) inverted numerically [30]. The solid curves show the results of direct numerical solution of Eqs. (4.1) and the GEMA results are shown with open circles. As discussed in Appendix A, the decay of the medium variables to equilibrium is biexponential for $\alpha > 4\gamma$ and is a damped oscillation for $\alpha < 4\gamma$. Both the underdamped and overdamped cases are represented in Figs. 1–6. Calculations for $c=0.5$ and for a variety of values of α and γ are shown in Figs. 1 and 2. In Fig. 1, $\gamma/w=10^{-2}$ and the curves from left to right were calculated for $\alpha/w=10^4$, 10^{-1}, 10^{-2}, 10^{-3}, and 10^{-4}. Each plot shows three regimes: an initial decay, a plateau, and a final decay. These regimes are readily interpreted in terms of an ensemble of two-site systems. Since $c=0.5$, in half of these systems, the walker's jump is initially blocked and in the other half, the jump is initially unblocked. Since $\gamma/w \ll 1$, the dynamics of the walker are rapid relative to those of the medium. In those systems with an initially unblocked jump, the walker will randomize its location between the two sites before any relaxation of the medium takes place. These dynamics are reflected in the initial decay, which takes place on the time scale associated with the jump rate w^{-1}. We show in Appendix B that for a static medium ($\gamma \to 0$), $G_{jj}(t)$ would decay to the value $1-c/2$. For a dynamic medium in which either $\alpha \ll w$ or $\gamma \ll w$, $G_{jj}(t)$ should therefore decay to a plateau at this value, which should persist until the medium begins to relax. The curves in Fig. 1 decay to a plateau at 0.75, in agreement with this reasoning. The time scale on which the medium relaxes depends on the relative values of α and γ, as may be seen explicitly from Eqs. (A4) and (A6). In the underdamped regime, the medium begins to relax on the time scale of the inverse of the frequency Ω, defined in Eq. (A5), while in the overdamped case, this relaxation begins on the time scale of the shorter of the two time constants in Eq. (A6). The decay that follows the plateau represents the randomization of probability between the two sites for those systems in which the jump was initially blocked. In this third regime, G_{jj} decays to its asymptotic value of 0.5

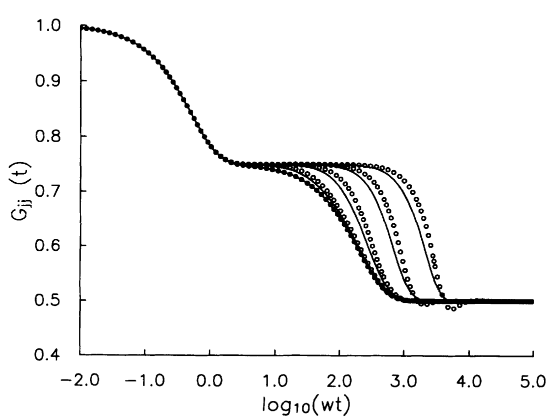

FIG. 1. The probability of remaining on the initial site G_{jj} is calculated for the two-site problem for $c=0.5$, $\gamma=10^{-2}w$, and, from left to right, $\alpha/w=10^4$, 10^{-1}, 10^{-2}, 10^{-3}, and 10^{-4}. The solid curves represent the exact solution, obtained by numerical integration of Eqs. (4.1). The open circles were calculated with the GEMA of Sec. III. The GEMA shows semiquantitative accuracy over a wide range of time scales.

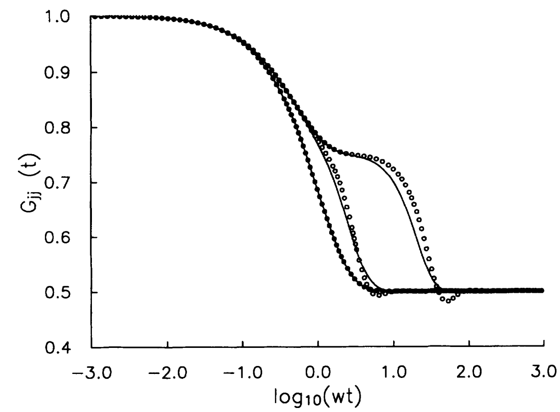

FIG. 2. The probability of remaining on the initial site G_{jj} is calculated for the two-site problem for $c=0.5$, $\gamma=10^2w$, and, from left to right, $\alpha/w=10^2$, 10^{-2}, and 10^{-4}. The solid curves represent the exact solution, obtained by numerical integration of Eqs. (4.1). The open circles were calculated with the GEMA of Sec. III. As the decay rate of the medium's memory kernel is diminished, a plateau develops in G_{jj}.

Comparison of the GEMA calculations to the exact results shows that the GEMA provides a semiquantitative description of the walker's dynamics over the three time regimes just described. In the leftmost curve with $\alpha/w=10^4$, the GEMA and exact results are indistinguishable. Agreement in this limit is to be expected, since for $\alpha \to \infty$, the GEMA is exactly correct for this model, as discussed following Eq. (4.1). Figure 1 shows that as α is decreased from an effectively infinite value of α/w, the GEMA continues to agree well with the numerical results. For very small values of α, the GEMA prediction incorrectly dips below $G_{jj}=0.5$ and approaches this asymptotic value from below.

Figure 2 shows $G_{jj}(t)$ for the same value of c as in Fig. 1, but for the case $\gamma \gg w$ ($\gamma/w=10^2$). From left to right, the curves were calculated for $\alpha/w=10^2$, 10^{-2}, and 10^{-4}. If $\alpha/w \gg 1$ and $\gamma/w \gg 1$, the medium dynamics are rapid compared to those of the walker and the plateau described in connection with Fig. 1 does not occur. For $\alpha/w \ll 1$, the medium relaxes slowly relative to the walker and G_{jj} displays a plateau at 0.75. As in Fig. 1, the GEMA curves agree well with the numerical results, except for the final approach to the asymptotic limit of 0.5.

Calculations for $c=0.4$ are shown in Figs. 3 and 4 and for $c=0.6$ in Figs. 5 and 6. In Fig. 3, $\gamma/w=10^{-2}$, and from left to right the curves were calculated for $\alpha/w=10^2$, 10^{-2}, and 10^{-3}. The behavior displayed in Fig. 3 is qualitatively similar to that in Fig. 1, since $\gamma/w \ll 1$ in both cases. The GEMA agrees well with exact results in each of the three regimes of decay. In Fig. 4, $\gamma/w=1$, and from left to right, $\alpha/w=10^2$, 1, and 0.1. The time dependence displayed in Fig. 4 is qualitatively

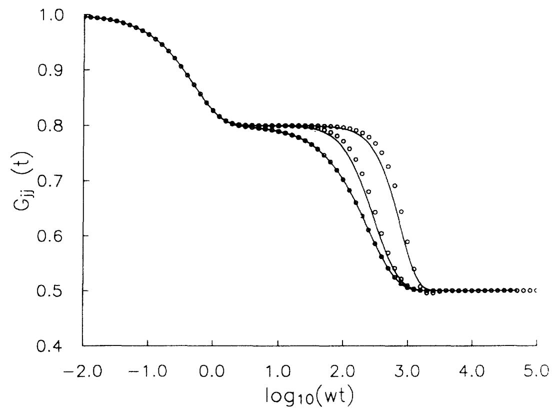

FIG. 3. The probability of remaining on the initial site G_{jj} is calculated for the two-site problem for $c=0.4$, $\gamma=10^{-2}w$, and, from left to right, $\alpha/w=10^2$, 10^{-2}, and 10^{-3}. The solid curves represent the exact solution, obtained by numerical integration of Eqs. (4.1). The open circles were calculated with the GEMA of Sec. III.

similar to that shown in Fig. 2: a plateau develops as α is decreased. Figure 5 repeats the calculations shown in Fig. 3, for $c=0.6$. In Fig. 5, $\gamma/w=10^{-2}$, and from left to right, $\alpha/w=10^2$, 10^{-2}, and 10^{-3}. Figure 6 repeats the calculations of Fig. 4 for $c=0.6$. For Fig. 6, $\gamma/w=1$, and from left to right, $\alpha/w=10^2$, 1, and 0.1. The trends displayed in Figs. 3 and 4 are also evident in Figs. 5 and 6. If $c\neq 0.5$, the medium variable at equilibrium is more likely to have one value than the other. The calculations shown in Figs. 3–6 demonstrate that the GEMA provides semiquantitative results for $c\neq 0.5$ as well as for the case $c=0.5$, in which blocked and unblocked jumps are equally likely.

V. ONE-DIMENSIONAL LATTICE

In Sec. IV, we assessed the accuracy of the GEMA by applying it to a two-site problem whose exact numerical

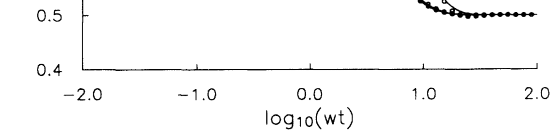

FIG. 4. The probability of remaining on the initial site G_{jj} is calculated for the two-site problem for $c=0.4$, $\gamma=w$, and, from left to right, $\alpha/w=10^2$, 1, and 10^{-1}. The solid curves represent the exact solution, obtained by numerical integration of Eqs. (4.1). The open circles were calculated with the GEMA of Sec. III.

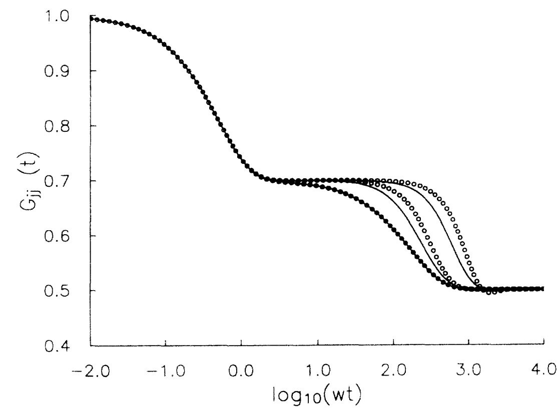

FIG. 5. The calculation of Fig. 3 is repeated for $c=0.6$.

solution is tractable. Having established that the GEMA provides a semiquantitative approximation over many orders of magnitude in time, we next turn to a problem whose exact solution is not available; a random walk with dynamical disorder on a one-dimensional lattice of infinite extent. Within the GEMA, the Laplace transform of the random walk propagator has the effective-medium form that is defined in Eq. (3.3). For the infinite, one-dimensional lattice, $\hat{\mathbf{G}}_e(s)$ is given by [31]

$$[\hat{\mathbf{G}}_e(s)]_{mn}=az^{|m-n|}\ , \tag{5.1a}$$

$$a=[s^2+4ws\psi(s)]^{-1/2}\ , \tag{5.1b}$$

$$z=\frac{s+2w\psi(s)-\sqrt{s^2+4ws\psi(s)}}{2w\psi(s)}\ . \tag{5.1c}$$

$\hat{\mathbf{G}}_e(s)$ has the form of the propagator for a random walk with nearest-neighbor steps and without disorder, with the jump rate w replaced by an effective, frequency-dependent jump rate $w\psi(s)$.

The effective medium function $\psi(s)$ is determined by solving the self-consistent equation, Eq. (3.20). This GEMA self-consistent equation contains the scalar h, which is defined in Eq. (3.19b) as a sum of elements of the matrix $\mathbf{H}$. The form of the inverse of $\mathbf{H}$ is given in Eqs. (3.18b) and (3.17b), in terms of a matrix $\hat{\mathbf{G}}_e^{(\alpha)}(s)$, which

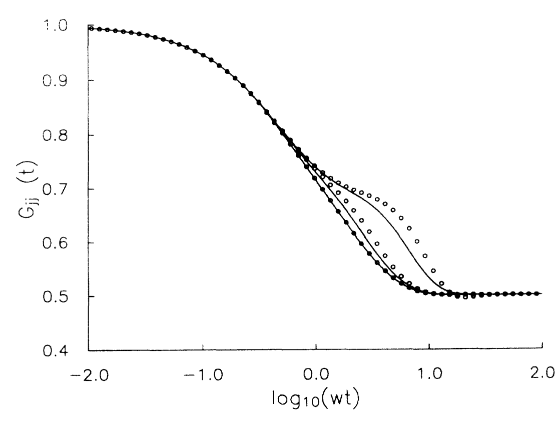

FIG. 6. The calculation of Fig. 4 is repeated for $c=0.6$.

according to Eq. (3.16b) is obtained from $\hat{\mathbf{G}}_e(s)$ by replacing s with $s+\alpha$, *except* in the argument of $\psi(s)$. The elements of this matrix are determined from (5.1) to be

$$[\hat{\mathbf{G}}_e^{(\alpha)}(s)]_{mn} = a^{(\alpha)}(z^{(\alpha)})^{|m-n|} , \tag{5.2a}$$

$$a^{(\alpha)} = [(s+\alpha)^2 + 4w(s+\alpha)\psi(s)]^{-1/2} , \tag{5.2b}$$

$$z^{(\alpha)} = \frac{s+\alpha+2w\psi(s) - \sqrt{(s+\alpha)^2+4w(s+\alpha)\psi(s)}}{2w\psi(s)} . \tag{5.2c}$$

Substitution of Eqs. (5.2) into Eq. (3.18b) yields the elements of the matrix $\mathbf{H}^{-1}$, whose inverse we seek:

$$[\mathbf{H}^{-1}]_{mn} \equiv h^{(-1)}(|m-n|) , \tag{5.3a}$$

$$h^{(-1)}(0) = s + 2w\psi(s) + \alpha\gamma a^{(\alpha)} , \tag{5.3b}$$

$$h^{(-1)}(1) = -w\psi(s) + \alpha\gamma a^{(\alpha)} z^{(\alpha)} , \tag{5.3c}$$

$$h^{(-1)}(k) = \alpha\gamma a^{(\alpha)}(z^{(\alpha)})^k, \quad k>1 . \tag{5.3d}$$

According to Eq. (5.3a), the elements of $\mathbf{H}^{-1}$ depend on their indices only through the difference of the indices. A matrix with this property is denoted a Toeplitz matrix [32] and the inverse of a Toeplitz matrix of infinite dimension is also of the Toeplitz form. We therefore define the coefficient $h(k)$, according to

$$H_{mn} = h(|m-n|) . \tag{5.4}$$

It may be verified by multiplication of $\mathbf{H}$ and $\mathbf{H}^{-1}$ that $h(k)$ is given by

$$h(k) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \frac{e^{-ik\theta}}{H^{(-1)}(\theta)} , \tag{5.5a}$$

$$H^{(-1)}(\theta) = \sum_{k=-\infty}^{\infty} h^{(-1)}(k) e^{ik\theta} . \tag{5.5b}$$

The function $H^{(-1)}(\theta)$ may be evaluated by substituting Eqs. (5.3b)–(5.3d) into Eq. (5.5b) and performing the summation to yield

$$H^{(-1)}(\theta) = \frac{\alpha_0 + \alpha_1\cos(\theta) + 4wz^{(\alpha)}\psi(s)\cos^2(\theta)}{1 - 2z^{(\alpha)}\cos(\theta) + (z^{(\alpha)})^2} , \tag{5.6a}$$

$$\alpha_0 = z^{(\alpha)}\{[s+2w\psi(s)][s+\alpha+2w\psi(s)] + \alpha\gamma\}/[w\psi(s)] , \tag{5.6b}$$

$$\alpha_1 = -2z^{(\alpha)}\{\alpha + 2[s+2w\psi(s)]\} . \tag{5.6c}$$

The scalar h that enters into the self-consistent equation in (3.20) may now be written as a one-dimensional integral

$$h = \frac{w}{\pi}\int_{-\pi}^{\pi} d\theta \frac{e^{-i\theta}-1}{H^{(-1)}(\theta)} . \tag{5.7}$$

The GEMA approximation to the time-domain random-walk propagator is determined as follows. Substitution of Eqs. (5.6) into the integrand of (5.7) and substitution of this result into Eq. (3.20) yields the GEMA self-consistent equation for the infinite one-dimensional lattice. The integration in (5.7) and the solution of (3.20) are accomplished numerically. Solution of (3.20) yields $\psi(s)$, which is then substituted into Eq. (5.1) to obtain the Laplace-space propagator. This Laplace transform is then numerically inverted [30].

Calculations of $G_{jj}(t)$, the probability that the walker, initially located at site j, can be found at that site after a time t, are shown in Figs. 7 and 8. The solid curves in Fig. 7 show $G_{jj}(t)$ for $c=0.5$, $\gamma/w=10^{-2}$, $\alpha/w=10^{-1}$ (leftmost curve), and $\alpha/w=10^{-6}$ (rightmost curve). The time dependence shown here is similar to that depicted for the same quantity in the two-site model in Fig. 1, in which γ/w has the same value. As was the case in Fig. 1, G_{jj} shows three regimes of behavior for the case $\gamma/w \ll 1$. Under these conditions, the walker's dynamics are rapid compared to those of the medium. On time scales short compared to the relaxation times of the medium, the walker finds itself on a cluster of lattice sites, connected to one another by unblocked jump rates. The boundary of the cluster is formed by blocked jump rates. The initial decay of G_{jj} represents the relaxation of the walker within such clusters. The second time regime is a plateau, which we show in Appendix B to occur at $G_{jj}=1-c$. This plateau persists until the medium begins to relax, which dissolves the clusters that had initially confined the walker. The third time regime represents the dynamics of the walker in a relaxed medium. The connection between the medium relaxation and walker dynamics is illustrated explicitly in Fig. 7. The broken curves show the probabilities that a bond variable initially in the state $\sigma=0$ has changed its state to $\sigma=1$ after a time t for $\alpha/w=10^{-1}$ (dotted curve) and for $\alpha/w=10^{-6}$ (dashed curve). For $\alpha/w=10^{-1}$, the medium is overdamped, and this probability approaches its equilibrium value of 0.5 as a biexponential. The medium is under-

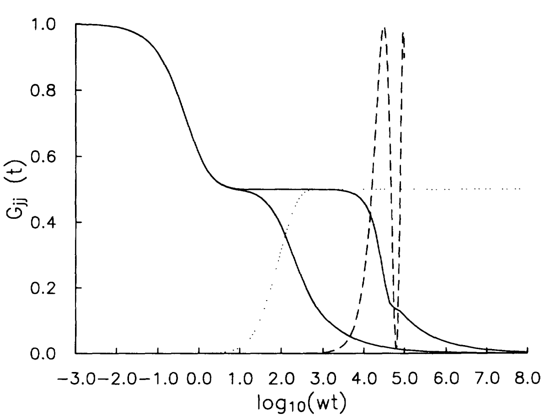

FIG. 7. The probability of remaining on the initial site G_{jj} is calculated for the one-dimensional lattice for $c=0.5$ and $\gamma=10^{-2}w$. The solid curves show G_{jj} calculated with the GEMA of Sec. III for $\alpha/w=10^{-1}$ (left) and 10^{-6} (right). The broken curves show $\Gamma_{10}(t)$, the probability that a jump rate which is initially forbidden has become permitted after a time t, for $\alpha/w=10^{-1}$ (dotted) and 10^{-6} (dashed). The medium dynamics are underdamped for $\alpha/w=10^{-6}$ and are overdamped for $\alpha/w=10^{-1}$. The dashed curve is terminated after one cycle for clarity. Comparison of the solid and broken curves shows that the plateau in the former decays as the medium relaxes.

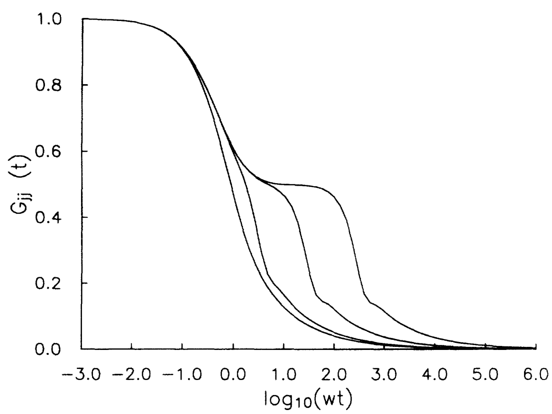

FIG. 8. The probability of remaining on the initial site G_{jj} is calculated for the one-dimensional lattice for $c=0.5$, $\gamma=10^2w$, and, from left to right, $\alpha/w=10^2$, 10^{-2}, 10^{-4}, and 10^{-6}, with the GEMA of Sec. III. As the decay rate of the medium's memory kernel is diminished, a plateau develops in G_{jj}.

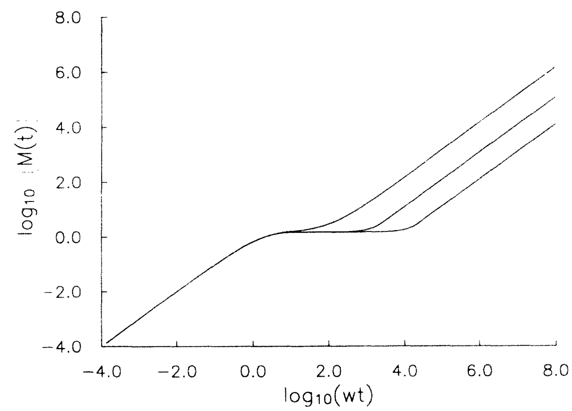

FIG. 9. The walker's mean-squared displacement, calculated from Eqs. (5.8), is plotted versus $\log_{10}(wt)$ for $c=0.5$, $\gamma=10^{-2}w$, and, from left to right, $\alpha/w=10^4$, 10^{-4}, and 10^{-6}. The initial regime represents diffusive motion within clusters of sites connected by finite jump rates, whose boundaries are formed by jump rates of value zero. The plateau represents times over which walkers have explored these clusters, but the clusters have not yet relaxed. A regime of terminal diffusion sets in after the clusters have relaxed.

damped for $\alpha/w=10^{-6}$, and this probability approaches 0.5 as a damped oscillation. The dashed curve has been terminated after one cycle for visual clarity. Comparing the solid and broken curves for a given value of α shows that the plateau in the walker dynamics ends as the medium begins to relax. Close inspection of G_{jj} for $\alpha=10^{-6}$ shows a small plateau following the principal plateau, which occurs at the time at which the transition probability for the medium variables has its first minimum. This behavior is generally displayed by G_{jj} in the underdamped regime, as may be seen from Fig. 8, which shows the time dependence of G_{jj} for $\gamma/w \gg 1$. In Fig. 8, $c=0.5$, $\gamma/w=10^2$, and, from left to right, $\alpha/w=10^2$, 10^{-2}, 10^{-4} and 10^{-6}. The time dependence in Fig. 8 is similar to that in Fig. 2 for the two-site problem, in which γ/w has the same value. For $\alpha/w \gg 1$, the walker dynamics are rapid compared to those of the medium and G_{jj} does not display a plateau. As α/w is decreased from this regime, a plateau develops.

Knowledge of the propagator in (5.1) permits the calculation of the walker's mean-squared displacement, whose Laplace transform is given by

$$\langle \hat{r}^2(s)\rangle = b^2 \sum_{j=-\infty}^{\infty} j^2 \hat{G}_{0j}(s) \tag{5.8a}$$

$$= 2ab^2 \left[\frac{z^2+z}{(1-z)^3} \right] . \tag{5.8b}$$

The lattice constant is denoted b in Eq. (5.8a) and a and z are defined in Eqs. (5.1b) and (5.1c). Calculations of $\langle r^2(t)\rangle$, obtained by numerical inversion of the Laplace transform in Eq. (5.8b), are shown in Fig. 9 for $c=0.5$, $\gamma/w=10^{-2}$, and, from left to right, $\alpha/w=10^4$, 10^{-4}, and 10^{-6}. The initial time regime represents diffusive motion within a cluster, the plateau represents the confinement of the walker within clusters, and the long-time diffusive regime represents dynamics on time scales long compared to the relaxation times of the clusters.

VI. CONCLUSION

In this work, we have presented an effective-medium approach to random walks with non-Markovian dynamical disorder. We conclude by comparing our general strategy to that underlying the EMA developed by Harrison and Zwanzig [3] and by Sahimi [4] for the Markovian case. In the EMA, the Laplace-space propagator for the disordered system is taken to have the form of the propagator in the absence of disorder, with the hopping rate replaced by an effective, frequency-dependent rate. This effective rate is determined by considering a system in which one rate fluctuates and the rest are assigned the mean-field value and by demanding that the averaged propagator for that system be identical to the effective propagator. In this approach, the fluctuations of one hopping rate are treated exactly, so that the EMA is exact for the Markovian limit of the two-site model treated in Sec. IV. The EMA is successful because the exact solution for the two-site problem with Markovian dynamical disorder has the form of the exact solution for the two-site problem in the absence of disorder, with the hopping rate replaced by a frequency-dependent scalar. If the medium variable dynamics are characterized by a memory function with finite decay time, the solution of the two-site problem no longer has this form. For this reason, we have made the additional approximations discussed in Sec. III, in order to preserve the convenient form of the effective medium propagator, in which all of the effects of the disorder are embodied in a scalar frequency-dependent hopping rate. The model treated by Harrison and Zwanzig [3] and by Sahimi [4] has proven to be relevant to a wide range of physical applications [9,12]. It is our hope that this range may be extended by the present work.

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APPENDIX A: DYNAMICS OF THE MEDIUM VARIABLES

In the random walk considered in this work, the values of the jump rates are determined by stochastic variables denoted the medium variables. The dynamics of the probability distribution of these medium variables are governed by Eq. (2.4). Equation (2.4) contains a memory function $K(t)$ of arbitrary form. In Sec. III, we specialized to the choice in (3.1), $K(t)=\alpha\gamma e^{-\alpha t}$. In this appendix, we provide the explicit solution of Eqs. (2.4) for this choice of memory function. For this case, Eqs. (2.4) take the form

$$\dot{\phi}(1,t)=\gamma\alpha\int_0^t d\tau\, e^{-\alpha(t-\tau)}[c\phi(0,\tau)-(1-c)\phi(1,\tau)] , \tag{A1}$$

$$\dot{\phi}(0,t)=-\dot{\phi}(1,t) . \tag{A2}$$

The solution of these equations may be expressed in terms of a propagator $\Gamma_{\sigma\sigma'}(t)$ that gives the probability that a medium variable has the value σ at time t, given that it had the value σ' at time 0:

$$\phi(\sigma,t)=\sum_{\sigma'}\Gamma_{\sigma\sigma'}(t)\phi(\sigma',0) . \tag{A3}$$

Since the right-hand side of Eq. (A1) has the form of a convolution, the Laplace transforms of Eqs. (A1) and (A2) are coupled linear equations and may be solved, and the Laplace transforms then inverted.

The form of the solution depends on the relative magnitudes of α, the decay rate of the memory function, and γ, the time integral of the memory function. For $\alpha<4\gamma$, the system is underdamped and the probabilities approach their equilibrium values with damped oscillations. For example, $\Gamma_{00}(t)$ is given by

$$\Gamma_{00}(t)=1-c+ce^{-\alpha t/2}[\cos\Omega t+(\alpha/2\Omega)\sin\Omega t] , \tag{A4}$$

$$\Omega=[\alpha\gamma-\alpha^2/4]^{1/2} . \tag{A5}$$

Γ_{11} may be obtained from Eq. (A4) by replacing c with $1-c$ and the off-diagonal terms may be determined from the requirement that $\Gamma_{00}+\Gamma_{10}=\Gamma_{11}+\Gamma_{01}=1$. If $\alpha>4\gamma$, the system is overdamped and the distributions approach equilibrium with a biexponential decay:

$$\Gamma_{00}(t)=1-c+ce^{-\alpha t/2}[\cosh\Omega' t+(\alpha/2\Omega')\sinh\Omega' t] , \tag{A6}$$

$$\Omega'=[\alpha^2/4-\alpha\gamma]^{1/2} . \tag{A7}$$

The behavior in the critically damped case may be obtained by taking the limit $\alpha\to 4\gamma$ in either (A4) or (A6):

$$\Gamma_{00}(t)=1-c+ce^{-\alpha t/2}[1-\alpha t/2] . \tag{A8}$$

In order for Eqs. (A1) and (A2) to provide an appropriate model for the dynamics of the medium variables, their solutions for the probabilities $\phi(1,t)$ and $\phi(0,t)$ must have values that lie between 0 and 1. For arbitrary values of the initial conditions $\phi(1,0)$ and $\phi(0,0)$, this condition will be satisfied if each of the propagator elements $\Gamma_{\sigma\sigma'}(t)$ is bounded from below by 0 and from above by 1. Inspection of Eqs. (A6) and (A8) confirms that this condition is satisfied in the overdamped and critically damped regimes. However, Eq. (A4) reveals that for certain values of c, α, and γ in the underdamped regime, $\phi(1,t)$ and $\phi(0,t)$ may take on values that are less than zero or greater than 1. Analysis of Eq. (A4) and the corresponding results for the other propagator elements demonstrates that these matrix elements have appropriately bounded values if the following condition is satisfied:

$$\left[\frac{1}{1-y}\right]^{1/2}\exp\left\{-\left[\frac{y}{1-y}\right]^{1/2}\times\left[\pi+\tan^{-1}\left[\frac{y}{1-y}\right]^{1/2}\right]\right\}\le F(c) , \tag{A9a}$$

$$y\equiv\alpha/4\gamma , \tag{A9b}$$

$$F(c)\equiv\begin{cases}(1-c)/c, & c\ge\frac{1}{2}\\ c/(1-c), & c\le\frac{1}{2} .\end{cases} \tag{A9c}$$

The condition shown in (A9a) depends on α and γ only through the variable y, defined in (A9b). The medium variable is underdamped if $y<1$ and overdamped if $y>1$. If the inequality in (A9a) is replaced by an equality, solution of the resulting equation for c as a function of y is shown in Fig. 10. This figure may be used to determine the physically reasonable values of α and γ for a given value of c denoted c^*. A horizontal line at $c=c^*$ intersects the curve at $y=y^*$. For $c=c^*$ and $y<y^*$, the solutions of Eqs. (A1) behave unphysically, in that quantities supposed to represent probabilities may have values

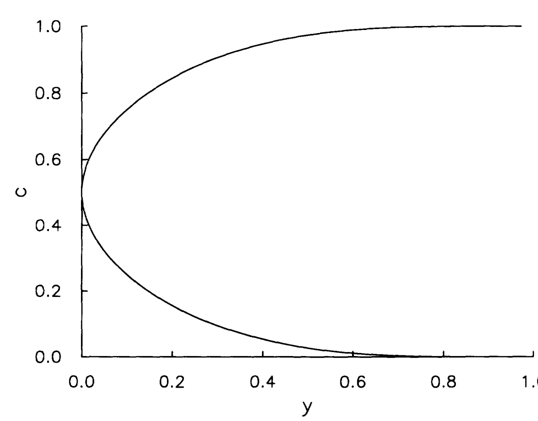

FIG. 10. The curve shows the solution of (A9a), written as an equation rather than an inequality, for c as a function of y. For a given value of c, values of y to the left of the curve yield unphysical solutions of Eqs. (A1) and (A2), while values of y on the right-hand side of the curve yield reasonable solutions of Eqs. (A1) and (A2). At $c=0.5$, all values of y give physical solutions.

that are negative or greater than unity. For $c=c^*$ and $y \geq y^*$, the solutions of Eqs. (A1) are properly bounded by 0 and 1. At $c^*=\frac{1}{2}$, $y^*=0$. When the equilibrium probabilities for the two states of the medium variable are equal, Eqs. (A1) are physically reasonable for all values of α and γ. As c approaches 0 or 1, y^* approaches 1, indicating that in the critically damped and overdamped regimes, the solutions of (A1) are physically reasonable for all values of α and γ. The preceding analysis demonstrates that Eqs. (A1) and (A2) represent valid equations of motion for the medium variables provided that the requirement in (A9a) is met. In Figs. 1–9, we show calculations of random walk dynamics that illustrate the influence on the walker of both underdamped and overdamped medium dynamics. In all cases, we have chosen values of c, α, and γ that satisfy Eq. (A9a).

APPENDIX B: THE PLATEAU IN $G_{jj}(t)$

Calculations of the probability that the walker, initially located at a given site, resides at that site at a later time, are presented in Sec. IV for the two-site problem and in Sec. V for a one-dimensional lattice of infinite extent. In both cases, the probability displays a plateau if the medium dynamics are slow compared to those of the walker. This condition is satisfied if the walker's hopping rate is large compared to either the decay rate of the medium's memory function ($w \gg \alpha$) or to the time-integrated memory function ($w \gg \gamma$). In this appendix, we derive expressions for the plateau height in both of these models.

The plateau value of $G_{jj}(t)$ for a slowly relaxing medium is identical to the infinite-time limit of $G_{jj}(t)$ for the case of a static medium $\alpha=0$ or $\gamma=0$. We denote this value G_{jj}^{∞}. We first calculate G_{jj}^{∞} for the two-site problem. The walker's jump is initially unblocked with probability c. If the jump is unblocked, the probability that the walker remains at the initial site decays to $\frac{1}{2}$, while if the jump is blocked, this probability remains equal to unity. The value of G_{jj}^{∞} is therefore $c/2+(1-c)=1-c/2$. The plateau values shown in Figs. 1–6 agree with this prediction. For the infinite lattice, we may express G_{jj}^{∞} in terms of $P(L)$, the probability that the initial site belongs to a cluster of L sites connected by unblocked jump rates, which is terminated at either end by a blocked jump rate:

$$G_{jj}^{\infty}=\sum_{L=1}^{\infty} L^{-1}P(L) \ . \tag{B1}$$

In (B1), the long-time limit of $G_{jj}(t)$ for a cluster of L sites, L^{-1}, is averaged over the distribution $P(L)$. Since medium variables associated with different pairs of sites are uncorrelated, $P(L)$ is given by

$$P(L)=Lc^{L-1}(1-c)^2 \ . \tag{B2}$$

The factor c^{L-1} is associated with the $L-1$ unblocked jump rates and the factor $(1-c)^2$ is contributed by the two blocked jump rates that terminate the cluster. The factor of L arises because any one of the L sites in the cluster could serve as the initial site for the random walk. Substitution of (B2) into (B1) yields the result discussed in Sec. V: $G_{jj}^{\infty}=1-c$.

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