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Theory of diffusion in finite random media with a dynamic boundary condition

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In the presence of a time-periodic incoming flow the diffusion problem on finite random media has been studied. Particular importance has been stressed on different boundary conditions (reflecting or absorbing). The problem has been worked out by generalizing the finite effective-medium approximation (FEMA). Thus a perturbative theory, in the time-asymptotic regime, has been built up in the Laplace representation (small-u parameter) for weak and strong site disorder. This theory separates in a natural way the contribution given by the effective medium (from other higher-order corrections) which appears as the zeroth-order step in the perturbation scheme. Asymptotic results for the current of probability (inside the finite domain) are obtained for different time-dependent incoming external flows. Exact results beyond FEMA are obtained for the low-frequency behavior of the evolution equation for the averaged Green's function on a finite lattice. Monte Carlo simulations have been carried out in order to compare them with our theoretical predictions. In the absence of an incoming external flow, the problem of the first passage time distribution through only one frontier (in a random media) and for different boundary conditions has been revisited. [S0163-1829(97)01033-3]

I. INTRODUCTION

Diffusion on random media has been a topic of long-standing interest, particularly because of its success in describing conductivity in amorphous materials.[1] Analytic techniques have been used to tackle this problem; special roles are played by the effective-medium approximation (EMA),[2] the continuous-time random-walk theory,[3] and its multistate approach.[4]

It is known that EMA gives the correct anomalous exponents for unbiased walks;[1,5] more complex systems, such as conductivity in granular metal film,[6] can also be described in the context of EMA. Also the study of the first passage time distribution (FPTD) in random media[7,8] has been done with success in the context of the finite effective-medium approximation (FEMA). Recently the FPTD has been studied in presence of bias[9] to get a direct access to the fluctuation of the quenched disorder, and to the evaluation on the mean time for particles to go across a random medium.

In random media, of particular importance is the study of the one-dimensional (1D) averaged probability distribution with special boundary conditions because this quantity carries information about the scaling properties on a finite system. In the presence of arbitrary boundary conditions, weak or strong disorder can, in principle, be worked out by doing a similar analysis as the one done with FEMA (i.e., in order to study the FPTD to leave a finite domain $D=[-L,L]$ (Ref. 7)).

In this paper we are interested in the study of the averaged probability distribution in the presence of periodically forced boundary conditions—on one extreme of the lattice. Therefore by studying the output flow of probability—close to the opposite extreme—we will be able to predict the type of disorder (in the sample) by measuring the time-dependent behavior of the probability distribution at the end of the lattice. The goal of this work is to study this profile in porous media,[10] giving in this way a direct access to the experimental measures made with the frequency response method,[11] or in the trap-limited electronic transport investigated by intensity modulated photocurrent spectroscopy.[12]

II. THEORY

Let us consider a general one-step Markovian random walk (RW) in a finite chain $\mathcal{D}\equiv[-L,L]$. The forward master equation has the general form[13]

$$\partial_t P(n,t|n_0,t_0)=\sum_{n'} \mathbf{H}_{n,n'} P(n',t|n_0,t_0), \qquad (2.1)$$

where $P(n,t|n_0,t_0)$ is the probability of being at site n at time t with the condition to start at $n_0 \in \mathcal{D}$ at time $t_0 < t$. Here $\mathbf{H}_{n,n'}$ is a finite square matrix whose indices run over the sites in the chain $n \in \mathcal{D}$.

Disorder is described as assigning a probability to each possible configuration of the hopping transition probability $\omega_{n\pm 1,n}$, per unit time, from site n to $n\pm 1$ of the chain. This assignment of probabilities defines a RW in random media. The statistical properties of this RW process can be obtained by averaging, over configurations of disorder, the expressions for the quantities of interest obtained for fixed hopping transitions $\omega_{n\pm 1,n}$.

We are interested in the particular situation when the master Hamiltonian $\mathbf{H}_{n,n'}$ models strong or weak disorder, and the diffusion is forced to time-periodic boundary conditions (BC) on site $-(L+1)$, and to a static absorbing BC on $L+1$; i.e., at the left frontier of $\mathcal{D}$ we have a dynamic BC and on the right frontier we have a static one. Let us consider a site-disorder model so that we can use the short notation $\omega_{n\pm 1,n} \equiv \omega_n$. If from the left side we introduce a flow J^e_{-L} (on site $-L$) the evolution equation for the conditional probability $P(-L,t|n_0,t_0) \equiv \mathbf{P}(t)_{-L,n_0}$ will read

$$\dot{\mathbf{P}}(t)_{-L,n_0} = \omega_{-L+1}\mathbf{P}(t)_{-L+1,n_0} - \omega_{-L}\mathbf{P}(t)_{-L,n_0} + J^e_{-L}. \tag{2.2}$$

The right side of $\mathcal{D}$ is assumed to be an absorbent site, so the evolution equation for the conditional probability $P(L,t|n_0,t_0) \equiv \mathbf{P}(t)_{L,n_0}$ is

$$\dot{\mathbf{P}}(t)_{L,n_0} = \omega_{L-1}\mathbf{P}(t)_{L-1,n_0} - 2\omega_L \mathbf{P}(t)_{L,n_0}. \tag{2.3}$$

The rest of the equations for $\mathbf{P}(t)_{n,n_0}$ (for $n \neq \pm L$) remain unchanged:

$$\dot{\mathbf{P}}(t)_{n,n_0} = \omega_{n+1}\mathbf{P}(t)_{n+1,n_0} + \omega_{n-1}\mathbf{P}(t)_{n-1,n_0} - 2\omega_n \mathbf{P}(t)_{n,n_0}. \tag{2.4}$$

The total set of equations for $\dot{\mathbf{P}}(t)_{n,n_0}$ can be written in a compact form. Consider a master Hamiltonian $\mathbf{H}^{\mathrm{RA}}_{n,n'}$, representing reflecting and absorbing boundary conditions on sites $\pm(L+1)$. Then introducing the matrix current $\mathbf{J}^e_{n,n_0}$, the problem posed from Eqs. (2.2) to (2.4) can be rewritten as

$$\dot{\mathbf{P}}(t)_{n,n_0} = \sum_{n'} \mathbf{H}^{\mathrm{RA}}_{n,n'}\mathbf{P}(t)_{n',n_0} + \mathbf{J}^e_{n,n_0}, \tag{2.5}$$

where $\mathbf{P}(t)$, $\mathbf{H}^{\mathrm{RA}}$, and $\mathbf{J}^e$ are $(2L+1)\times(2L+1)$ matrices. The master Hamiltonian $\mathbf{H}^{\mathrm{RA}}_{n,n'}$ is

$$\mathbf{H}^{\mathrm{RA}} \equiv \begin{pmatrix} -\omega_{-L} & \omega_{-L+1} & 0 & & & \\ \omega_{-L} & -2\omega_{-L+1} & \cdots & & & \\ 0 & \omega_{-L+1} & \cdots & . & & \\ \cdots & 0 & \cdots & \cdots & \cdots & \\ & \cdots & . & \cdots & 0 & \cdots \\ & & . & \cdots & \omega_{L-1} & 0 \\ & & & \cdots & -2\omega_{L-1} & \omega_L \\ & & & 0 & \omega_{L-1} & -2\omega_L \end{pmatrix} \tag{2.6}$$

and matrix $\mathbf{J}^e$ represents an incoming flow at site $-L$:

$$\mathbf{J}^e_{n,n'} = J^e(t)\,\delta_{n,-L}. \tag{2.7}$$

Taking the Laplace transform $\{t \leftrightarrow u\}$ in Eq. (2.5), the formal solution $\mathbf{P}(u)$ is

$$\mathbf{P}(u) = (u\mathbf{1} - \mathbf{H}^{\mathrm{RA}})^{-1}[\mathbf{P}(t=0) + \mathbf{J}^e(u)]. \tag{2.8}$$

For the particular case when the current is a constant in time we get for the Laplace transform of Eq. (2.7)

$$\mathbf{J}^e(u) = \frac{1}{u}\mathbf{J}^e.$$

Therefore in general the average over the disorder gives

$$\langle \mathbf{P}(u)\rangle = \langle \mathbf{G}^{\mathrm{RA}}(u)\rangle [\mathbf{P}(t=0) + \mathbf{J}^e(u)]. \tag{2.9}$$

Here we have assumed that the initial condition $\mathbf{P}(t=0)$ and the current $\mathbf{J}^e(u)$ do not depend on the different configurations of disorder, thus we only need to know the averaged Green's function $\langle \mathbf{G}^{\mathrm{RA}}(u)\rangle = \langle (u\mathbf{1} - \mathbf{H}^{\mathrm{RA}})^{-1}\rangle$. This matrix can be calculated in the context of an effective media. Of course the averaged Green's function will depend on the particular BC that we impose on the master Hamiltonian $\mathbf{H}$. For the absorbing-absorbing case this calculation was done using Terwiel's cumulant[7,14] by introducing a diagrammatic perturbation theory. This perturbation corresponds to the one-loop resummation in diagrammatic representations, known as the single-site approximation in condensed matter.[5]

By using the method of images[15] we have worked out in Appendix A the corresponding *ordered* Green's function $\mathbf{G}^{\mathrm{RA}}(u)$; i.e., with reflecting-absorbing BC. In Appendix B we have summarized the mathematical details to obtain $\langle \mathbf{G}^{\mathrm{RA}}(u)\rangle$. Section IV is concerned with the absorbing-absorbing case with an incoming flow $\mathbf{J}^e$ at any arbitrary site

n^e and considering different domains $\mathcal{D}=[-L,L]$ and $\mathcal{D}_1=[1,L_1]$.

The result for the reflecting-absorbing case, with $m,n \in \mathcal{D}\equiv[-L,L]$, gives

$$\mathbf{G}^{\mathrm{RA}}(u)_{n,m}=B(u)[A^{|n-m|}+KA^{2L+1}R_{nm}], \tag{2.10}$$

where

$$R_{nm}\equiv R_{nm}(u)=A^{n+m}-A^{4L+n+m+3}+A^{6L-n+m+5} -A^{2L-n+m+2}-A^{-n-m+1}+A^{4L-n-m+4} +A^{6L+n-m+5}-A^{2L+n-m+2}, \tag{2.11}$$

$$A\equiv A(u)=1+\frac{u}{2\mu}-\left[\frac{u}{\mu}+\frac{u^2}{4\mu^2}\right]^{1/2}, \tag{2.12}$$

$$K\equiv K(u)=(1-A^{8L+6})^{-1}, \tag{2.13}$$

$$B(u)=\frac{1}{2\mu}\left[\frac{u}{\mu}+\frac{u^2}{4\mu^2}\right]^{-1/2}, \tag{2.14}$$

and μ is the hopping transition rate (see Appendix A).

The long time limit of the Green's function (2.10) can be studied by analyzing the limit $u\rightarrow 0$ in its Laplace representation:

$$\mathbf{G}^{\mathrm{RA}}(u)_{n,m}\cong\frac{(1+L-\max[n,m])}{\mu}+\mathcal{O}(u^{3/2}); \tag{2.15}$$

here $n,m\in\mathcal{D}$.

A. Taking the average in a site-disorder model

As we have mentioned before, a diffusion process in random media forced to a dynamic and static BC is characterized by Eq. (2.9). For the particular reflecting-absorbing situation, the effective hopping transition $\mu(u)$ must be obtained from the self-consistent equation (see Appendix B)

$$\left\langle\frac{\omega-\mu(u)}{1-[\omega-\mu(u)]\mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(u)}\right\rangle_{\Pi(\omega)}=0; \tag{2.16}$$

here $\Pi(\omega)$ is the probability measure characterizing the type of disorder on the random medium and

$$\mathbf{H}^0=[\mathbf{E}^+ +\mathbf{E}^- -2]$$

is the ordered master Hamiltonian for an infinite lattice, where $\mathbf{E}^{\pm}$ are shifting operators:

$$\mathbf{E}^{\pm}\mathbf{G}^{\mathrm{RA}}(u)_{n,m}=\mathbf{G}^{\mathrm{RA}}(u)_{n\pm 1,m}.$$

The ordered Green's function $\mathbf{G}^{\mathrm{RA}}$ (in time representation) is the solution of the initial-value problem

$$\partial_t\mathbf{G}^{\mathrm{RA}}(t|t')=\mu\mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(t|t'), \tag{2.17}$$

$$\mathbf{G}^{\mathrm{RA}}(t|t)=\mathbf{1},$$

with absorbing BC at $n=L+1$:

$$\mathbf{G}^{\mathrm{RA}}_{L+1,m}(t|t')=0$$

and a reflecting BC placed midway between sites $n=-(L+1)$ and $-L$.[15] The solution of Eq. (2.17), in the Laplace representation, is the one given by Eq. (2.10).

The average over the disorder is easily obtained by replacing $\mu\rightarrow\mu(u)$ in Eq. (2.10), i.e.,

$$\langle\mathbf{G}^{\mathrm{RA}}\rangle=[\mathbf{G}^{\mathrm{RA}}]_{\mu=\mu(u)}. \tag{2.18}$$

Another important quantity in Eq. (2.16) to work out is $\mathcal{J}(u)_{n,m}\equiv\mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(u)_{n,m}$, which in the asymptotic regime (see Appendix A) is characterized by

$$\mathcal{J}(u)_{n,m}\cong-\frac{1}{\mu}\delta_{n,m}+\frac{1+L-\max(n,m)}{\mu^2}\,u+\mathcal{O}(u^2). \tag{2.19}$$

Specifying the probability measure $\Pi(\omega)$ and using Eq. (2.19) in Eq. (2.16) we can obtain in a self-consistent way $\mu(u)$, and therefore we can study different random media. The type of disorder that we have considered in this paper is the same that one of us studied in Ref. 7. Thus from Eq. (2.16) we get:

(1) For weak disorder (model A of Ref. 1), all the inverse moments $\beta_k\equiv\langle 1/\omega_n^k\rangle$, $k=1,2,\ldots,$ are finite, therefore, from Eq. (2.16) in the $u\rightarrow 0$ limit we get

$$\mu(u=0)^{-1}=\langle 1/\omega\rangle_{\Pi(\omega)}=\beta_1. \tag{2.20}$$

(2) Model B of Ref. 1. The probability distribution for each statistical independent variable ω_n is

$$\Pi(\omega)=\begin{cases}1 & \text{if } \omega\in[0,1],\\ 0 & \text{otherwise,}\end{cases}$$

therefore from Eq. (2.16) in the $u\rightarrow 0$ limit we get

$$\mu(u)\cong-(\ln u)^{-1}\left(1-\frac{\ln(L+1)}{\ln u}+\cdots\right). \tag{2.21}$$

(3) Model C of Ref. 1. The probability distribution for each statistical independent variable ω_n is

$$\Pi(\omega)=\begin{cases}(1-\alpha)\quad\omega^{-\alpha} & \text{if } \omega\in[0,1],\\ 0 \quad \text{otherwise,}\end{cases}$$

therefore from Eq. (2.16) in the $u\rightarrow 0$ limit we get

$$\mu(u)\cong(L+1)^{\alpha}\frac{\sin(\pi\alpha)}{\pi(1-\alpha)}u^{\alpha}. \tag{2.22}$$

Using these effective hopping transitions $\mu(u)$ we can calculate from Eqs. (2.9) and (2.18)—for different type of disorders—the long-time limit behavior of the averaged probability distribution for the proposed problem. We want to remark that FEMA, as well as EMA, give the correct exponent in the asymptotic long-time regime, nevertheless for strong disorder the coefficient of $\mu(u)$ is overestimated (see, for example, Refs. 7 and 5 and Appendix C).

B. The long-time limit

Let us consider the weak disorder model A and the situation when the current J^e is constant in time. In this case we get from Eqs. (2.7), (2.9), and (2.18) in the $u\rightarrow 0$ limit

$$\langle \mathbf{P}(u)_{n,n_0}\rangle \sim \sum_m \frac{1+L-\max[n,m]}{\mu(u)}\left[\mathbf{P}(t=0)+\frac{1}{u}\mathbf{J}^e\right]_{m,n_0}. \tag{2.23}$$

For this case, from Eq. (2.20) $\mu(u=0)=\langle 1/\omega\rangle^{-1}$, then using the matrix expression of $\mathbf{J}^e_{m,n}$ we immediately see that in the long-time regime and for weak disorder, the averaged RW probability distribution is given by

$$\langle \mathbf{P}(t)_{n,n_0}\rangle \sim J^e\left\langle \frac{1}{\omega}\right\rangle (1+L-n). \tag{2.24}$$

Therefore we have got, inside the lattice, a renormalized current flow of probability; its time-scale is now characterized by the disorder in terms of the inverse moment $\langle 1/\omega\rangle^{-1}$. As expected, in the long-time regime the probability distribution $\langle \mathbf{P}(t)_{n,n_0}\rangle$ is independent of the initial condition n_0 and it has its minimum at the absorbing barrier $\langle \mathbf{P}(t)_{L,n_0}\rangle \sim J^e\langle 1/\omega\rangle$.

Model B of disorder gives

$$\langle \mathbf{P}(t)_{n,n_0}\rangle \sim J^e(\ln t+\gamma)(1+L-n); \tag{2.25}$$

here $\gamma=0.5772156\cdots$ is the Euler's constant, and we have taken from Eqs. (2.21) and (2.23) the inverse Laplace transform of the dominant contribution ($\ln u/u$).

Let us now consider the strong disorder model C. In this case from Eqs. (2.22), (2.23) and using a Tauberian theorem we get

$$\langle \mathbf{P}(t)_{n,n_0}\rangle \sim J^e(1+L-n)(L+1)^{-\alpha}\frac{\pi(1-\alpha)}{\sin(\pi\alpha)}t^{\alpha}. \tag{2.26}$$

These remarkable results, show that, for strong disorder, the averaged RW probability distribution increases with time. We can understand this result if we think that the disorder promotes the localization of the diffusion particles and therefore the particles cannot freely diffuse in a disordered lattice. This fact is ultimately responsible for the increase of the probability distribution in the long-time regime. Figure 1 shows the comparison of our theoretical predictions for strong disorder against Monte Carlo simulations. We remark that this power low is an exact result in the asymptotic regime. Nevertheless, as was pointed out before, the correct coefficient of $\langle \mathbf{P}(t\rightarrow\infty)_{n,n_0}\rangle$ for strong disorder is overestimated in the framework of FEMA (see Appendix C).

C. Time-periodic boundary condition

Of particular importance, in solid state physics, is the behavior of the averaged probability distribution in presence of a periodic incoming flow of particles. This problem can also be studied in terms of the analysis that we have carried out in the previous sections. To do this we just need to introduce a time-periodic current in Eq. (2.7). Let for example the current be proportional to $|\sin(\Omega t)|$; in this case the long-time regime of the averaged probability distribution is characterized as before by Eq. (2.23), but now considering the Laplace transform of Eq. (2.7) with $J^e(t)\sim|\sin(\Omega t)|$, and $\mathbf{P}(t=0)=0$ we get

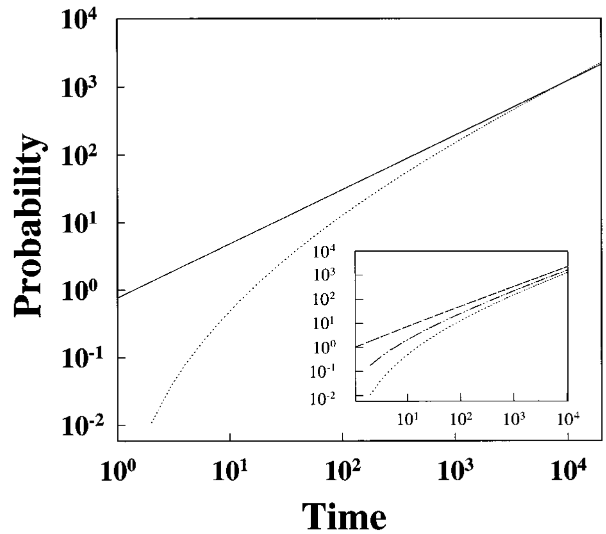

FIG. 1. Disorder-averaged RW probability distribution at site $n=L$, plotted as a function of time for strong disorder (model C with $\alpha=0.8$) and in the presence of an external incoming constant flow $J^e=1$ at site $n^e=-L$. The inset shows the same function for different positions [from top to bottom n $(=-1,0,1)$]. All the plots correspond to a lattice with $L=1$. The continuous line is the FEMA result and the dotted line is the Monte Carlo simulations with 10^5 realizations.

$$\langle \mathbf{P}(u)_{n,n_0}\rangle \sim \frac{1+L-n}{\mu(u)}\frac{\Omega}{u^2+\Omega^2}\coth\left(\frac{\pi u}{2\Omega}\right). \tag{2.27}$$

As before the disorder enters in the explicit expression for the effective hopping transition rate $\mu(u)$. For the time-periodic case it must be understood that the long-time limit is also a time average over one period of time $2\pi/\Omega$. Thus in order to get a nonzero average current we could consider a periodic modulation superimposed over a constant flow $\mathcal{A}^e$, so we show here a typical time-periodic modulation such as[16]

$$J^e=\mathcal{A}^e-\cos\Omega t. \tag{2.28}$$

Therefore we have to use

$$\mathbf{J}^e(u)_{n,n'}=\left[\frac{1}{u}\mathcal{A}^e-\frac{u}{u^2+\Omega^2}\right]\delta_{n,-L} \tag{2.29}$$

for the Laplace representation of the matrix $\mathbf{J}^e(u)$ appearing in Eq. (2.9). Thus in presence of the incoming flow (2.28) on site $n=-L$, the long-time averaged RW probability distribution is given by

$$\langle \mathbf{P}(u)_{n,n_0}\rangle \sim \frac{1+L-n}{\mu(u)}\left(\frac{1}{u}\mathcal{A}^e-\frac{u}{u^2+\Omega^2}\right), \tag{2.30}$$

where $\mu(u)$ is given by Eqs. (2.20)–(2.22) depending on the type of disorder. In Fig. 2 we show—at the long-time regime—the comparison of our theoretical predictions [from Eq. (2.30) for strong disorder]

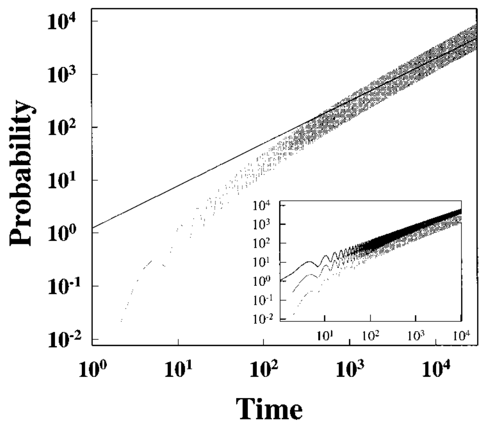

FIG. 2. Disorder-averaged RW probability distribution at site $n=L$, plotted as a function of time for strong disorder (with $\alpha=0.8$) and in presence of an external incoming time-periodic flow $J^e(t)=2-\cos t$ at site $n^e=-L$. The inset shows the same function for different positions [from top to bottom n $(=-1,0,1)$]. All the plots correspond to a lattice with $L=1$. The continuous black line is the FEMA result, and the shaded lines correspond to Monte Carlo simulations with 10^5 realizations.

$$\langle \mathbf{P}(t)_{n,n_0}\rangle \sim \mathcal{A}^e(1+L-n)(L+1)^{-\alpha}\frac{\pi(1-\alpha)}{\sin(\pi\alpha)}t^{\alpha} \tag{2.31}$$

against the corresponding Monte Carlo simulations. The agreement is very good for all types of disorder (strong or weak). Note that other dynamical incoming flows can also be considered in the framework of the present theory, just by changing $\mathbf{J}^e(u)_{n,n'}$.

Thus we see that due to the strong disorder there will be an increasing current of probability at site $n=L$ [i.e., $\langle \mathbf{P}(t)_{L,n_0}\rangle \sim t^{\alpha}$]. This is a remarkable result that is only present in strong disordered random media. Thus, formulas (2.31) provide a way to classify different types of materials by using a suitable experimental device which measures the out-coming flow of probability on the opposite side of the sample.

III. MEAN FIRST PASSAGE TIME

In Ref. 7 the FPTD—in random media—to leave the interval $[-L,L]$ was investigated taking into account different types of disorder. A related problem is the calculation of the first passage time through a specific frontier, i.e., for example, through the site $n=L$. This physical problem can be mapped into the calculation of the survival probability in the presence of an absorbing site $n=L+1$ and a reflecting one, midway between sites $(-L-1,-L)$. Thus the results of the previous sections can be used to calculate the required MFPT in disordered media.

As we have mentioned before, a diffusion process in random media with reflecting-absorbing frontiers can be analyzed by using Eq. (2.9). For the particular situation when $J^e_{-L}=0$ the FPTD through the border $n=+L$ can be studied in terms of the survival probability $F_{n_0}(t|t_0)$, i.e., the probability to still be in $\mathcal{D}$ if the walker had started at time t_0 from site n_0. Thus distribution $F_n(t|0)$ fulfills the evolution equation

$$\partial_t F(t)=[\mathbf{H}^{\mathrm{RA}}]^{\dagger}F(t), \tag{3.1}$$

where the matrix $[\mathbf{H}^{\mathrm{RA}}]^{\dagger}$ is the adjoint of the one given in Eq. (2.6) and $F(t)$ is a vector with components $[F(t)]_n \equiv F_n(t)$. The initial condition for Eq. (3.1) is $F_n(t=0)=1$ for all $n\in[-L,L]\equiv\mathcal{D}$. For the ordered case the exact solution of Eq. (3.1) in the Laplace representation is

$$F_n(u)=B(u)\left\{\sum_{m=-L}^{n-1}A^{n-m}+\sum_{m=n}^{L}A^{m-n} + \sum_{m=-L}^{L}KA^{2L+1}R_{nm}\right\}, \tag{3.2}$$

where R_{nm}, A, K, $B(u)$ were given in Eqs. (2.11)–(2.14). From Eq. (3.2) it is simple to calculate the exact expression of the MFPT, $T_n=\int_0^\infty F_n(t)dt\equiv F_n(u=0)$:

$$T_n=\frac{2+5L+3L^2-n-2Ln-n^2}{2\mu}. \tag{3.3}$$

In random media, the average MFPT can be calculated in the framework of the present perturbation theory (see Appendix B) by introducing the effective media. Therefore μ has to be replaced by the effective hopping transition $\mu(u)$ solution of the self-consistent Eq. (2.16).

It could be necessary to know the equivalent formulas (3.3) for a different domain, i.e., for example, $\mathcal{D}_1\equiv[1,L_1]$ with the reflecting BC at $n=0$ and the absorbing one at $n=L_1+1$. Therefore instead of Eq. (3.3) we get

$$T_{n_1}=\frac{1}{2\mu}[L_1(L_1+1)-n_1(n_1-1)]. \tag{3.4}$$

Note that with the scaling $n_1\equiv L+1+n$ and $L_1=2L+1$ from Eq. (3.4) we reobtain Eq. (3.3).

MFPT through $n=+L$ for disordered media.

(1) Disorder model A: using Eq. (2.20) in Eq. (3.3) we get

$$\langle T_n\rangle=\frac{2+5L+3L^2-n-2Ln-n^2}{2}\left\langle\frac{1}{\omega}\right\rangle. \tag{3.5}$$

(2) Disorder model B: for this case the MFPT diverges. Using Eq. (2.21) we get the following divergency low:

$$-\frac{2+5L+3L^2-n-2Ln-n^2}{2}\lim_{u\to 0}\ln u. \tag{3.6}$$

Thus the same localization phenomena—as for the case with two absorbing frontiers—occurs for the present problem. The only difference with Eq. (4.25) of Ref. 7 is the coefficient of proportionality.

(3) Disorder model C: for this case the MFPT also diverges. Using Eq. (2.22) we get the following power low:

$$\frac{2+5L+3L^2-n-2Ln-n^2}{2}(L+1)^{-\alpha}\frac{\pi(1-\alpha)}{\sin(\pi\alpha)}\lim_{u\to 0}u^{-\alpha}. \tag{3.7}$$

As expected there is also localization due to the strength of the disorder. The difference with Eq. (4.29) of Ref. 7 is the coefficient.

We remark that for weak disorder the MFPT passing through the frontier $n=+L$ is proportional to $(2+5L+3L^2-n-2Ln-n^2)$. This coefficient is quite different from the MFPT leaving the domain $\mathcal{D}=[-L,+L]$, which is proportional to the distance between the initial position leaving the nearest neighboring frontier.

For weak disorder and when the domain is $\mathcal{D}_1\equiv[1,L_1]$ the averaged MFPT can be analyzed in a similar way as was done in Eq. (3.4) for the ordered case.

IV. INCOMING FLOW AT ANY ARBITRARY SITE

In order to consider other geometrical (physical) problems it could be interesting to know the average probability distribution for other types of BC, and the position for the incoming flow J_n^e. In this case the problem must be reformulated considering a master Hamiltonian $\mathbf{H}_{n,m}^{\mathrm{AA}}$, which in fact is quite similar to the one written in Eq. (2.6), with the only difference being its element $\mathbf{H}_{-L,-L}^{\mathrm{AA}}=-2\omega_{-L}$. To solve this problem we need to know the Green's function for the absorbing-absorbing case, which has already been obtained in Ref. 7.

As in Sec. I, we are interested in the particular situation when $\mathbf{H}_{n,n'}^{\mathrm{AA}}$ models strong or weak site disorder. But now we consider the situation that there is an incoming flow (in general, time periodic) on the arbitrary site n^e. Thus the BC to be considered are absorbing sites $\pm(L+1)$. Other BC's could also be considered in a similar way.[18] The evolution equation for the probability $\mathbf{P}(t)_{n,n_0}$ will now read

$$\dot{\mathbf{P}}(t)_{n,n_0}=\sum_{n'}\mathbf{H}_{n,n'}^{\mathrm{AA}}\mathbf{P}(t)_{n',n_0}+\mathbf{J}_{n,n_0}^{e},\qquad(4.1)$$

where, as before, the $\mathbf{P}(t)$, $\mathbf{H}^{\mathrm{AA}}$, and $\mathbf{J}^e$ are $(2L+1)\times(2L+1)$ matrices. Here $\mathbf{J}^e(t)$ represents an incoming flow on site n^e, thus their elements are characterized by

$$\mathbf{J}_{n,n'}^{e}(t)=J^e(t)\,\delta_{n,n^e}.\qquad(4.2)$$

As before, in the Laplace representation, the formal solution of $\mathbf{P}(u)$ is

$$\mathbf{P}(u)=(u\mathbf{1}-\mathbf{H}^{\mathrm{AA}})^{-1}[\mathbf{P}(t=0)+\mathbf{J}^e(u)]$$
$$\equiv\mathbf{G}^{\mathrm{AA}}(u)[\mathbf{P}(t=0)+\mathbf{J}^e(u)],\qquad(4.3)$$

where, in general, the current $J^e(u)$, from Eq. (4.2), is a Laplace-dependent function.

The ordered Green's function[7] has elements n,m given by

$$\mathbf{G}^{\mathrm{AA}}(u)_{n,m}=B(u)K(u)[A^{|n-m|}-A^{2L+2}(A^{-(n+m)}+A^{n+m})$$
$$+A^{4L+4}(A^{-|n-m|})],\qquad(4.4)$$

where

$$A\equiv A(u)=1+\frac{u}{2\mu}-\left[\frac{u}{\mu}+\frac{u^2}{4\mu^2}\right]^{1/2},\qquad(4.5)$$

$$K(u)=(1-A^{4L+4})^{-1},\qquad(4.6)$$

$$B(u)=\frac{1}{2\mu}\left[\frac{u}{\mu}+\frac{u^2}{4\mu^2}\right]^{-1/2}.\qquad(4.7)$$

The long-time limit of this Green's function is obtained by taking the $u\to0$ limit in its Laplace representation:

$$\mathbf{G}^{\mathrm{AA}}(u)_{n,m}\cong\frac{(1+L+\min[n,m])(1+L-\max[n,m])}{2\mu(1+L)}$$
$$+\mathcal{O}(u^{3/2});\qquad(4.8)$$

here, as before, $n,m\in\mathcal{D}$.

The disordered case can now be studied by changing μ to $\mu(u)$, the effective hopping transition rate which is solution of an analogous self-consistent equation

$$\left\langle\frac{\omega-\mu(u)}{1-[\omega-\mu(u)]\mathbf{H}^0\mathbf{G}^{\mathrm{AA}}(u)}\right\rangle_{\Pi(\omega)}=0.\qquad(4.9)$$

For this particular absorbing-absorbing case, the effective hopping transition rate $\mu(u)$ has been calculated in Ref. 7. Therefore in the asymptotic regime we get from Eqs. (4.3) and (4.8) in the $u\to0$ limit

$$\langle\mathbf{P}(u)_{n,n_0}\rangle\cong\sum_m\frac{(1+L+\min[n,m])(1+L-\max[n,m])}{2\mu(u)(1+L)}$$
$$\times[\mathbf{P}(t=0)+\mathbf{J}^e(u)]_{m,n_0}.\qquad(4.10)$$

Using the matrix representation of $\mathbf{J}_{m,n}^e$ (for $J^e=$const in time) we immediately see that for weak disorder, the averaged RW distribution is nonhomogeneous on the lattice and is given by

$$\langle\mathbf{P}(t)_{n,m_0}\rangle\cong J^e\left\langle\frac{1}{\omega}\right\rangle$$
$$\times\frac{(1+L+\min[n,n^e])(1+L-\max[n,n^e])}{2(1+L)}.\qquad(4.11)$$

Model B of disorder gives

$$\langle\mathbf{P}(t)_{n,m_0}\rangle$$
$$\cong J^e|\ln t|\frac{(1+L+\min[n,n^e])(1+L-\max[n,n^e])}{2(1+L)}.\qquad(4.12)$$

Considering strong disorder, model C, we get

$$\langle\mathbf{P}(t)_{n,m_0}\rangle\cong J^e\frac{(1+L+\min[n,n^e])(1+L-\max[n,n^e])}{2(1+L)}$$
$$\times\left(\frac{L+1}{2}\right)^{-\alpha}\frac{\pi(1-\alpha)}{\sin(\pi\alpha)}t^{\alpha}.\qquad(4.13)$$

The disordered case with a time-periodic incoming flow $J^e(t)=\mathcal{A}^e-\cos\Omega t$ (at site $n^e=0$), is immediately obtained

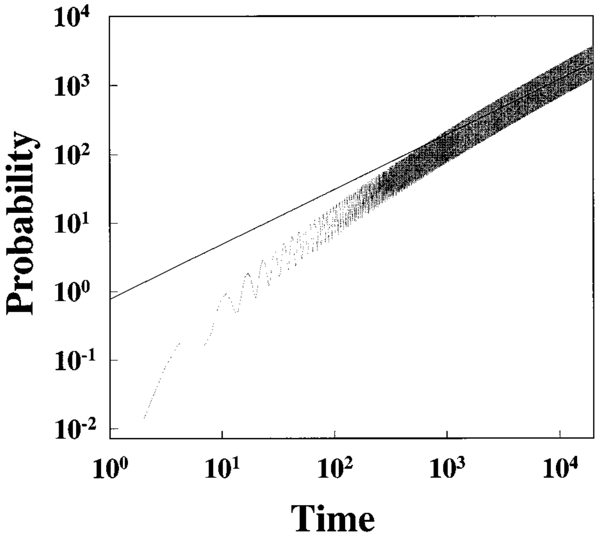

FIG. 3. Disorder-averaged RW probability distribution (over strong disorder $\alpha=0.8$) at site $n=L$, plotted as a function of time and in the presence of an external incoming time-periodic flow: $J^e(t)=2-\cos t$ (at site $n^e=0$). Note that in this plot the BC are absorbing-absorbing and the lattice has five sites (i.e., $L=2$). The continuous black line is the FEMA result and the continuous gray line is the Monte Carlo simulation with 10^5 realizations.

from Eq. (4.10) by changing $J^e \to J^e(u)=[(1/u)\mathcal{A}^e-u/(u^2+\Omega^2)]$, using the Laplace transform of Eq. (2.28). The averaged RW probability distribution inside the sample is given by

$$\langle \mathbf{P}(t)_{n,m_0}\rangle \cong \mathcal{A}^e \frac{(1+L+\min[n,0])(1+L-\max[n,0])}{2(1+L)} \times \left(\frac{L+1}{2}\right)^{-\alpha} \frac{\pi(1-\alpha)}{\sin(\pi\alpha)} t^{\alpha}; \quad (4.14)$$

here we have used strong disorder Model C. This long-time anomalous prediction has been checked with a Monte Carlo simulation. Figure 3 shows the excellent agreement between FEMA and the simulation.

The situation when the domain is $\mathcal{D}_1=[1,L_1]$ instead of $\mathcal{D}=[-L,L]$ can also be analyzed in a similar way as we have shown in Eq. (3.4).

V. CONCLUSIONS

The topic addressed here was the study of diffusion in a finite disordered 1D lattice, in presence of a time-dependent incoming flow J^e. Disorder was represented by random variables appearing in the master equation matrix $\mathbf{H}$. This matrix was split into a disordered and an ordered part. The fairly general method FEMA, based on projection-operator techniques and Terwiel's cumulant, was generalized to tackle some special boundary conditions required for the present physical problem. This method was applied in detail to the side-disorder model (weak and strong) but can also be applied to other models of disorder.

The inhomogeneous averaged probability distribution $\langle \mathbf{P}(t)_{n,m_0}\rangle$ was characterized in its long-time asymptotic regime. We have used arbitrary initial condition on $\mathbf{P}(t)$ and external incoming flow, which let us apply our method to different dynamical models of $J^e(t)$. Particular importance was put on the case when the flow $J^e(t)$ is periodic in time. In that case the asymptotic probability $\langle \mathbf{P}(t)_{n,m_0}\rangle$ was also characterized depending on the degree of disorder.

In the strong disorder case (Model C), and when the incoming external flow (applied on the left side of $\mathcal{D}$) is time periodic [i.e., $J^e(t)=\mathcal{A}^e-\cos\Omega t$] an anomalous long-time behavior was found: $\langle \mathbf{P}(t)_{n,m_0}\rangle \sim t^{\alpha}$. Note that for weak disorder the expected probability current on the right side of $\mathcal{D}$ should be constant. This method provides a very clear mechanism for characterizing (experimentally) the presence of strong disorder on the sample. In general, and for any arbitrary time-periodic incoming flow, the degree of disorder (into the sample) can be characterized by measuring the slope of the log-log plot $\langle \mathbf{P}(t)_{n,m_0}\rangle$ as a function of time. For the weak disorder case the present approach gives, immediately, the quantity $\langle 1/\omega\rangle$ by analyzing the current probability given in Eq. (2.24). Thus the transport of photogenerated carriers through a porous network, consisting of nanometer sized particles,[12] can theoretically be studied by the present approach. Work along this line is in progress and will be presented elsewhere.

Also the problem of the first passage time through one frontier $(+L)$ was revisited. The exact behavior of the averaged mean first passage time was found. Generalizations to other domains such as $\mathcal{D}=[1,L_1]$ was also given. As was reported before in a related problem,[7] models B and C of disorder predict a divergence in the averaged mean first passage time $\langle T_n\rangle$.

In this paper we presented a diagrammatic calculation scheme which fully incorporates the effects coming from the disorder on a random walk in a finite lattice, and in presence of an external incoming flow. The present generalization of FEMA was introduced to take into account the nonperturbative effects appearing with the issue of strong disorder. A formal self-consistent perturbation theory (in the small-u Laplace variable) was presented for the particular situation when the boundary conditions are reflecting-absorbing. The reflecting boundary condition introduces some difficulties in the formulation of the perturbation theory, nevertheless we have overcome this issue by characterizing the error $\mathcal{O}(u^2)$ introduced in the calculation of the propagator $\mathcal{J}_{n,m}$ appearing in the perturbation around FEMA. Thus, this method gives a systematic (in small u) procedure to work out reflecting boundary conditions.

We have proof (in Appendix C) that FEMA gives the exact leading behavior, in the small-u parameter, for models of disorder A and B. We also proved that for model C (strong disorder), FEMA gives the exact power low (long-time tail) and got the exact $\mathcal{O}(u^{\alpha})$ correction to the calculation of the coefficient—which is overestimated by FEMA. The mathematical details can be found in Appendixes A, B, and C.

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APPENDIX A: THE GREEN'S FUNCTION FOR THE REFLECTING-ABSORBING CASE

The problem of solving a finite-dimensional Green's function such as $\mathbf{G}^{\mathrm{RA}}(t|0)$ with reflecting BC (between $\{-L-1,-L\}$) and absorbing BC (at $n=L+1$) is reduced to that of solving Eq. (2.17) with the infinite-dimensional operator $\mathbf{H}^0=[\mathbf{E}^+ +\mathbf{E}^- -2]$ with suitable BC's. The RW method of the images consists of summing to the free Green's function $\mathbf{G}^0_{nm}(t|0)$, with indices in $\mathcal{D}$, terms of the form $\pm\mathbf{G}^0_{km}(t|0)$ with k being the specular images of n with respect to the boundary considered. In the case of the reflecting BC the images must be positive, and should be negative through an absorbing mirror. From this fact it is possible to see that the reflecting-absorbing BC's are satisfied if we write

$$\begin{aligned}\mathbf{G}^{\mathrm{RA}}_{n,m}=\mathbf{G}^0_{0,0}&+\sum_{k=0}^{\infty}(-1)^k\mathbf{G}^0_{n+(2L+1)+k(4L+3),-m}\\&+\sum_{k=1}^{\infty}(-1)^k\mathbf{G}^0_{-n+k(4L+3),-m}\\&+\sum_{k=0}^{\infty}(-1)^{k+1}\mathbf{G}^0_{2L+2+k(4L+3)-n,m}\\&+\sum_{k=1}^{\infty}(-1)^k\mathbf{G}^0_{n+k(4L+3),m}.\end{aligned}\tag{A1}$$

Using the fact that the free Green's function (in time representation) is given by

$$\mathbf{G}^0_{nm}(t|t')=\exp[-2\mu(t-t')]I_{|n-m|}[2\mu(t-t')];\tag{A2}$$

here $I_{|r|}(\tau)$ is a modified Bessel function. In the Laplace representation $(t\to u)$ the sum (A1) can be evaluated. Thus we obtain for the Laplace transformed Green's function $\mathbf{G}^{\mathrm{RA}}(u)_{n,m}$ in the interval $[-L,L]$ the expression (2.10). From Eq. (A1) it is possible to see that the BC at $n=L+1$ is fulfilled: $\mathbf{G}^{\mathrm{RA}}(u)_{L+1,m}=0$. The reflecting BC is satisfied by the mirror construction located midway between $-(L+1)$ and $-L$.

Another important quantity in the context of Terwiel's cumulant theory is the propagator $\mathcal{J}(u)_{n,m}\equiv\mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(u)_{n,m}$. From Eq. (A1) this quantity can be calculated. In the asymptotic regime, operating $[\mathbf{E}^+ +\mathbf{E}^- -2]$ on $\mathbf{G}^{\mathrm{RA}}(u)$ we get

$$\mathcal{J}(u)_{n,m}=-\frac{1}{\mu}\delta_{n,m}+\frac{1+L-\max(n,m)}{\mu^2}\,u+\mathcal{O}(u^2).\tag{A3}$$

In order to work out an effective-medium perturbation theory for the reflecting-absorbing problem, it is useful to know the asymptotic behavior of $\Delta\mathbf{G}^{\mathrm{RA}}(u)_{-L,m}\equiv\mathbf{G}^{\mathrm{RA}}(u)_{-L-1,m}-\mathbf{G}^{\mathrm{RA}}(u)_{-L,m}$. From Eq. (A1) it is possible to see that its long-time regime is characterized by

$$\begin{aligned}\Delta\mathbf{G}^{\mathrm{RA}}(u)_{-L,m}=[&L^5(361)+L^4(1425-285m)+L^3(2265\\&-800m-110m^2)+L^2(1815-855m\\&-270m^2+30m^3)+L(734-410m-225m^2\\&+40m^3+5m^4)+(120-74m-65m^2\\&+15m^3+5m^4-m^5)]u^2+\mathcal{O}(u^3).\end{aligned}\tag{A4}$$

APPENDIX B: FEMA FOR REFLECTING-ABSORBING BC

It was shown in the context of the FPTD (Ref. 7) that strong disorder introduces nonperturbative effects which need further rearrangement when compared to a perturbation theory for weak disorder. In order to establish whether the present FEMA gives the exact result for the small-u behavior of $\langle\mathbf{P}(u)_{n,n_0}\rangle$ we need to know some properties of the Terwiel cumulants[14] appearing in the diagrammatic perturbation theory (see Appendix C). Here we are going to sketch FEMA for reflecting-absorbing BC.

Following past experience[7] we propose to do a sort of perturbative analysis around an effective medium to study the u dependence of $\langle\mathbf{G}^{\mathrm{RA}}(u)_{n,n_0}\rangle$. First of all, we write the disordered version of Eq. (2.17) in the Laplace representation, adding and subtracting a homogeneous mean-field term $\Lambda[\mathbf{E}^+ +\mathbf{E}^- -2]^{\mathrm{RA}}\equiv\Lambda\mathbf{H}^D$, Λ being an arbitrary effective rate to be determined below:

$$\begin{aligned}u\mathbf{P}(u)_{n,m}-\mathbf{P}(t=0)_{n,m}=&\Lambda[\mathbf{E}^+ +\mathbf{E}^- -2]^{\mathrm{RA}}\mathbf{P}(u)_{n,m}\\&+[\mathbf{E}^+ +\mathbf{E}^- -2]^{\mathrm{RA}}(\mu+\xi_n-\Lambda)\\&\times\mathbf{P}(u)_{n,m}.\end{aligned}\tag{B1}$$

Here we understand that the notation $\mathbf{E}^{\pm}\xi_n\mathbf{P}(u)_{n,m}=\xi_{n\pm1}\mathbf{P}(u)_{n\pm1,m}$. The superscript RA is put in order to remark that we are working in a finite-lattice with reflecting-absorbing BC. In order to compare Eq. (B1) with Eq. (2.5), for $\mathbf{J}^e=0$, note that $\mu+\xi_n=\omega_n$, i.e., Eq. (B1) corresponds to a site disorder model where ξ_n, with $m\in D$, are statistical independent random variables with mean value zero, and preserving the positive condition $\omega_n\geqslant0$.

By defining the quantities $\eta_n=\omega_n-\Lambda$, we can rewrite Eq. (B1) in time representation:

$$\partial_t\mathbf{P}(t)=[\Lambda\mathbf{H}^D+\Theta_D]\mathbf{P}(t).\tag{B2}$$

Here

$$\Theta_D\mathbf{P}(t)_{n,m}=[\mathbf{E}^+ +\mathbf{E}^- -2]^{\mathrm{RA}}\eta_n\mathbf{P}(t)_{n,m}\equiv\mathbf{H}^D\eta_n\mathbf{P}(t)_{n,m}.$$

The average of Eq. (B2) over the realization of η_n leads to and effective evolution equation (non-Markovian). This average can formally be carried out introducing a projector operator $\mathcal{P}$ that averages over the disorder:[7]

$$\langle\mathbf{P}\rangle=\mathcal{P}\mathbf{P},\quad\mathbf{P}=\langle\mathbf{P}\rangle+(1-\mathcal{P})\mathbf{P}.\tag{B3}$$

A close exact evolution equation can be obtained operating with this projector technique:

$$\partial_t\langle \mathbf{P}(t)\rangle = \Lambda \mathbf{H}^D\langle \mathbf{P}\rangle + \left\langle \sum_{k=0}^{\infty} [\Theta_D \mathbf{M}(1-\mathcal{P})]^k \Theta_D \right\rangle \langle \mathbf{P}\rangle, \tag{B4}$$

where $\mathbf{M}$ is a finite-dimensional convolution operator:

$$[\mathbf{ML}(t)]_n \equiv \sum_m \int_0^t dt' \, \mathbf{G}^{\mathrm{RA}}_{n,m}(t|t')\mathbf{L}_m(t'). \tag{B5}$$

Equation (B4) requires that the statistics of the random variable η_n for each particular model are specified. Note that Eq. (B4) contains the Green's function on a finite domain $\mathcal{D}$ with reflecting-absorbing BC [i.e., Eq. (2.17) with $\mu \to \Lambda$]. Introducing Terwiel's cumulant of the random variable η_n, using past experience and the explicit form of Θ_D and $\mathbf{H}^D$, we can rewrite the evolution equation (B4) (in Laplace representation) in the following way:

$$u\langle \mathbf{P}(u)_{n,m_0}\rangle - \mathbf{P}(t=0)_{n,m_0}$$
$$\simeq \Lambda \mathbf{H}^D \langle \mathbf{P}(u)_{n,m_0}\rangle + \sum_{p=0}^{\infty} \sum_{n_1\neq n; n_2\neq n_1;\cdots;n_p\neq n_{p-1}} \times \langle \Psi_n \Psi_{n_1}\cdots\Psi_{n_p}\rangle_T \times \mathcal{J}_{n,n_1}\mathcal{J}_{n_1,n_2}\cdots\mathcal{J}_{n_{p-1},n_p}\mathbf{H}^D\langle \mathbf{P}(u)_{n_p,m_0}\rangle, \tag{B6}$$

where the random operator $\Psi_n \equiv \Psi_n(\Lambda,u)$—acting on the right—has been defined as in Ref. 7 and the indices $n_p \in \mathcal{D}$:

$$\Psi_k(\Lambda,u) = \mathcal{M}_k(\Lambda,u) - \frac{\mathcal{M}_k(\Lambda,u)\mathcal{J}_{k,k}(\Lambda,u)}{1+\langle \mathcal{M}_k(\Lambda,u)\rangle \mathcal{J}_{k,k}(\Lambda,u)} \times \mathcal{P}\mathcal{M}_k(\Lambda,u) \tag{B7}$$

with

$$\mathcal{M}_k(\Lambda,u) \equiv \frac{\eta_k}{1-\eta_k \mathcal{J}_{k,k}(\Lambda,u)}. \tag{B8}$$

Note that $\eta_k \equiv \eta_k(u)$ through the implicit dependence on Λ. The propagator $\mathcal{J}_{n,n_1} \equiv \mathcal{J}_{n,n_1}(\Lambda,u) = \mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{n,n_1}$ is given in terms of the free Green's function $\mathbf{G}^{\mathrm{RA}}$. We remark that in Eq. (B4) the true propagator is $\mathcal{J}_{n,n_1}(\Lambda,u) = \mathbf{H}^D\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{n,n_1}$, but in Eq. (B6) $\mathbf{H}^D$ has been replaced by $\mathbf{H}^0$ in the definition of $\mathcal{J}_{n,n_1}$. Noting that the indices n_p in the sum (B6) run from $-L$ to L, and that the absorbing BC on $n=L+1$ ensures that $\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{L+1,n}=0$, we see that we can use $\mathcal{J}_{n,n_1}(\Lambda,u) = \mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{n,n_1}$. Nevertheless the reflecting BC on the right frontier of the domain $\mathcal{D}$ does not allow for this replacement. This is in remarkable contrast to the case studied in Ref. 7 where the absorbing-absorbing BC allowed for the simplification $\mathbf{H}^D \to \mathbf{H}^0$. Therefore, in order to be able to continue with the present perturbation theory, we ought to justify this replacement.

It is possible to check that the error introduced by doing this replacement is of $\mathcal{O}(u^2)$. To see this, note that the difference between $\mathcal{J}_{n,n_1}(\Lambda,u) = \mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{n,n_1}$ and $\mathcal{J}_{n,n_1}(\Lambda,u) = \mathbf{H}^D\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{n,n_1}$ is characterized by $\Delta\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{-L,m}$. Thus from Eq. (A4) we see that this quantity is of $\mathcal{O}(u^2)$. The steps made so far are formally the same as those realized in Ref. 7 for the problem of averaging the survival probability to obtain the MFPT to leave the domain $[-L,L]$. In that paper a diagrammatic analysis of the perturbation series was introduced. We remark that by the introduction of the random operator $\Psi_n(\Lambda,u)$, we have summed up all the terms containing the diagonal parts $\mathcal{J}_{n,n}(\Lambda,u) \equiv \mathcal{J}_{n,n}$. This is equivalent to one-loop perturbation in field theory. Nevertheless note that in the present paper Eq. (B6) is only an approximation, so this is different when compared with original FEMA theory.[7] Terwiel's diagrams allow us to realize that the best election for Λ (the still undefined mean field) is that given by the solution $\langle \Psi_n(\Lambda,u)\rangle = 0$. This is the best choice in the sense that it allows the vanishing of an infinite number of diagrams. In the present physical problem it is impossible to have $\langle \Psi_n(\Lambda,u)\rangle = 0$ for all the values of n because the BC implicit in the construction of $\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{n,n_1}$ destroys the translational invariance (see Appendix A). Nevertheless, we can tentatively define Λ by $\langle \Psi_n(\Lambda,u)\rangle = 0$ at some particular site n, and after this explore the consequences of such an election.

In the following, Λ will be taken as the solution of

$$\langle \Psi_0(\Lambda,u)\rangle = 0. \tag{B9}$$

It will turn out that this election is a very convenient one because, although it does not produce a drastic simplification to the diagrams appearing in Eq. (B6), it makes an approach related to EMA useful.[5] The analogous approximation in the present problem would consist of reducing Eq. (B6) to

$$u\langle \mathbf{P}(u)\rangle - \mathbf{P}(t=0) = \Lambda \mathbf{H}^D \langle \mathbf{P}(\mathbf{u})\rangle,$$

with Λ defined by Eq. (B9) or, more explicitly, using Eqs. (B7), (B8), and $\eta_0 = \omega_0 - \Lambda$:

$$\left\langle \frac{\omega_0 - \Lambda}{1-(\omega_0-\Lambda)\mathcal{J}_{00}(\Lambda,u)} \right\rangle_{\Pi(\omega)} = 0, \tag{B10}$$

which is Eq. (2.16) after we identify $\Lambda \equiv \mu(u)$, $\omega_0 \equiv \omega$, and $\mathcal{J}_{00}(\Lambda,u) = (\mathbf{E}^+ + \mathbf{E}^- - 2)\mathbf{G}^{\mathrm{RA}}(\Lambda,u)_{0,0} \equiv \mathbf{H}^0\mathbf{G}^{\mathrm{RA}}(u)_{0,0}$.

APPENDIX C: ANALYSIS OF CORRECTIONS TO THE FEMA WITH REFLECTING-ABSORBING BC

In this appendix we study Eq. (B6) in order to establish whether the FEMA (for reflecting-absorbing BC) gives the exact result for the small-u behavior of $\langle \mathbf{P}(u)_{n,m_0}\rangle$. To this end we need to use some properties[14] of Terwiel's cumulant:

$$\langle \Psi_n \Psi_{n_1}\cdots\Psi_{n_p}\rangle_T \equiv \mathcal{P}\Psi_n\mathcal{P}(1-\mathcal{P})\Psi_{n_1}(1-\mathcal{P})\cdots(1-\mathcal{P})\Psi_{n_p}, \tag{C1}$$

appearing in Eq. (B6). Using the definition of the random operator Ψ_n, it is possible to see that there exists a cluster structure in terms of Terwiel's cumulant and moments.[7]

For the moments of Ψ_n [see Eqs. (B7) and (B8)] we show some explicit examples,

$$\langle \Psi_1\rangle = \langle \mathcal{M}_1\rangle - \langle \mathcal{M}_1\rangle \mathcal{N}_1 \langle \mathcal{M}_1\rangle, \tag{C2}$$

$$\langle\Psi_1\Psi_2\rangle=\langle\mathcal{M}_1\mathcal{M}_2\rangle-\langle\mathcal{M}_1\rangle\mathcal{N}_1\langle\mathcal{M}_1\mathcal{M}_2\rangle-\langle\mathcal{M}_1\mathcal{M}_2\rangle\mathcal{N}_2\langle\mathcal{M}_2\rangle+\langle\mathcal{M}_1\rangle\mathcal{N}_1\langle\mathcal{M}_1\mathcal{M}_2\rangle\mathcal{N}_2\langle\mathcal{M}_2\rangle, \tag{C3}$$

$$\begin{aligned}\langle\Psi_1\Psi_2\Psi_3\rangle=&\langle\mathcal{M}_1\mathcal{M}_2\mathcal{M}_3\rangle-\langle\mathcal{M}_1\rangle\mathcal{N}_1\langle\mathcal{M}_1\mathcal{M}_2\mathcal{M}_3\rangle\\&-\langle\mathcal{M}_1\mathcal{M}_2\rangle\mathcal{N}_2\langle\mathcal{M}_2\mathcal{M}_3\rangle\\&-\langle\mathcal{M}_1\mathcal{M}_2\mathcal{M}_3\rangle\mathcal{N}_3\langle\mathcal{M}_3\rangle\\&+\langle\mathcal{M}_1\rangle\mathcal{N}_1\langle\mathcal{M}_1\mathcal{M}_2\rangle\mathcal{N}_2\langle\mathcal{M}_2\mathcal{M}_3\rangle\\&+\langle\mathcal{M}_1\mathcal{M}_2\rangle\mathcal{N}_2\langle\mathcal{M}_2\mathcal{M}_3\rangle\mathcal{N}_3\langle\mathcal{M}_3\rangle\\&+\langle\mathcal{M}_1\rangle\mathcal{N}_1\langle\mathcal{M}_1\mathcal{M}_2\mathcal{M}_3\rangle\mathcal{N}_3\langle\mathcal{M}_3\rangle\\&-\langle\mathcal{M}_1\rangle\mathcal{N}_1\langle\mathcal{M}_1\mathcal{M}_2\rangle\mathcal{N}_2\langle\mathcal{M}_2\mathcal{M}_3\rangle\mathcal{N}_3\langle\mathcal{M}_3\rangle,\end{aligned} \tag{C4}$$

etc., where we have defined

$$\mathcal{N}_k\equiv\frac{\mathcal{J}_{k,k}(\Lambda,u)}{1+\langle\mathcal{M}_k\rangle\mathcal{J}_{k,k}(\Lambda,u)}. \tag{C5}$$

In order to know the Terwiel cumulant $\langle\Psi_1\Psi_2\Psi_3\rangle_T$ we have to use Eqs. (C2)–(C4) in the cluster (C1) itself. Due to the fact that the Green's function breaks the translational invariance there is not a drastic simplification (in Terwiel's diagrams) by demanding the FEMA condition, i.e., $\langle\Psi_n\rangle_T \neq 0$ if $n\neq 0$. For example,

$$\langle\Psi_1\Psi_2\Psi_3\rangle_T=\langle\Psi_1\Psi_2\Psi_3\rangle-\langle\Psi_1\rangle\langle\Psi_2\Psi_3\rangle-\langle\Psi_1\Psi_2\rangle\langle\Psi_3\rangle+\langle\Psi_1\rangle\langle\Psi_2\rangle\langle\Psi_3\rangle.$$

For more details see Ref. 7.

Following past experience we introduce a convenient expression for $\mathcal{M}_n$ in Eq. (B8):

$$\mathcal{M}_n=[\Lambda+\mathcal{R}_n]\frac{\omega_n-\Lambda}{\omega_n+\mathcal{R}_n}, \tag{C6}$$

where we have used $\eta_n=\omega_n-\Lambda$ and the definition

$$\mathcal{R}_n=-\Lambda-\frac{1}{\mathcal{J}_{nn}}\simeq(L+1-n)u+\mathcal{O}(u^2)\equiv g_nu+\cdots. \tag{C7}$$

Note that in the asymptotic behavior we have assumed, $\lim_{u\to 0}(u/\Lambda)\to 0$. This fact is true for all types of disorder considered in this paper. In order to estimate the contribution coming from the *diagrammatic* terms of Eq. (B6) we have to evaluate

$$\langle\Psi_n\Psi_{n_1}\cdots\Psi_{n_p}\rangle_T\mathcal{J}_{n,n_1}\mathcal{J}_{n_1,n_2}\cdots\mathcal{J}_{n_{p-1},n_p}\quad \text{if } p\neq 0,$$
$$\langle\Psi_n\rangle\quad \text{if } p=0. \tag{C8}$$

If these contributions are smaller than $\Lambda\equiv\mu(u)$, FEMA would not need any correction from diagrams with $p\geqslant 0$.

Even when the indices n_l run from $-L$ to L there exists an infinite number of those diagrams with different values of p. Among these diagrams, all of them with different vertices will vanish due to the Terwiel property (for example, if $p=1$, we get $\langle\Psi_n\Psi_{n_1}\rangle_T=0$ because of the statistical independence for $n\neq n_1$). Therefore we will only be interested in Terwiel's cumulant of the type

$$\text{for } p=0,\ \langle\Psi_n\rangle_T\neq 0\quad \text{if}\quad n\neq 0,$$
$$\text{for } p=2,\ \langle\Psi_n\Psi_1\Psi_n\rangle_T\neq 0,$$
$$\text{for } p=3,\ \langle\Psi_n\Psi_1\Psi_n\Psi_1\rangle_T\neq 0,\ \langle\Psi_n\Psi_1\Psi_2\Psi_n\rangle_T\neq 0,\ \text{etc.} \tag{C9}$$

Note from Eq. (B6) that index n is fixed, so in Eq. (C9), repeated natural indices mean that they must be summed with the corresponding $\mathcal{J}_{n_1,n_2}$ (nice drawings of these diagrams can also be designed, for example, in a similar context; see Ref. 5).

Due to the fact that the present demonstration is similar to the one given in Ref. 7, we shall only give here a swift proof for models A, B, and C of disorder.

Weak disorder. In this case and from Eq. (B10),

$$\Lambda\equiv\mu(u\to 0)\simeq(\beta_1)^{-1}\left[1+(L+1)\left(\frac{\beta_2-(\beta_1)^2}{\beta_1}\right)u\right]+\mathcal{O}(u^2). \tag{C10}$$

Remember that $\beta_k\equiv\langle 1/\omega^k\rangle$ is finite for all k.

From the definitions (B7), (B8), and (C8) it is possible to see that the first important diagram is

$$\langle\Psi_n\rangle_T\sim-\frac{\beta_2-(\beta_1)^2}{\beta_1}\ nu+\mathcal{O}(u^2), \tag{C11}$$

so the correction $p=0$ is beyond FEMA because $\Lambda\equiv\mu(u=0)\sim\mathcal{O}(u^0)$. Note that Eq. (C11) is in agreement with the self-consistent condition $\langle\Psi_0(\Lambda,u)\rangle_T=0$.

The general analysis of correction comes from the following considerations. For this case $\mu(u)\sim\mathcal{O}(u^0)$, thus from Eq. (A3) $\mathcal{J}_{n_1,n_2}\sim\mathcal{O}(u^1)$ for $n_1\neq n_2$, and $\mathcal{N}_n\sim\mathcal{O}(u^0)$. From Eqs. (C6) and (C7) it follows that $\langle\mathcal{M}_n^N\rangle\sim\mathcal{O}(u^0)$ for all N, therefore Terwiel's cumulants, such as (C9), are of $\mathcal{O}(u^0)$ [see Eqs. (C2)–(C4)]. With all this information we can see from Eq. (C8) that any corrections from $p\neq 0$ are of $\mathcal{O}(u^p)$. Then FEMA is the dominant contribution for weak disorder. Due to the fact that the diagram for $p=1$ vanishes, we see that the first correction ($p=0$) beyond FEMA—and consistent with the analysis of reflecting-absorbing BC—is given by Eq. (C11). The contribution $p=2$ cannot be considered in this case because the error introduced in Eq. (B6) was $\mathcal{O}(u^2)$, as we noted in Eq. (A4). Therefore, for weak disorder FEMA gives the exact leading order. On the other hand, the present approach allows us to go beyond FEMA. For model A and up to $\mathcal{O}(u)$ the long-time evolution equation is characterized by

$$u\langle\mathbf{P}(u)_{n,m_0}\rangle-\mathbf{P}(t=0)_{n,m_0}=\left[\beta_1^{-1}-\frac{\beta_2-(\beta_1)^2}{\beta_1}\ nu\right]\times\mathbf{H}^D\langle\mathbf{P}(u)_{n,m_0}\rangle. \tag{C12}$$

From Eq. (C12) we see that at $\mathcal{O}(u)$, the variance of the quenched disorder turns out to be important. The correction to go beyond FEMA, Eq. (C12), introduces explicit n dependence in the coefficient of the finite master equation; nevertheless, standard methods[17] can be used to tackle Eq. (C12). A similar situation appeared in the study of the FPTD in presence of bias.[9]

Disorder model B. For this case using Eq. (B10) we get

$$\Lambda \equiv \mu(u\sim 0) \simeq \frac{1}{|\ln u|}\left(1+\frac{\ln g_0}{|\ln u|}+\cdots\right), \qquad \text{(C13)}$$

with g_0 defined in Eq. (C7). From Eq. (A3) we get

$$\mathcal{J}(u)_{n,m} \simeq -\frac{1}{\Lambda}\delta_{n,m}+\frac{1+L-\max(n,m)}{\Lambda^2}\;u+\mathcal{O}(u^2). \qquad \text{(C14)}$$

Thus, from Eq. (C5) in the small-u limit we obtain

$$\mathcal{N}_n \simeq -\left(\frac{1}{\Lambda}+\ln\frac{g_n}{g_0}+\cdots\right). \qquad \text{(C15)}$$

In general for model B, using Eqs. (C6) and (C7) it is possible to see that

$$\langle \mathcal{M}_n\rangle \simeq \Lambda^2 \ln\frac{g_n}{g_0} = \frac{1}{|\ln u|^2}\ln\left(1-\frac{n}{L+1}\right),$$

$$\langle \mathcal{M}_n^N\rangle \simeq u(-\Lambda^2/u)^N. \qquad \text{(C16)}$$

Note that $\langle \mathcal{M}_n\rangle$ is in agreement with the self-consistent condition $\langle \Psi_0(\Lambda,u)\rangle_T = \langle \mathcal{M}_0\rangle - \mathcal{N}_0\langle \mathcal{M}_0\rangle^2 = 0$. Using Eqs. (C13)–(C16), it is possible to see that the leading contribution (for small u) in the type of diagrams appearing in Eq. (C9) are characterized [see Eqs. (C2)–(C4)] for the mean values

$$\langle \mathcal{M}_{n_0}\mathcal{M}_{n_0}\cdots \mathcal{M}_{n_2}\mathcal{M}_{n_2}\cdots \mathcal{M}_{n_p}\mathcal{M}_{n_p}\rangle \sim \langle \mathcal{M}_{i_1}^{m_1}\rangle\langle \mathcal{M}_{i_2}^{m_2}\rangle\cdots\langle \mathcal{M}_{i_I}^{m_I}\rangle \sim u^I(\Lambda^2/u)^{p+1}, \quad \text{(C17)}$$

in which only I of the indices $\{n_0,n_1,\cdots,n_p\}$ are different $(\Sigma_j{}^I m_j = p+1)$. Thus, using Eqs. (C14) and (C17) we prove that the order of correction in Eq. (C8) is

$$\sim u^I(\Lambda^2/u)^{p+1}(u/\Lambda^2)^p = \mathcal{O}[u^I(\Lambda^2/u)] \quad \text{if } p\geqslant 2,$$

$$\mathcal{O}\left(\Lambda^2\ln\frac{g_n}{g_0}\right) \quad \text{if } p=0. \qquad \text{(C18)}$$

This means that FEMA gives the exact leading contribution for small u. Note that for $p\geqslant 2$ the corrections are independent of p, thus in order to obtain higher systematic corrections to FEMA, an infinite number of diagrams with different values of $p\geqslant 2$ must be summed up. Beyond FEMA and up to $\mathcal{O}(\Lambda^2)$—for model B—we should consider the long-time evolution equation

$$u\langle \mathbf{P}(u)_{n,m_0}\rangle - \mathbf{P}(t=0)_{n,m_0} = \frac{1}{|\ln u|}\left[1+\frac{1}{|\ln u|}\ln\left(1-\frac{n}{L+1}\right)\right] \times \mathbf{H}^D\langle \mathbf{P}(u)_{n,m_0}\rangle. \qquad \text{(C19)}$$

Strong disorder model C. For this case, using Eq. (B10) and taking the average in Eq. (C6) with care, it is possible to see that

$$\Lambda \equiv \mu(u\sim 0) \simeq \frac{[R_0(u)]^\alpha}{(1-\alpha)B(1-\alpha,\alpha)} = \frac{(L+1)^\alpha}{(1-\alpha)}\frac{\sin \pi\alpha}{\pi}u^\alpha, \qquad \text{(C20)}$$

with R_0 defined in Eq. (C7) and where $B(x,y)$ is the β function (note that the difference in the effective rate with Ref. 7 is a factor 2^α). As before we know that $\mathcal{J}(u)_{n,m}$ is given by Eq. (C14) with Λ characterized by Eq. (C20), and from Eq. (C5) $\mathcal{N}_n \sim \mathcal{O}(-1/\Lambda)$. Using Eqs. (C6) and (C7) it is possible to see that

$$\langle \mathcal{M}_n\rangle \simeq [1-(L+1)^\alpha/(L+1-n)^\alpha]\Lambda,$$

$$\langle \mathcal{M}_n^N\rangle \simeq \mathcal{O}[-(\Lambda^2/u)^N u^{1-\alpha}]. \qquad \text{(C21)}$$

Note that $\langle \mathcal{M}_n\rangle$ is in agreement with the self-consistent condition $\langle \mathcal{M}_0\rangle = 0$. From Eqs. (C20) and (C21) we can see that the leading contribution (for small u) in the moments of $\mathcal{M}_n$ are characterized for the mean value:

$$\langle \mathcal{M}_{n_0}\mathcal{M}_{n_0}\cdots \mathcal{M}_{n_2}\mathcal{M}_{n_2}\cdots \mathcal{M}_{n_p}\mathcal{M}_{n_p}\rangle \sim (\Lambda^2/u)^{p+1}u^{I(1-\alpha)}, \qquad \text{(C22)}$$

in which only I of the indices $\{n_0,n_1,\ldots,n_p\}$ are different $(\Sigma_j{}^I m_j = p+1)$.

We remark that now there is a difference with model B; here all the partitions appearing in the moments such as $\langle \Psi_{n_0}\Psi_{n_1}\cdots\Psi_{n_p}\rangle$ are of the same order. See, for example, Eqs. (C2)–(C4). Thus a specific coefficient must be considered in front of a term such as $\langle \mathcal{M}_{n_0}\mathcal{M}_{n_1}\cdots\mathcal{M}_{n_p}\rangle$.

Using Eqs. (C14) [with Λ given by Eqs. (C20)] and (C22) we prove that the corrections in Eq. (C8) are of the order

$$\sim u^{I(1-\alpha)}(\Lambda^2/u)^{p+1}(u/\Lambda^2)^p = \mathcal{O}[(\Lambda^2/u)u^{I(1-\alpha)}] \quad \text{if } p\geqslant 2,$$

$$\mathcal{O}(\Lambda) \quad \text{if } p=0. \qquad \text{(C23)}$$

This means that FEMA gives the correct power low for small u but, as we have remarked before, its coefficient needs a correction from the diagram corresponding to $p=0$. For $p\geqslant 2$ the corrections are independent of p, thus in order to obtain higher systematic corrections in u an infinite number of diagrams with different values of p must be summed up.

In order to estimate the importance of the correction in the coefficient of FEMA—for strong disorder model C—we should solve the equation which contains the whole dominant $\mathcal{O}(u^\alpha)$ dependence:

$$u\langle \mathbf{P}(u)_{n,m_0}\rangle - \mathbf{P}(t=0)_{n,m_0} = \Lambda\left\{1+\left[1-\left(\frac{L+1}{L+1-n}\right)^{\alpha}\right] + \left[1-\left(\frac{L+1}{L+1-n}\right)^{\alpha}\right]^2\right\}\mathbf{H}^D\langle \mathbf{P}(u)_{n,m_0}\rangle. \quad \text{(C24)}$$

This last expression has been obtained by considering the Terwiel cumulant $\langle\Psi_n\rangle_T = \langle\mathcal{M}_n\rangle - \langle\mathcal{M}_n\rangle\mathcal{N}_n\langle\mathcal{M}_n\rangle$ in the diagrammatic representation (C8).

Previous experience has also shown similar conclusions.[7] For the present problem and in the case $(\alpha\approx 0.8)$ the error introduced in the coefficient was about 19% for a lattice of $L=1$. This fact can be seen in our figures where the agreement with the power law is excellent, but there is a little constant shift when compared with the Monte Carlo simulations.

Thus we have finished the proof that for reflecting-absorbing BC problems, FEMA gives the correct leading small-u behavior of $\langle \mathbf{P}(u)_{n,m_0}\rangle$ (for all the types of disorder considered in this paper).

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[16] If $\mathbf{J}^e(t) = J^e(t)\delta_{n,n^e}$ were negative (at any time), it would mean that we should have the possibility to extract particles from site n^e. In this paper we are only interested on injecting particles into the lattice, thus $J^e(t)$ is always positive, therefore $\mathcal{A}^e > 1$.

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[18] For example, for the case when there is some incoming flow J_n^e at site n^e and the lattice has reflecting-reflecting BC. The same procedures can be followed and then we can see interesting phenomena appearing on the averaged RW probability distribution. Work along this line will be presented in the future.