RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 41, NUMBER 8 15 APRIL 1990

Characterizing strong disorder by the divergence of a diffusion time

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(Received 11 August 1989)

We propose to characterize strong disorder and the degree of disorder (in anomalous diffusion problems) by the divergence and the divergence law, respectively, of the mean first passage time to leave an arbitrary interval of finite size. Exact results for the exponents and amplitudes characterizing the divergence are given for certain models.

A stochastic process $x(t)$ admits, in general, two complementary descriptions. In the first one (most often used), the process is described by the time-dependent statistical properties of the variable x. A second alternative is to look for the statistical properties of the time t at which the process $x(t)$ reaches a prescribed value L from a given initial condition for the first time. This corresponds to focusing on the inverse stochastic function of $x(t)$, $t(x)$, which is characterized by a first-passage-time distribution (FPTD).[1] The second alternative emphasizes the role of the individual realizations of the process.

The problem of transport in disordered media[2] modeled by random walk (RW) in a chain with quenched disorder has usually been characterized by the time-dependent behavior of $\langle x^2\rangle$. Anomalous diffusion of the subdiffusive type, in which $\langle x^2\rangle$ grows slower than linearly with time, is found in several cases. A hierarchy of disorder can be associated with the different asymptotic laws in time for $\langle x^2\rangle$. For weak disorder [model A of Ref. 2(a)], $\langle x^2\rangle \approx t$, but with a diffusion constant modified by the disorder. For strong disorder [model C of Ref. 2(a)], $\langle x^2\rangle \approx t^\delta$, $\delta<1$, and $\delta=0$ in the extreme case in which configurations with perfectly absorbing sites are allowed. Intermediate cases are model B of Ref. 2(a) with $\langle x^2\rangle \approx t/\ln t$ and the Sinai model[3] with $\langle x^2\rangle \approx (\ln t)^4$. A natural question which we address here is the study of RW in a disordered chain by the passage times, characterizing anomalous diffusion and the degree of disorder by a FPTD.

Such a question corresponds to the meaningful physical problem of the time that a particle takes to leave a given interval in the presence of disorder. A naive answer to the problem is to invert the function $\langle x^2\rangle(t)$ obtaining $t\approx L^{2/\delta}$ for strong disorder. This generally does not give a correct answer due to the importance of the tails of the FPTD. In particular, configurations of the disorder with small statistical weight can dominate the average passage time.

While transport in chains with quenched disorder is a problem of long-lasting interest, it is only recently that a few attempts at characterization in terms of a FPTD have been reported.[4-7] A different but related problem for which a FPTD characterization has been used is that of calculating the survival probability for normal diffusion in a medium with randomly distributed traps.[2(c)] Our results here are for a model defined by a master equation describing RW in an infinite disordered chain

$$\partial_t P_n(t) = (E^+ + E^- - 2)\omega_n P_n(t)\,, \qquad (1)$$

where $P_n(t)$ is the probability of finding the walker at site n at time t. $E^\pm$ are shift operators such that $E^\pm P_n = P_{n\pm1}$. The quantities ω_n are independent random variables with a given probability distribution. The model (1) is usually called[2(a),2(b)] the random trap model.

We consider a site-percolating model in which the jump rates ω_n from site n take values 0 or 1 with probability $\frac{1}{2}$, and the version of models A, B, and C of Ref. 2(a) defined by Eq. (1). For these models we analyze the FPTD for leaving a finite interval $[-L,L]$ of the chain. Previous results in this context refer to continuous models,[4] continuous-time random-walk models[5] (CTRW), or to the Sinai model.[2(c),6] Other results are for the time to leave an interval with a reflecting boundary in one extreme in cases of weak disorder or local bias.[7] A novelty of the problem that we consider here is that, except for model A, the mean first passage time (MFPT) diverges independently of the size of the interval. This fact is easy to understand for the site-percolating model defined above in which there are always configurations where the time to escape from $[-L,L]$ is infinity. For models B and C, the value of the MFPT is not so obvious because the walker leaves any finite interval with probability one. In spite of this, it turns out that the MFPT is also infinity for any finite interval [this makes it clear that it cannot be obtained by an inversion of $\langle x^2\rangle(t)$]. In other models, such as the Sinai model, and in the absence of trapping, the MFPT is finite for finite intervals.[6] This implies a clear-cut difference among models that can be classified as having an intermediate degree of disorder when considering the time dependence of $\langle x^2\rangle$. Our proposal here is to associate the concept of strong disorder with a divergent MFPT and to characterize, in these cases, the degree of disorder by the divergence law in a survival probability. We present here exact results for the exponents and amplitudes characterizing the divergence laws for intervals of any size. The exponents are independent of the size of the interval and the initial condition. This implies an interesting scaling form for the divergence law.

Equation (1) can be averaged over the probability distribution of the ω_n giving rise to an effective master equation with non-Markovian characteristics.[8] This equation gives information on the statistical properties of the moments, but it does not contain the required information on the process to be a correct starting point for us to calculate the passage-time statistics of the process (1) averaged over the distribution of ω_n. To this end we need to consider the equation satisfied by the survival probability $F^L_{n_0}(t)$

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for a given configuration of disorder. This is the probability that the walker is still at time t in the interval $[-L,L]$ starting at time $t=0$ at a site n_0 belonging to this interval. It is obvious that $F^L_{n_0}(0)=1$. The FPTD $f^L_{n_0}(t)$ is given by $f^L_{n_0}(t)=-dF^L_{n_0}(t)/dt$. The MFPT T is obtained from the Laplace transform $\hat{F}^L_{n_0}(z)$ as $T=\hat{F}^L_{n_0}(z=0)$. We are interested in the asymptotic dependence for $z\rightarrow 0$ of $\hat{F}^L_{n_0}(z)$ averaged over the configurations of ω_n. Such dependence characterizes the possible divergence of the averaged MFPT $\langle T\rangle$. For large z, and given the initial condition at $t=0$, it is obvious that $\langle \hat{F}^L_{n_0}(z)\rangle \sim z^{-1}$ for all types of disorder. The survival probability $F^L_{n_0}(t)$ obeys the adjoint or backwards equation associated with Eq. (1), but with the evolution operator adjusted so that stochastic paths reentering the interval from the outside are eliminated.[9] The equation for $F^L_{n_0}(t)$ is

$$\partial_t F^L_{n_0}(t)=\omega_{n_0}(E^{+}+E^{-}-2)F^L_{n_0}(t)\,. \qquad (2)$$

The adjustment of the evolution operator is easily done since the process is Markovian for a given configuration of the disorder. It consists of imposing the boundary condition $E^{\pm}F^L_{n_0=\pm L}=0$, or equivalently, $F^L_{n_0}=0$ for any $n_0\notin[-L,L]$. Equation (2) takes into account the exact statistics of the passage-time problem for a given configuration of ω_{n_0}. For a finite value of L, Eq. (2) in the Laplace space is a linear algebraic equation that can be solved for $\hat{F}^L_{n_0}(z)$ and then averaged over the distribution of quenched disorder. This gives a correct calculational method from first principles and of practical use for small values of L. In the site-percolating problem defined above, the asymptotic behavior of $\langle \hat{F}^L_{n_0}(z)\rangle$ as $z\rightarrow 0$ can be obtained independently of (2). For this problem it is obvious that the probability of leaving the interval is less than one: $\langle \hat{f}^L_{n_0}(z=0)\rangle = p<1$. This implies that $\langle \hat{F}^L_{n_0}(z\rightarrow 0)\rangle \approx (1-p)/z$. The consequence is that the asymptotic dependence of $\langle \hat{F}^L_{n_0}(z)\rangle$ is the same $(\sim z^{-1})$ for small and large z. The divergence of the MFPT determined by the divergence as $z\rightarrow 0$ is characterized by the probability $1-p$ of no escape from the interval. For example, the average of the solution of (2) for $L=1$ and $n_0=0$ is obtained by simple configuration counting as

$$\langle \hat{F}^{L=1}_{n_0=0}\rangle = [(5/z)+2(z^2+4z+2)/z(z+3)(z+1)+(z+4)/(z^2+4z+2)]/8\,. \qquad (3)$$

This reproduces the announced law z^{-1} for $z\ll 1$ and gives the result $p=\frac{5}{24}$. We have also obtained the result for $\hat{F}^L_0(z)$ for $L=2$ and 3 by solving (2) and doing the average numerically by exactly enumerating all the possible configurations of disorder. The result is shown in Fig. 1. We obtain $p=\frac{7}{80}$ and $p=\frac{503}{13440}$ for $L=2$ and 3, respectively.

We next consider three models of varying strength of the disorder, but for which the probability of escaping from the interval is always $p=1$. We first consider model A of weak disorder for which no anomalous diffusion exists. We define it by Eq. (1) and ω_n taking the values $\frac{1}{2}$ and $\frac{3}{2}$ with probability $\frac{1}{2}$ so that the inverse moments $\langle \omega_n^{-M}\rangle$ are finite for any M. The number of possible configurations of the disorder is finite and we have calculated $\langle \hat{F}^L_{n_0}(z)\rangle$, for $L=1$, 2, and 3 and different initial conditions n_0, by solving (2) and averaging by the exact enumeration of configurations. Our results are shown in Fig. 2(a), where the expected dependence for $z\gg 1$, $\langle \hat{F}^L_{n_0}(z)\rangle \sim z^{-1}$ is observed. We find that $\langle \hat{F}^L_{n_0}(z\rightarrow 0)\rangle$ tends to a finite quantity $\Omega^A(L,n_0)$. This gives a finite value for the MFPT. Disorder models B and C are defined by a probability distribution ρ for the ω_n with diverging inverse moments $\rho(\omega_n)=(1-\alpha)\omega_n^{-\alpha}$, $0\le\alpha<1$. The limiting case $\alpha=0$ defines model B. Again we have calculated $\langle \hat{F}^L_{n_0}(z)\rangle$ for $L=1$, 2, and 3, different initial conditions, and several values of α. Here the average with $\rho(\omega_n)$ has been made by a Monte Carlo sampling of the different configurations. The delicate dependence on configurations with small statistical weight has required samples of 10^7 configurations. Results for $\alpha=0$ and $\frac{1}{2}$ are shown in Figs. 2(b) and 2(c). Similar results are obtained for other values of α. Besides the expected z^{-1} dependence for $z\gg 1$, for $z\ll 1$ our results are well fitted by $\langle \hat{F}^L_{n_0}(z)\rangle \sim \Omega^B(L,n_0)|\ln z|$ for model B, and by $\langle \hat{F}^L_{n_0}(z)\rangle \sim \Omega^C(L,n_0)z^{-\alpha}$ for model C. In fact, these are the exact asymptotic behaviors, as will be commented on below. These results characterize the divergence of the MFPT and provide us with a novel quantitative description of the strong disorder. In the sense proposed here, model B is a model of strong disorder, but not the Sinai model, for which the MFPT is finite[6] for finite L.

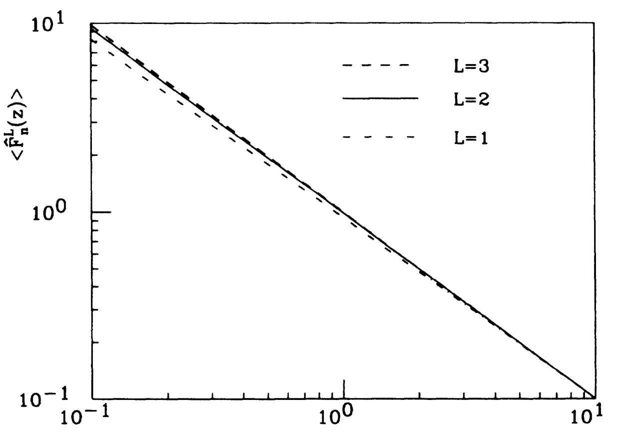

FIG. 1. Survival probability for the site-percolation model for several values of L. Initial condition: $n=0$.

It is interesting for us to comment on the relation between our results and those of a CTRW approach. An approximation to the general model of Eq. (1) is obtained by associating it with a CTRW. This is done by constructing a waiting time distribution $\psi(t)$ to jump from one site to its neighbor site by averaging over $\rho(\omega_n)$ the exponential waiting-time distribution associated[10] with (1) for fixed $\omega_n=\omega$. For our model C, one finds for $z\ll 1$, $\hat{\psi}(z)\approx 1-A_0(\alpha)z^{1-\alpha}+O(z)$. This is the form of $\psi(t)$ used in Ref. 5. It is known that this association gives an incorrect

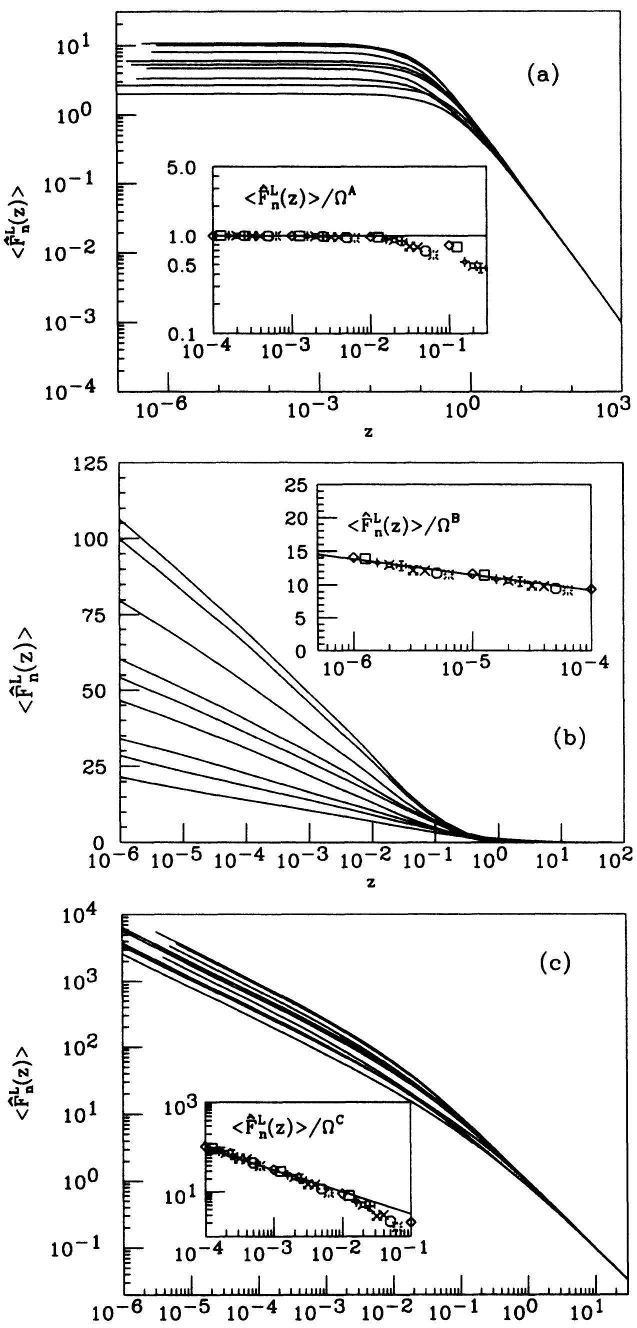

FIG. 2. Survival probability for different models of disorder: (a) weak disorder (model A); (b) strong disorder (model B); (c) strong disorder (model C, $\alpha=\frac{1}{2}$). Curves with different values of (L,n) are plotted; from top to bottom: $(L,n)=(3,0)$, (3,1), (3,2), (2,0), (2,1), (3,3), (2,2), (1,0), and (1,1). A scaled form of the survival probability is shown in the insets; different symbols are for different values of (L,n); the solid line is the small-z prediction of the finite-effective-medium approximation.

exponent δ of the law $\langle x^2\rangle \sim t^\delta$. [For model C one finds[2,8(b)] $\delta=2(1-\alpha)/(2-\alpha)$, while δ obtained from the associated CTRW is $\delta=1-\alpha$.] However, it happens that the exact dependence $\langle \hat{F}^L_{n_0}(z)\rangle \sim z^{-\alpha}$ obtained here for model C coincides with the one obtained[5] by a renormalization-group argument in the large-L limit for the corresponding CTRW model.

Our results for $\langle \hat{F}^L_{n_0}(z)\rangle$ and small L discussed above can be understood within the context of a general theory, which will be described in detail elsewhere.[11] The basic idea is to average (2) by a projector method[8] similar to the one used in Ref. 8(b). Such a straightforward averaging does not define a good perturbative series for small z. In order to construct a good perturbation theory we introduce a sort of effective medium characterized by effective non-Markovian rates $\Gamma(z)$ between nearest-neighbor sites. The rates $\Gamma(z)$ are determineed so that a straightforward perturbation theory around such mean-field approximations has good convergence properties for $z \ll 1$. This approximation has a number of peculiarities associated with boundary conditions due to the fact that (2) is defined for finite intervals. To differentiate it from the standard-effective-medium approximation (EMA) for the calculation of a frequency-dependent diffusion coefficient,[2(a),2(b),8(b)] we wish to call it the finite-EMA (F-EMA). The F-EMA for the calculation of the survival probability is given by

$$z\langle \hat{F}^L_n\rangle - 1 = \Gamma(z)(E^+ + E^- - 2)\langle \hat{F}^L_n\rangle , \qquad (4)$$

with $\Gamma(z)$ defined in a self-consistent way by

$$\left\langle \frac{\omega_0-\Gamma(z)}{1-[\omega_0-\Gamma(z)](E^+ + E^- -2)G_{00}[\Gamma(z),z]} \right\rangle = 0 , \qquad (5)$$

where $G_{00}(\Gamma,z)$ is the Green's function for a RW with effective rates Γ and absorbing boundary conditions.

Two important things have to be noted about the F-EMA. The first one is that it generally does not coincide with the adjoint or backwards equation of the standard EMA. The second one is that the analysis of the corrections to the F-EMA shows[11] that it gives the exact result for the exponent in the leading contribution to $\langle \hat{F}^L_{n_0}(z)\rangle$ as $z \to 0$ for all models of disorder considered here. Moreover, it can be demonstrated[11] that the F-EMA also gives the exact amplitude $\Omega(L,n_0)$ for models A and B. For model C, corrections to the amplitude given by Eqs. (4) and (5) can be shown to be generally very small. Explicit evidence of this fact is seen in the inset of Fig. 2(c). The results obtained from Eqs. (4) and (5) confirm the asymptotic dependence of $\langle \hat{F}^L_{n_0}(z)\rangle$ on z numerically established before, giving the following values for the amplitudes:

$$\Omega^B(L,n_0) = [(L+1)^2 - n_0^2]/2 ,$$

$$\Omega^A(L,n_0) = \Omega^B(L,n_0)\langle \omega^{-1}\rangle ,$$

$$\Omega^C(L,n_0) = \Omega^B(L,n_0)\pi(1-\alpha)2^\alpha/[(L+1)^\alpha \sin(\pi\alpha)] .$$

We first note that the exact result for the averaged MFPT for model A, $\langle T\rangle = \Omega^A(n_0,L)$, only involves the static limit of the frequency-dependent diffusion coefficient $D(z=0)=\langle \omega^{-1}\rangle^{-1}$. The important fact is that for all the models studied here the dependence on n_0 and L of the asymptotic law for $\langle \hat{F}^L_{n_0}(z)\rangle$ only appears through the amplitudes Ω. This permits us to scale out such dependence. The scaling form is manifested in the insets of Fig. 2. Our numerical calculation gives a rather convincing check of the exponents and amplitudes that follow from the theory sketched above.

Financial support from Dirección General de Investigación Científica y Técnica (DGICYT) (Spain) Project No. PB-86-0534 is acknowledged. M.O.C. acknowledges support from DGICYT (Spain) and Consejo Nacional de Investigaciones Científicas y Técnicas, Resolución No. 1857/88 (Argentina).

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