Fluctuations and self-averaging in random trapping transport: The diffusion coefficient

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On the basis of a self-consistent cluster effective-medium approximation for random trapping transport, we study the problem of self-averaging of the diffusion coefficient in a nonstationary formulation. In the long-time domain, we investigate different cases that correspond to the increasing degree of disorder. In the regular and subregular cases the diffusion coefficient is found to be a self-averaging quantity—its relative fluctuations (relative standard deviation) decay in time in a power-law fashion. In the subdispersive case the diffusion coefficient is self-averaging in three dimensions (3D) and weakly self-averaging in two dimensions (2D) and one dimension (1D), when its relative fluctuations decay anomalously slowly logarithmically. In the dispersive case, the diffusion coefficient is self-averaging in 3D, weakly self-averaging in 2D, and non-self-averaging in 1D. When non-self-averaging, its fluctuations remain of the same order as, or larger than, its average value. In the irreversible case, the diffusion coefficient is non-self-averaging in any dimension. In general, with the decreasing dimension and/or increasing disorder, the self-averaging worsens and eventually disappears. In the cases of weak self-averaging and, especially, non-self-averaging, the reliable reproducible experimental measurements are highly problematic. In all the cases under consideration, asymptotics with prefactors are obtained beyond the scaling laws. Transition between all cases is analyzed as the disorder increases.

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I. INTRODUCTION

The problem of hopping transport or diffusion of particles in a system with random traps is quite common in the kinetics of condensed media. Some examples are the exciton migration in molecular crystals, in amorphous solids, and in biological systems, and sensitized luminescence and photochemistry, conductivity of extrinsic semiconductors, spin diffusion, and kinetics of diffusion-controlled reactions [1–6].

Such processes are studied in the frameworks of chemical kinetics (both classical and fluctuational) [1,7–10], and of the stochastic transport theory of disordered systems [2–6,11–46]. In the latter case the rigorous description of the incoherent (Markov) hopping can be constructed on the basis of the master equation [2–6]. The analogy with the quantum theory of disordered systems makes possible the use of the Green's function technique [11–17,19–26,31–33].

Most complete is the study of symmetric transition rates that correspond to the structural disorder [2–5,11,13]. Less studied is the case of the nonzero spread of energy levels, when the hopping rate is asymmetric in site indices between which the transfer takes place [6,12,14–16].

An important particular case of asymmetric transition rates is the transport with random trapping. Diffusion with a chemical reaction (equivalent to trapping by mobile sinks) has been considered by Smoluchowski [7] within an approximation of mean-field type. The exact decay of the concentration of the surviving particles in the fluctuation regime at long time $\approx \exp[-\text{const}\, t^{d/(d+2)}]$ has been found in Refs. [8,9]. The approach to equilibrium in a reversible chemical reaction [10] at long time (trapping corresponds to one of the components being frozen) has been demonstrated to be of a slow power-law type $\approx (Dt)^{-d/2}$.

A diagram technique has been developed for exciton migration in a solution with sinks [11,12], and two- and three-site self-consistent approximations have been built. In one dimension, the hopping on a chain with traps has been studied rigorously in Refs. [15,16]. A diverse evolution in a system with diffusion, annihilation, and reproduction of particles has been investigated [17,18]. The spatial evolution of particles diffusing in the presence of traps has been studied [19]. The effect of the applied electric field on the trapping kinetics has been analyzed [20].

For the problem of particle migration on a lattice with random traps (random positions, random depths), we have built a self-consistent cluster effective-medium approximation [21–26]. We demonstrated that the method is accurate in most limiting cases. On this basis, we analyzed the evolution of the diffusion coefficient and the kinetics of relaxation of the spectral population to equilibrium. We also considered the question of self-averaging of the diffusion coefficient and of the partial (spectral) populations in some cases, primarily for the regular regime of reversible trapping and for the dispersive and subdispersive regimes. The term self-averaging is used to characterize the evolution of the relative fluctuations, whether they vanish with time or not.

An alternative method termed CTRW (continuous time random walk) [27–30] has been justified for the calculation of averaged quantities like conductivity [29]. However, the classic CTRW [27,28] chaotizes the trajectories or, in other words, neglects their self-intersections. Every hop is considered to be independent of all the preceding ones. All hops are

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characterized by the same averaged waiting-time distribution. Thus, the spatial fluctuations that originate from the static disorder within the classic CTRW are averaged out at the start. It makes impossible the correct calculation of correlations of fluctuating quantities. Clearly, this inconsistency is crucial for the variances formed by disorder, though it is tolerable for the average quantities.

A generalization of the classic CTRW [27,28] method has been used to retain spatial inhomogeneities in [42,46]. However, it contains some approximations (like "coarse graining") and leads back to a kind of random trapping–type model. Our approach to random trapping, constructed previously in [21–24], is transparent, rigorous, controllable, and it is suitable for the construction of approximation schemes for any correlators.

In the stochastic formulation, the problem of self-averaging has been addressed in a number of studies [15,23–26,31–46]. Within the master-equation approach to disordered systems, self-averaging has been considered in Refs. [15,23–26]. Since then, numerous processes have been studied from the point of view of self-averaging properties. Processes of spin relaxation in the course of random walks on disordered lattices are self-averaging [31]. Directed percolation leads to non-self-averaging [32]. With the help of the renormalization group method it has been shown that near the critical point self-averaging depends crucially on the interrelation of the system size and the correlation length [33]. Occupation-time distribution for the diffusion on a disordered chain demonstrates loss of self-averaging and big sample-to-sample fluctuations [34]. The fractal dimension in diffusion-limited aggregation is a weakly self-averaging quantity [35]. Record statistics for random walks and Levy flights are non-self-averaging [36]. Particle concentration for a continuous time random walk is not self-averaging either [37]. The ratio between diffusivity and admittance in a disordered non-self-averaging system may be viewed as a stochastic effective temperature [38]. Certain classes of percolation models are not self-averaging in the thermodynamic limit [39]. The lack of self-averaging has been demonstrated for transient subdiffusion in corrugated potentials with spatial correlations [40]. The first-passage-time distribution in the presence of quenched traps is non-self-averaging [41]. Self-averaging and ergodicity of subdiffusion in quenched random media have been studied [42,46]. The fluctuations of the single-particle diffusivity far exceed the results of the annealed theory [43]. The distribution function for the diffusion coefficient in quenched disorder is that of Mittag-Leffler in three dimensions (3D), and of modified Mittag-Leffler in one dimension (1D) and two dimensions (2D) [44]. The previous calculation of the distribution function has been extended to fractal lattices as well [45].

The goal of this paper is to present a unified rigorous systematic theoretical study of the self-averaging properties of the nonstationary diffusion coefficient in all possible regimes within the random trapping model. At present, a complete analysis of all the possible cases beyond scaling laws is still lacking. Under what circumstances will the measurements in the ensemble of samples with disorder produce close and reproducible results? If the fluctuations are large, will they decay in time and, if so, which way? To answer these questions we calculate and analyze the variance of the diffusion coefficient as a function of time, of the disorder magnitude, and of the dimensionality of the system. We also compare our results to the other approaches.

II. MODEL

Let us consider a particle that performs incoherent Markov hops between neighboring sites on a d-dimensional lattice. Each site can be a trap with some random escape rate w, characterized by a specified distribution function $\rho(w)$. For a given site, the hopping rates w to any of its z nearest neighbors are equal. The traps are distributed in space at random in an uncorrelated macroscopically uniform manner. The concentration of traps and the dispersion of the hopping rates do not have to be small. In fact, all the sites can be called traps.

The incoherent migration of a particle on a lattice is governed by the master equation for the populations of sites:

$$dP_{j,i}/dt = \sum_{k(j)} w_{j,k}P_{k,i} - \sum_{l(j)} w_{l,j}P_{j,i}. \tag{1}$$

Here $P_{j,i}(t)$ is the probability for finding the particle at site j at time t, if initially it was at site i. Thus $P_{j,i}(t)$ is the Green's function of the problem with the initial conditions $P_{j,i}(t=0) = \delta_{j,i}$. The normalization of $P_{j,i}(t)$ or, in other words, the number of particles, is preserved in time. The summation over $k(j)$ in Eq. (1) runs over the nearest neighbors of j. The hopping rate $w_{j,k}$ from site k to site j in this model is determined by the level the particle is leaving, but does not depend upon the level at which it arrives. Therefore, the hopping rate in fact is the function of the second index solely; $w_{j,k} = w_k$.

There is no explicit Langevin-type noise in the model. The noise is averaged out in the master-equation approach from the start.

In experimentation, this situation may correspond, for example, to the migration of particles on a set of impurities of low concentration. The qualitative picture is that of a particle activated thermally to the conduction band—with a subsequent relaxation to the other impurity site. The activation energy to the bottom of the conduction band depends on the trap depth only—in contrast to the situation of quantum tunneling between closely positioned impurities, when the transition rate depends upon both levels.

Besides the picture of random hopping rates w, another equivalent representation of the disorder distribution is possible. The idea of it is the following. The particle exits the trap activationally at rate $w_k \approx \text{const} \exp(-\Delta_k/T)$ [2–5]. Here Δ_k is the depth of trap k with T being the temperature in energy units. Let the trap levels be positioned on the energy scale at random with some average "concentration" T_0^{-1}. Then the distribution ρ_Δ of trap depths is of an exponential type, $\rho_\Delta(\Delta_k) = T_0^{-1} \exp(-\Delta_k/T_0)$. Going over from the distribution of trap depths Δ_k (as the independent parameter) to the distribution of hopping rates w_k, one finds the distribution function of a power-law type $\rho(w_k) \approx \text{const} w_k^\beta$ [2], where

$$\beta = (T/T_0) - 1. \tag{2}$$

The first interpretation of the problem in terms of escape rates $\rho(w)$ is more general. The second picture of "trap levels Δ_k, randomly distributed on the energy scale" is more

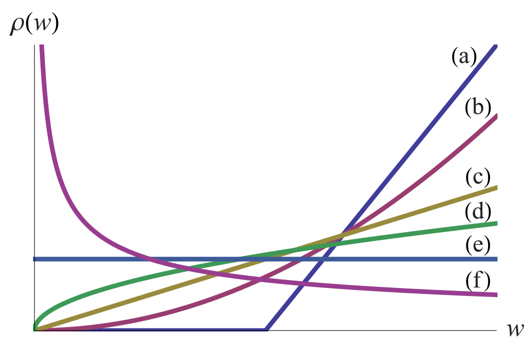

FIG. 1. Examples of rate distribution functions $\rho(w)$, cases (a)–(f). The classification is governed by the deep-trap tail of the distribution of the hopping rates w, i.e., by the $w \to 0$ asymptotics of $\rho(w)$.

transparent. In the second formulation the different regimes, considered below, may be qualitatively interpreted as a kind of "phase diagram," a function of temperature. The definitions of different regimes are provided below in both formulations.

Several different classes of distributions $\rho(w)$ that lead to qualitatively different long-time behaviors of the kinetic characteristics can be defined. The classification is governed by the limiting behavior of the distribution $\rho_\Delta(\Delta_k)$ for deep traps $\Delta_k \to \infty$ or, equivalently, by the distribution of the low escape rates $\rho(w)$ for $w \to 0$. In the present consideration of the fluctuations of the kinetic characteristics the classification should be somewhat enlarged in comparison to its counterpart for the average kinetic characteristics [21–26]. The sequence of cases corresponds to the increasing disorder or to the lowering temperature T, Fig. 1.

(a) If the deep-trap tail of the distribution $\rho_\Delta(\Delta_k)$ is identically zero in the vicinity of zero escape rates $w = 0$, we call it the regular case, Fig. 1, curve (a). The hopping rate distribution below some value w_γ obeys

$$\rho(w < w_\gamma) = 0. \tag{3a}$$

(b) If the deep-trap tail of the distribution $\rho_\Delta(\Delta_k)$ decays faster than exponential $\mathrm{const}\exp(-\Delta_k/T_0)$, or if $T > 2T_0$, then we call this case the subregular 1, Fig. 1, curve (b). The hopping rate distribution $\rho(w)$ vanishes for $w \to 0$ in a power-law fashion with the exponent $\beta > 1$ or faster:

$$\rho(w) = Aw^\beta, \quad A = (1+\beta)w_0^{-1-\beta}, \quad \beta > 1,\ 0 < w < w_0. \tag{3b}$$

Here w_0 is the upper cutoff for the escape rate w. The definition of β (2) is equal to $-\alpha$ in Refs. [21–26].

(c) The case $T = 2T_0$ in Eq. (3b) or, equivalently,

$$\beta = 1, \tag{3c}$$

we call the subregular 2 case, Fig. 1, curve (c).

(d) The case $T_0 < T < 2T_0$ or, equivalently,

$$0 < \beta < 1 \tag{3d}$$

we call subregular 3 case, Fig. 1, curve (d).

In the regular (3a) and all the subregular (3b)–(3d) cases the *average* evolutions at long time in the main terms are qualitatively similar to one another and satisfy diffusion-type scaling. Therefore, we united them all in the single regular case in Refs. [21–26]. The fluctuations considered here, however, in these cases are qualitatively different, as we demonstrate below.

(e) The intermediate subdispersive case corresponds to $T = T_0$ or to $\beta = 0$, so that the limiting probability density at $w \to 0$ is a nonzero constant $\rho(0) = \mathrm{const}$, Fig. 1, curve (e). For definiteness, we consider the particular distribution:

$$\rho(w) = w_0^{-1}, \quad 0 < w < w_0. \tag{3e}$$

The long-time leading terms have similar time dependencies for any particular distribution within each case. In this particular case (3e) the leading long-time asymptotics will be determined by the limiting value $\rho(0) = w_0^{-1}$ solely.

(f) In the dispersive case $0 < T < T_0$ the distribution of the hopping rates $\rho(w)$ diverges in an integrable way in the vicinity of $w = 0$. We consider the distribution [Fig. 1, curve (f)]:

$$\rho(w) = Aw^{-\alpha}, \quad A = (1-\alpha)w_0^{-1+\alpha},$$
$$0 < \alpha < 1, \quad 0 < w < w_0. \tag{3f}$$

Instead of the variable β in Eqs. (3b)–(3e) it is more convenient to use here $\alpha = -\beta$, as in Refs. [21–26].

(g) The irreversible case of trapping by infinitely deep traps or sinks of finite concentration c contains a δ function in the distribution:

$$\rho(w) = c\delta(w) + \rho_1(w), \quad \rho_1(w = 0) = 0. \tag{3g}$$

To study all these regimes (3a)–(3g) in the random trapping model we constructed a self-consistent cluster effective-medium approximation based on the multiple-scattering formalism from the quantum theory of disordered systems [21–26]. We studied a number of kinetic characteristics that include the generalized diffusion coefficient, the frequency-dependent conductivity, and the spectral relaxation of partial populations. We also considered the problem of self-averaging of the diffusion coefficient and of the spectral populations in some cases. The term self-averaging is used to characterize the reliable measurability of the diffusion coefficient in the experiments on (or computer simulations of) stochastic transport in disordered systems. In the present paper, we consider to the end the problem of self-averaging of the diffusion coefficient in the other cases, which were not addressed in Refs. [15,23–26].

III. BASIC RELATIONS

Below we provide some basic relations [21–25] that our consideration relies upon.

The master equation (1) for the Green's function $\tilde{\mathbf{P}}$ in matrix form, Laplace transformed, is

$$(\varepsilon\mathbf{I} - \mathbf{W})\tilde{\mathbf{P}} = \mathbf{I}, \tag{4}$$

where $I_{i,j} = \delta_{i,j}$ is the unit matrix in site representation. The Laplace parameter is denoted by ε. All the functions of ε are marked by a tilde. The transition rate matrix $\mathbf{W}$ in Eq. (4) is

$$W_{j,k} = (1 - \delta_{j,k})w_k - \delta_{j,k}zw_j. \tag{5}$$

The initial disordered system in zero-order approximation is modeled by a uniform effective medium. The corresponding effective transition rate $\tilde{w}^{\text{eff}}$ is assumed to be a function of ε. Later $\tilde{w}^{\text{eff}}$ is chosen in an optimized self-consistent way. It can also be noted that in real space the modeling system corresponds to partly coherent transfer with memory, described by a generalized master equation.

The difference between the initial disordered system $\mathbf{W}$ and the effective one $\tilde{\mathbf{W}}^{\text{eff}}$,

$$\tilde{W}^{\text{eff}}_{j,k} = (1 - \delta_{j,k})\tilde{w}^{\text{eff}} - \delta_{j,k} z \tilde{w}^{\text{eff}}, \tag{6}$$

constitutes the perturbation $\Delta\tilde{\mathbf{W}}$. The particle propagates in the effective medium and gets "scattered" on that perturbation:

$$\Delta\tilde{\mathbf{W}} = \mathbf{W} - \tilde{\mathbf{W}}^{\text{eff}}. \tag{7}$$

The perturbation matrix can be represented as a sum of contributions from local perturbing clusters:

$$\Delta\tilde{\mathbf{W}} = \sum_m \Delta\tilde{\mathbf{W}}_m. \tag{8}$$

Important is the choice of the perturbing cluster. We have chosen it in the following way [21–25]: One cluster perturbation comprises all the hops from one site (from within one trap) to all of its nearest neighbors. All the other hops (including the ones from the nearest neighbors into the trap under consideration) do not enter that perturbation, but belong to the other (neighboring) clusters. Thus the following essential conditions are met: (a) One perturbation comprises the correlated hopping rates (in our case all of them are equal within the cluster), (b) different clusters are not correlated with one another, (c) the clusters do not overlap in space, and (d) being put together in space, the clusters reproduce the initial disordered system like a mosaic.

Then the corresponding local perturbation matrix for site m is

$$\Delta\tilde{\mathbf{W}}_m = \Delta\tilde{w}_m \mathbf{M}_m, \tag{9}$$

$$\Delta\tilde{w}_m = w_m - \tilde{w}^{\text{eff}}. \tag{10}$$

$$(\mathbf{M}_m)_{n,l} = \sum_{m'(m)} \delta_{n,m'}\delta_{l,m} - z\delta_{n,m}\delta_{l,m}. \tag{11}$$

Summation over m' in $m'(m)$ runs over the nearest neighbors of m.

The Dyson equation follows from (4) and (7):

$$\tilde{\mathbf{P}} = \tilde{\mathbf{P}}^{\text{eff}} + \tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}\tilde{\mathbf{P}}, \tag{12}$$

where $\tilde{\mathbf{P}}^{\text{eff}} = (\varepsilon\mathbf{I} - \tilde{\mathbf{W}}^{\text{eff}})^{-1}$ is the Green's function of the effective medium.

Iterations of Eq. (12) provide the perturbation series in scattering on local clusters:

$$\tilde{\mathbf{P}} = \tilde{\mathbf{P}}^{\text{eff}} + \sum_m \tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}_m\tilde{\mathbf{P}}^{\text{eff}} + \sum_{m,n} \tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}_m\tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}_n\tilde{\mathbf{P}}^{\text{eff}} + \cdots. \tag{13}$$

Next in Eq. (13) all the terms that correspond to successive scattering on one cluster are combined in a $\mathbf{t}$ matrix:

$$\tilde{\mathbf{t}}_m = \Delta\tilde{\mathbf{W}}_m + \Delta\tilde{\mathbf{W}}_m\tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}_m + \Delta\tilde{\mathbf{W}}_m\tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}_m\tilde{\mathbf{P}}^{\text{eff}}\Delta\tilde{\mathbf{W}}_m + \cdots. \tag{14}$$

The result for $\tilde{\mathbf{t}}_m$ is

$$\tilde{\mathbf{t}}_m = \tilde{F}_m \mathbf{M}_m, \tag{15}$$

$$\tilde{F}_m = \tilde{w}^{\text{eff}} \frac{w_m - \tilde{w}^{\text{eff}}}{w_m - \varepsilon\tilde{P}^{\text{eff}}_{1,1}(w_m - \tilde{w}^{\text{eff}})}. \tag{16}$$

The matrix $\mathbf{M}$ in (15) is specified in Eq. (11), and $\tilde{P}^{\text{eff}}_{1,1}$ is the diagonal element of the Green's function. The superscript *eff* always refers to the effective medium. In the $\mathbf{t}$ matrix (14) all the one-loop diagrams that take account of all the consecutive scattering on one site are summed up.

The renormalized series (13) in $\mathbf{t}$ matrices takes the following form:

$$\tilde{\mathbf{P}} = \tilde{\mathbf{P}}^{\text{eff}} + \sum_m \tilde{\mathbf{P}}^{\text{eff}}\tilde{\mathbf{t}}_m\tilde{\mathbf{P}}^{\text{eff}} + \sum_{\substack{m,n \\ m\neq n}} \tilde{\mathbf{P}}^{\text{eff}}\tilde{\mathbf{t}}_m\tilde{\mathbf{P}}^{\text{eff}}\tilde{\mathbf{t}}_n\tilde{\mathbf{P}}^{\text{eff}} + \sum_{\substack{m,n,k \\ m\neq n, n\neq k}} \tilde{\mathbf{P}}^{\text{eff}}\tilde{\mathbf{t}}_m\tilde{\mathbf{P}}^{\text{eff}}\tilde{\mathbf{t}}_n\tilde{\mathbf{P}}^{\text{eff}}\tilde{\mathbf{t}}_k\tilde{\mathbf{P}}^{\text{eff}} + \cdots. \tag{17}$$

Next we determine the effective hopping rate $\tilde{w}^{\text{eff}}$ by the self-consistency condition [21–26]:

$$\langle \tilde{F}_m \rangle = 0. \tag{18}$$

The expression for $\tilde{F}_m$ is specified in Eq. (16). The angular brackets denote averaging over the random hopping rates w_m. The ensemble for averaging is constituted by the realizations of the disorder.

The self-consistency condition (18) is an equation to be solved for $\tilde{w}^{\text{eff}}$.

Let us analyze the renormalized perturbation series (17) under the condition (18).

The first term $\tilde{\mathbf{P}}^{\text{eff}}$ in Eq. (17) is the zero-order propagation in the self-consistent effective medium. The next terms correspond to "scattering" on one, two, etc., clusters. As all the consecutive scattering on one site is summed up in the $\mathbf{t}$ matrix, the summation in Eq. (17) runs over all the sites of the lattice with the following limitation: The indices of the neighboring $\mathbf{t}$ matrices cannot coincide.

The perturbing clusters have been selected in such a way that the scattering events on different clusters are independent and do factorize. So do the $\tilde{F}_m$ factors in the $\mathbf{t}$ matrices in Eq. (17).

The analysis [21–23] of the series for the Green's function (17) with the self-consistency condition (18) demonstrates that nearly all the trajectories are accounted for. The exception is the rather exotic class of the "all-self-intersecting" trajectories, such that every site visited is visited at least twice.

To see that, let us consider an arbitrary term in the averaged series (17). The scalar factors $\tilde{F}_m$ in the corresponding matrix product factorize. If among the $\mathbf{t}$ matrices (or, equivalently, among the sites in that trajectory) there is at least one $\mathbf{t}$ matrix (site) that enters the product (trajectory) a single time, the corresponding factor $\tilde{F}_m$ factorizes out from the product $\langle \tilde{F}_m \rangle \langle \tilde{F}_i \cdots \tilde{F}_j \rangle$ and vanishes according to the self-consistency condition (18). It means that all such "non-all-self-intersecting" trajectories are accounted for by the self-consistent effective-medium approximation correctly.

In particular, in Eq. (17) for the averaged Green's function the second, third, and fourth terms are zero. The first correction term, non-accounted-for, appears in the fourth order.

Let N be the total number of sites in the lattice. Then the non-accounted-for term of the fourth order is just one versus $(N-2)(N-3)$ terms in that order that become zero due to (18) and, consequently, that are taken into account correctly. Thus, in the limit $N \to \infty$ the following ratio: "the number of neglected terms in any order divided by the number of terms, correctly accounted for in that order" tends to zero. Obviously, such an approximation should be typically very accurate, apart from some special exotic cases, which select precisely these rare untypical all-self-intersecting trajectories.

We note, however, that such all-self-intersecting trajectories play an important role at long time in percolation-type problems, when the particle gets "trapped" on an isolated cluster and its trajectory winds up densely in a low-dimensional space. However, there are no such topological limitations in the present problem.

Nevertheless, in the problem of traps there is one regime which selects indirectly these all-self-intersecting trajectories. This is the case of irreversible trapping by sinks of finite concentration, Eq. (3g). In the long-time limit the particles survive in random trap-free cavities only, while in the regions with more or less uniformly distributed traps they decay effectively [8]. Besides the presence of sinks of finite concentration, another condition is implied. This condition is that the trapped particle not only gets "frozen" in the infinitely deep trap forever, but it also falls out from the normalization; i.e., it is considered as having disappeared in the sink. It is this second condition of surviving particles that selects only the exotic all-self-intersecting trajectories in the fluctuation regime at long time and that renders nonessential the regular paths.

In the regimes (3a)–(3f) under consideration, however, both these conditions are not met. Therefore, the method utilized provides correct results, at least up to the prefactor [21–26]. In other words, in the absence of infinitely deep traps of finite concentration and with the account of all the particles (not the survivors only), the kinetic characteristics are formed by all the trajectories, while the exotic all-self-intersecting ones have zero weight. In the irreversible case (3g), however, the present results form the correct intermediate-time asymptotics and neglect the purely fluctuational long-time tail of survivors, as explained above.

Further approximations of higher order on top of the effective medium for the calculation of correlators can be built.

IV. FLUCTUATIONS AND SELF-AVERAGING

The effective hopping rate $\tilde{w}^{\mathrm{eff}}$ is obtained as the solution to the self-consistency equation (18). The generalized diffusion coefficient $D(t)$ is determined through the mean-square displacement via the inverse Laplace transform $\hat{L}^{-1}$:

$$D(t) = a^2 w^{\mathrm{eff}}(t) = a^2 t^{-1} \hat{L}^{-1}[\tilde{w}^{\mathrm{eff}} \varepsilon^{-2}], \qquad (19)$$

where a is the intersite distance, assumed to be unity hereafter. Then the time-dependent effective hopping rate $w^{\mathrm{eff}}(t)$, defined by Eq. (19), can be used interchangeably with $D(t)$.

As the mean-square displacement in a disordered system typically grows nonlinearly, the diffusion coefficient is time dependent. The initial conditions for the calculated quantities correspond to the particle initially localized at site 0.

We are looking for the answers to the following questions: The calculated average values of the kinetic coefficients, such as (19)—are they well determined at long time and therefore reliably measurable in experiments, or do their fluctuations (variations of the values, measured in different samples or different realizations of disorder) remain substantial?

To find the answer we calculate the variance of the mean-square displacement,

$$\mathrm{Var}[R^2] = \sum_{j,k} R_{ji}^2 R_{ki}^2 (\langle P_{ji} P_{ki} \rangle - \langle P_{ji} \rangle \langle P_{ki} \rangle), \qquad (20)$$

and analyze its time dependence with respect to the mean-square displacement itself.

The correlator in Eq. (20) we calculate with the help of the series for the Green's function (17). In the lowest order in $\mathbf{t}$ matrices (15), (16), and (11) with the account of the self-consistency condition (18) and of the limitations on summation in Eq. (17) we obtain

$$\langle \tilde{P}_{ji} \tilde{P}_{ki} \rangle = \tilde{P}_{ji}^{\mathrm{eff}} \tilde{P}_{ki}^{\mathrm{eff}} + \sum_{m} (\tilde{P}^{\mathrm{eff}} \tilde{t}_m \tilde{P}^{\mathrm{eff}})_{ji} (\tilde{P}^{\mathrm{eff}} \tilde{t}_m \tilde{P}^{\mathrm{eff}})_{ki} + \cdots . \qquad (21)$$

In Eq. (21) we neglected some terms of the fourth and higher orders in the $\mathbf{t}$ matrices. However, an overwhelming majority of terms in all higher orders have been accounted for in Eq. (21) correctly. These are all the non-all-self-intersecting trajectories [cf. the reasoning following Eq. (17)] that vanish due to the self-consistency condition (18). The neglected all-self-intersecting trajectories obviously become essential in the long-time limit only in the irreversible case of trapping by sinks (3g), as noted in Sec. III. In the last case, the result is correct as an intermediate-long-time asymptotics, prior to the fluctuation long-time tail. The accurate long-time fluctuation asymptotics for case (3g) are being considered in [47] within a different approach.

In contrast to Refs. [21–25], the decoupling of nonlocal correlators $\langle P_{ji} P_{ki} \rangle = \delta_{k,j} \langle P_{ji}{}^2 \rangle + (1 - \delta_{k,j}) \langle P_{ji} \rangle \langle P_{ki} \rangle$ is not used.

With the account of Eqs. (21) and (15) the formula for the variance of the diffusion coefficient (20) finally takes the following form:

$$\mathrm{Var}[\tilde{R}^2] = \langle \tilde{F}^2 \rangle \tilde{w}^{\mathrm{eff}^{-2}} \sum_{j,k,m} R_{ji}^2 R_{ki}{}^2 \times \left(\varepsilon \tilde{P}_{jm}^{\mathrm{eff}} - \delta_{jm}\right)\left(\varepsilon \tilde{P}_{km}^{\mathrm{eff}} - \delta_{km}\right) \tilde{P}_{mi}^{\mathrm{eff}^2}. \qquad (22)$$

It is accurate up to the third order in $\mathbf{t}$ matrices and it takes into account most high-order terms, as discussed above.

The sums in Eq. (22) cannot be calculated in the general form. We do the calculations below for every particular case (3a)–(3g) and for every dimension separately. First, the solutions to the corresponding self-consistency equations (18) are required and then the explicit expressions for the Green's functions of the effective medium $\tilde{P}^{\mathrm{eff}}$ are utilized.

V. RESULTS

The short-time limit $w^{\mathrm{eff}}(t)t \ll 1$ is the most simple.

A. Short-time domain

The diffusion coefficient (19) in all the cases (3a)–(3g)) is determined by the average rate of the first hop [21–24]:

$$D(t) = \langle w \rangle - \cdots . \tag{23}$$

Its variance (22),

$$\mathrm{Var}[D(t)] = \langle w^2 \rangle - \langle w \rangle^2 + \cdots , \tag{24}$$

is not small if the traps are not shallow. Therefore, at short time the diffusion coefficient in general is not a well-determined self-averaging quantity. Its dispersion in different samples is proportional to the degree of disorder.

B. Long-time domain

More complicated is the long-time limit $w^{\mathrm{eff}}(t)t \gg 1$.

1. Regular and subregular cases

The long-time diffusion coefficient (19) in the regular and all the subregular cases (3a)–(3d) is provided by a single formula in all the dimensions [21–24], which follows from Eq. (18):

$$D(t) = \langle w^{-1} \rangle^{-1} + \cdots . \tag{25}$$

The reciprocal standard deviation (square root of the variance, divided by the average value) of the diffusion coefficient (19) and (22) in the regular case (3a) can be found to decay in any dimension d in a power-law manner [15,23]:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = A_1^{(d)} \left(\left\langle \frac{1}{w^2} \right\rangle \left\langle \frac{1}{w} \right\rangle^{-2} - 1 \right)^{1/2} \left(\left\langle \frac{1}{w} \right\rangle^{-1} t \right)^{-d/4} + \cdots , \tag{26}$$

where $A_1^{(1)} = 2[3\,\Gamma(3/4)]^{-1}$ for $d = 1$, $A_1^{(2)} = 17^{1/2} 15^{-1/2} \pi^{-1}$ for $d = 2$ and $A_1^{(3)} = \sqrt{2}[\sqrt{\pi}\,\Gamma(1/4)]^{-1}$ for $d = 3$. This corresponds to normal slow self-averaging. It is illustrated by Fig. 2.

In the subregular 1 case, Eq. (3b), the variance of the diffusion coefficient coincides with the regular case (3a). It is provided by the same Eq. (26), which corresponds to power-law self-averaging. The qualitative illustration is provided by the same Fig. 2.

In the subregular 2 case, Eq. (3c), the reciprocal standard deviation of the diffusion coefficient decays at long time somewhat slower—with an additional logarithmic factor:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = A_2^{(d)} \frac{\ln^{1/2}(w^{\mathrm{eff}} t)}{(w^{\mathrm{eff}} t)^{d/4}} + \cdots , \tag{27}$$

where $A_2^{(1)} = [3\,\Gamma(3/4)]^{-1}$, $A_2^{(2)} = \sqrt{17/30}\,\pi^{-1}$, $A_2^{(3)} = [\sqrt{\pi}\,\Gamma(1/4)]^{-1}$, and w^{eff} is determined by Eqs. (19) and (25). The increasing disorder (fraction of deep traps) slows down the process of self-averaging. The process of self-averaging is depicted on a qualitative level in Fig. 2, the dispersion area getting slightly larger in comparison to case (3b).

Subregular 3 case (3d). Due to the increase of the disorder, the reciprocal standard deviation of the diffusion coefficient decays slower at long time in a power-law manner. In one

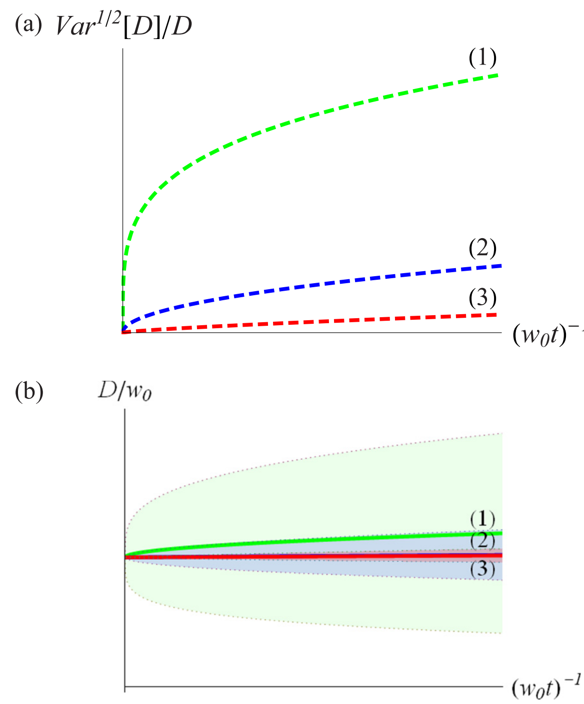

FIG. 2. Illustrative plots of the self-averaging in the regular and subregular cases (a)–(d) in the long-time limit, $(w_0 t)^{-1} \to 0$. (a) Plot of the reciprocal standard deviation of the diffusion coefficient, as a function of inversed time. Curves (1)–(3) are for the dimensions $d = 1,\ 2,\ 3$ correspondingly. (b) Plots of the average diffusion coefficients in dimensions $d = 1,\ 2,\ 3$; solid lines are marked as (1)–(3), correspondingly. The averaged curves for $d = 2$ and $d = 3$ nearly coincide. The dispersion areas, ranging from $D - \mathrm{Var}^{1/2}[D]$ to $D + \mathrm{Var}^{1/2}[D]$, are shaded and marked with dashed lines on their borders. The dispersion area for $d = 1$ is the biggest; the one for $d = 3$ is the smallest. The left ends of the curves correspond to $t \to \infty$. All the values are scaled to w_0.

dimension it is

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_3^{(1)}}{(w^{\mathrm{eff}} t)^{\beta/4}} + \cdots , \tag{28}$$

where $A_3^{(1)} = \frac{\sqrt{\pi}\,\beta^{(2+\beta)/2}}{2^{(1+\beta)/2}\Gamma(2-\beta/4)\sqrt{\sin(\pi\beta)}(\beta+1)^{\beta/2}}$, and w^{eff}, as before, is specified by Eqs. (19) and (25).

In two dimensions, an additional logarithmic correction emerges:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_3^{(2)}}{(w^{\mathrm{eff}} t)^{\beta/2} \ln^{(1-\beta)/2}(w^{\mathrm{eff}} t)} + \cdots , \tag{29}$$

where $A_3^{(2)} = \frac{\sqrt{17}\,\beta^{(2+\beta)/2}}{2G_2^{(1-\beta)/2}\Gamma(2-\beta/2)\sqrt{15\sin(\pi\beta)}(\beta+1)^{\beta/2}}$ and G_d is a constant, specific for the lattice type.

In three dimensions, we get

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_3^{(3)}}{(w^{\mathrm{eff}} t)^{(1+2\beta)/4}} + \cdots , \tag{30}$$

with $A_3^{(3)} = \frac{\beta^{(2+\beta)/2}}{2^{3/2}G_3^{(1-\beta)/2}\Gamma(7/4-\beta/2)\sqrt{\sin(\pi\beta)}(\beta+1)^{\beta/2}}$.

The subregular 3 case has larger fluctuations and self-averages slower than the subregular 2. As always, the increasing disorder (decreasing β) slows down the self-averaging.

Another effect of the increasing disorder is the following: The effectiveness of the self-averaging depends somewhat more on the dimensionality than before—with the growing dimension, the self-averaging accelerates faster.

In the limit $\beta \to 1$, the time dependencies go back to the subregular 2 case (27) up to a logarithmic correction. In addition, the factor $\sqrt{\sin(\pi\beta)}$ in the denominator of the coefficient $A_3^{(d)}$ goes to zero and that heralds the appearance of the additional logarithm in the numerator (27). An accurate derivation in the limit $\beta \to 1$ reproduces the form (27) correctly.

With $\beta \to 0$ the relaxation of fluctuations in one- and two-dimensional cases (but not in three dimensions) ceases to be of power-law type.

The subregular 3 case is illustrated qualitatively by the same shapes in Fig. 2, the dispersion area decaying with $t \to \infty$ somewhat slower than before.

We have obtained the result (26) for the regular case (3a) before [15,23]. The subregular (3b)–(3d) asymptotics with prefactors (27)–(30) are new. Scaling laws of the type (27)–(30) without prefactors have been obtained recently by another approximate method in [46].

2. Subdispersive case

In the long-time subdispersive case (3e) the diffusion coefficient (19) goes to zero in an extremely slow logarithmic way:

$$D(t) = A_4^{(d)} w_0 \ln^{-1}(w_0 t), \tag{31}$$

with the following factors for different dimensions d: $A_4^{(1)} = 2$ and $A_4^{(2)} = A_4^{(3)} = 1$, Refs. [21–26].

The reciprocal standard deviation of the diffusion coefficient (22) decays anomalously slowly in one- and two-dimensional systems:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_5^{(1)}}{\ln^{1/2}(w_0 t)} + \cdots, \quad d = 1, \tag{32}$$

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_5^{(2)}}{\ln(w_0 t)} + \cdots, \quad d = 2, \tag{33}$$

where $A_5^{(1)} = 1$ and $A_5^{(2)} = 17^{1/2} 2^{-1} (15\pi G_2)^{-1/2}$. Formally self-averaging takes place, but this is weak self-averaging with a logarithmic decay of fluctuations. It is much slower than the power-law decay in the previous cases. Within this weak self-averaging the fluctuations in the one-dimensional case are, as usual, bigger, and decay slower, $\approx \ln^{-1/2}(w_0 t)$, than in two dimensions $\approx \ln^{-1}(w_0 t)$.

In three dimensions, the decay of the reciprocal standard deviation of the diffusion coefficient remains of the power-law type:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_5^{(3)}}{[w_0 t \ln(w_0 t)]^{1/4}} + \cdots, \quad d = 3, \tag{34}$$

where $A_5^{(3)} = 2^{1/2} [7\Gamma(3/4)]^{-1} (\pi G_3)^{-1/2}$. The 3D subdispersive diffusion coefficient is still self-averaging. The curves of the reciprocal standard deviation and of the dispersion area of the diffusion coefficient are illustrated by Fig. 3.

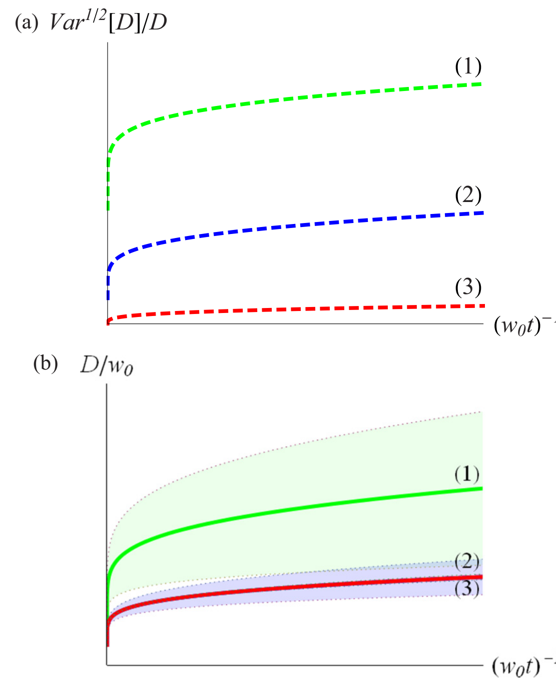

FIG. 3. Self-averaging in the subdispersive case (3e) in the long-time limit, $(w_0 t)^{-1} \to 0$. (a) Plot of the reciprocal standard deviation of the diffusion coefficient, as a function of inversed time. Curves (1)–(3) correspond to dimensions $d = 1, 2, 3$. (b) Plots of the average diffusion coefficients in dimensions $d = 1, 2, 3$; solid lines are marked as (1), (2), and (3) correspondingly. The averaged curves for $d = 2$ and $d = 3$ nearly coincide. The dispersion areas, ranging from $D - \mathrm{Var}^{1/2}[D]$ to $D + \mathrm{Var}^{1/2}[D]$, are shaded and marked with dashed lines on their borders. The dispersion area for $d = 1$ is the biggest; the one for $d = 3$ is the smallest. The left ends of the curves correspond to $t \to \infty$. All the values are scaled to w_0.

The subregular 3 results (28)–(30) in the corresponding limit $\beta \to 0$ reproduce the leading power-law dependencies (32)–(34) up to logarithmic corrections.

The results in the form (32)–(34) are new. We have obtained time dependencies of this kind previously in [26], though without prefactors.

3. Dispersive case

The dispersive case (3f). Note the change of the variables: $\alpha = -\beta$, $0 < \alpha < 1$ in the notations of Refs. [21–26]. The diffusion coefficient (19) in the long-time limit vanishes in a power-law fashion [21–25]:

$$D(t) = A_6^{(1)} (w_0 t)^{-\alpha/(2-\alpha)}, \quad d = 1, \tag{35}$$

$$D(t) = A_6^{(2)} (w_0 t)^{-\alpha} \ln^{\alpha}(w_0 t), \quad d = 2, \tag{36}$$

$$D(t) = A_6^{(3)} (w_0 t)^{-\alpha}, \quad d = 3, \tag{37}$$

where $A_6^{(1)} = [\frac{\sin(\pi\alpha)}{\pi 2^{\alpha}}]^{\frac{2}{2-\alpha}} \frac{w_0}{\Gamma[(4-3\alpha)/(2-\alpha)]}$, $A_6^{(2)} = \frac{G_2^{\alpha} \sin(\pi\alpha)(1-\alpha)^{\alpha} w_0}{\pi\Gamma(2-\alpha)}$, $A_6^{(3)} = \frac{G_3^{\alpha} \sin(\pi\alpha) w_0}{\pi\Gamma(2-\alpha)}$.

In the one-dimensional dispersive case we observe non-self-averaging—the reciprocal standard deviation of the diffusion coefficient does not vanish at long time:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \sqrt{\frac{\alpha}{2(1-\alpha)}} + \cdots, \quad d = 1. \tag{38}$$

The diffusion coefficient in this case ceases to be a well-determined quantity. Its fluctuations remain of the same order as its average value.

In two dimensions the self-averaging exists, but is pretty weak:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_7^{(2)}}{\ln^{1/2}(w_0 t)} + \cdots, \quad d = 2. \tag{39}$$

where $A_7^{(2)} = \frac{\sqrt{17}\alpha^{1/2}}{2\sqrt{15\pi}G_2^{1/2}(1-\alpha)}$.

In the three-dimensional case we find the regular power-law self-averaging:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = \frac{A_7^{(3)}}{(w_0 t)^{(1-\alpha)/4}} + \cdots, \quad d = 3. \tag{40}$$

with $A_7^{(3)} = \frac{\alpha^{1/2}\Gamma(2-\alpha)}{2^{3/2}\pi^{1/4}(1-\alpha)^{1/2}\Gamma(7/4-3\alpha/4)G_3^{1/2+\alpha/4}\sin^{1/4}(\pi\alpha)}$.

The process of self-averaging in the dispersive case (3f) is illustrated by Fig. 4.

In the limit $\alpha \to 0$ the dependencies of the preceding subdispersive case (32)–(34) are reproduced up to logarithmic factors. In the other limit $\alpha \to 1$, the relative fluctuations grow. In particular, in 1D the variations of the diffusion coefficient reveal the tendency to a faster growth in time, compared to its average value. In 2D the relative standard deviation reveals the tendency to a loss of weak self-averaging. In 3D the tendency to a loss of self-averaging in favor of weak self-averaging is revealed.

We have obtained previously [25] the asymptotics (38)–(40) with approximate values of the prefactors. Scaling laws of this type (without prefactors) have been found also in [46].

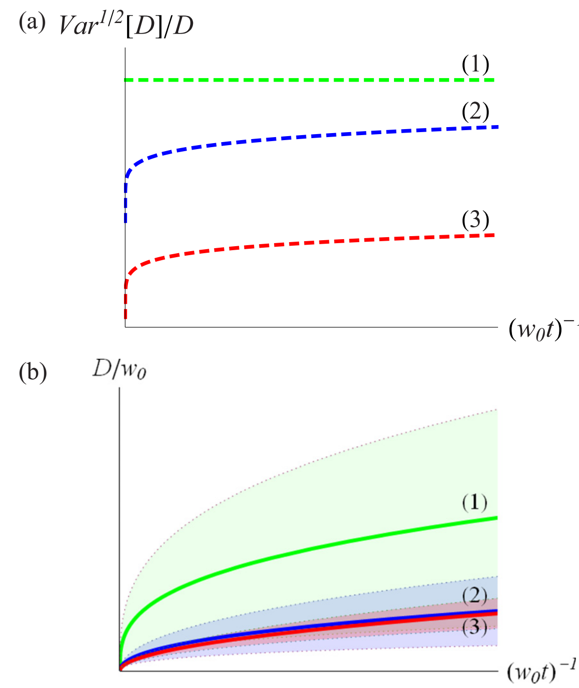

FIG. 4. Self-averaging and non-self-averaging in the dispersive case (3f) in the long-time limit, $(w_0 t)^{-1} \to 0$. (a) Plot of the reciprocal standard deviation of the diffusion coefficient, as a function of inversed time. Curves (1), (2), and (3) correspond to dimensions $d = 1, 2, 3$. In one dimension the leading term is a nonzero constant, so that curve (1) signifies non-self-averaging. (b) Plots of the average diffusion coefficients in dimensions $d = 1, 2, 3$; solid lines are marked as (1)–(3) correspondingly. The averaged curves for $d = 2$ and $d = 3$ nearly overlap. The dispersion areas from $D - \mathrm{Var}^{1/2}[D]$ to $D + \mathrm{Var}^{1/2}[D]$ are shaded and marked with dashed lines on their borders. The dispersion area for $d = 1$ is the biggest; the one for $d = 3$ is the smallest. The left ends of the curves correspond to $t \to \infty$. All the values are scaled to w_0.

4. Irreversible case

In the case of irreversible trapping (3g) with the account of all the particles (not only the survivors) within the effective-medium approximation, the mean-square displacement at long time tends to a constant:

$$D(t) = A_8^{(d)} t^{-1}, \tag{41}$$

where $A_8^{(1)} = 2^{-2}(1-c^2)c^{-2}$, $A_8^{(2)}$ is the solution of the equation $A_8^{(2)} = G_2 c^{-1} \ln A_8^{(2)}$ and $A_8^{(3)} = G_3 c^{-1}$.

This formula, in accordance with the discussion that follows Eqs. (17) and (18), is the intermediate long-time asymptotics that determines the evolution of the majority of the particles—though it does not reproduce the long-time fluctuation tail. The fluctuation regime we address separately in [47]. Here and below in the study of the irreversible case we limit ourselves to the intermediate long-time mean-field-type dependencies.

The diffusion coefficient for irreversible trapping in all dimensions is a non-self-averaging quantity. Its relative standard deviation at long time does not vanish, but goes to a nonzero constant:

$$\frac{\mathrm{Var}^{1/2}[D(t)]}{D(t)} = A_9^{(d)}, \tag{42}$$

where $A_9^{(1)} = 2^{-1/2}(1-c)^{-3/4}(1+c)^{-1/4}$, $A_9^{(2)} = 17^{1/2}[60\pi c(1-c)A_8^{(2)}]^{-1/2}$ and $A_9^{(3)} = c^{1/4}[2^{3/2}\pi^{1/2}G_3^{3/4}(1-c)^{1/2}]^{-1}$.

In the limit $c \to 0$ of "weak" irreversible disorder the process of self-averaging (42) depends on the dimensionality of the system. In 1D the relative standard deviation remains nonzero, so the diffusion coefficient is not self-averaging. In 2D the relative standard deviation vanishes logarithmically $\approx(-\ln c)^{-1/2}$, and this is a tendency to a weak self-averaging. This agrees qualitatively with the weak self-averaging $\approx\ln^{-1/2}(w_0 t)$ in the preceding 2D dispersive case. In three dimensions with $c \to 0$ the relative standard deviation vanishes in a power-law fashion $\approx c^{1/4}$, which demonstrates the tendency to a normal power-law self-averaging. This agrees qualitatively with the self-averaging of the diffusion coefficient $\approx(w_0 t)^{(1-\alpha)/4}$ in the preceding dispersive case $d = 3$.

In the limit $c \to 1$ of "strong" irreversible disorder, the relative fluctuations of the diffusion coefficient grow unboundedly as $(1-c)^{-3/4}$ in 1D and, somewhat slower, as $(1-c)^{-1/2}$ in 2D and 3D. In other words, for $c \to 1$ the diffusion coefficient is strongly non-self-averaging in all dimensions.

The intermediate-long-time asymptotics (42) for the reciprocal standard deviation of the diffusion coefficient for irreversible trapping within the self-consistent effective-medium approximation is another result of the present study. The plots of the dependences (41) and (42) are not provided here, as their shapes are trivial.

The corresponding result for the true long-time fluctuation tail (non-self-averaging) we found and analyzed recently in [47] with the use of the method of fluctuational cavities.

VI. DISCUSSION

First, let us discuss the accuracy of the self-consistent effective-medium approximation [21–24] that our consideration relies upon.

A. Accuracy

The leading terms of the short-time expansions (23) and (24) are exact [21,22]. This is obvious from their appearance: They are governed by the first hop.

Now let us address the long-time domain. The reasoning that follows Eqs. (17) and (18) seems to provide a clear qualitative picture. The overwhelming majority of the trajectories are correctly accounted for—with the exception of the case of sinks, when the neglected exotic trajectories start to provide the leading contribution.

Quantitatively, the estimate of the neglected terms in Ref. [21] suggests that in the regular-type cases, Eqs. (3a)–(3d), the leading long-time term of the diffusion coefficient is exact within the considered self-consistent effective-medium approximation. In the subdispersive (3e) and dispersive (3f) cases, the result should be accurate up to a numerical prefactor. In the case (3g) of irreversible trapping or sinks the fluctuational long-time tail is not reproduced; the self-consistent effective-medium approximation provides a correct intermediate-time asymptotics only.

The results of the self-consistent effective-medium approximation can also be compared to the exact solutions known. First, let us consider the average value of the diffusion coefficient. In one dimension the exact value of the diffusion coefficient in the regular-type cases (3a)–(3d) [2,15] is reproduced by the present method exactly. An electric analogy, provided in [21], proves that the result for the regular-type cases (3a)–(3d) is exact in any dimension as well. In the one-dimensional subdispersive (3d) and dispersive (3e) cases the exact result [2] is reproduced by the self-consistent effective-medium approximation up to a numerical prefactor.

The variance of the diffusion coefficient in the regular case (3a) in any dimension is reproduced by the present method exactly [15,23,24].

All these facts signify the high accuracy of the method, except for the long-time limit for irreversible trapping by sinks. The latter we consider here within the applicability range of the method, in the intermediate-time domain. The corresponding long-time fluctuation tail we study in [47] within a different approach.

In addition, our analytic results (26)–(30) and (38)–(40) agree with the scaling laws, obtained without prefactors in Refs. [42,46]. The fact that similar results have been obtained by a different analytic method provides another proof of their accuracy.

The numerical simulations provided in [42,46] confirm their scaling laws and, equally, our time dependencies.

B. Models and methods

We would like also to make some remarks concerning the methods and the models.

We do not introduce explicit Langevin-type noise in the evolution. We start with the master equation, where thermal Langevin fluctuations are accounted for in an averaged form. In our opinion, if the number of particles is large, the self-averaging properties are governed by the quenched disorder and not by the explicit noise. This is backed up by the fact that the scaling laws, obtained in Refs. [42,46], agree with our results.

Typical situations involve a macroscopic number of contributing particles. Then, description in terms of noise-averaged site populations (or concentration of particles in space) instead of noise-driven single-particle trajectories is typically quite adequate. This simpler noise-averaged formulation enables a rigorous and transparent study of the leading effect of quenched disorder. The explicit account of Langevin noise, in our opinion, is necessary when one has to trace single or a few particles.

We do not have any time averages in the course of our solution. As noted above, we do not introduce noise ensemble or noise averages. Therefore, we do not discuss ergodicity. The only ensemble we have is constituted of the realizations of the static disorder.

The method, based on the statistics of distinct sites, visited by a random walk on a regular lattice seems to be of a limited applicability. It is satisfactory for a random trap model, when the escape rates from a trap are the same for the exit to any of its nearest neighbors. Then the topology of the trajectories is similar to the ones in a regular system and, consequently, some statistics for regular systems can be used. In the other cases, when the exit probabilities to the nearest neighbors are not the same, the topology of the trajectories changes drastically. A clear example of this is a percolation-type system with isolated clusters, where the statistics and the results are entirely different; cf. [23]. In all such cases, averaging with the statistics for trajectories in regular systems becomes inaccurate. In the models of disorder, except for random traps, the process of “sampling” is inseparable from the correct account of the topology of the trajectories. In our treatment, the correct trajectories are generated by the perturbation expansions (13) and (17) automatically.

C. Qualitative picture

Next, after having provided the quantitative results in Sec. V, let us discuss the dilemma of “self-averaging” or “non-self-averaging” on a qualitative level. The qualitative picture becomes more transparent if we focus on the time dependence of the reciprocal standard deviation of the diffusion coefficient

TABLE I. The long-time evolution of the average value of the diffusion coefficient $D(\tau)$ and of its reciprocal standard deviation $\mathrm{Var}^{1/2}[D(\tau)]/D(\tau)$, as functions of dimensionless time $\tau = w_0 t,\ \tau \gg 1$. The power-law decay of the reciprocal standard deviation signifies self-averaging. Logarithmic decay corresponds to weak self-averaging. Nonvanishing of the reciprocal standard deviation manifests non-self-averaging. In table headings we use abbreviated notations for the cases (3a)–(3g).

	Reg Eq. (3a) +subreg 1 Eq. (3b), $\beta > 1$	Subreg 2 Eq. (3c), $\beta = 1$	Subreg 3 Eq. (3d), $0 < \beta < 1$	Subdisp Eq. (3e), $\beta = 0$	Disp Eq. (3f), $0 < \alpha = -\beta < 1$	Irreg Eq. (3g)
$D(\tau)$		$\approx\tau^0$, Eq. (25)		$\approx\ln^{-1}\tau$, Eq. (31)	$\approx\tau^{-\frac{\alpha}{2-\alpha}}$, $d = 1$, Eq. (35) $\approx\tau^{-\alpha}\ln^{\alpha}\tau$, $d = 2$, Eq. (36) $\approx\tau^{-\alpha}$, $d = 3$, Eq. (37)	$\approx\tau^{-1}$, Eq. (41)
$\frac{\mathrm{Var}^{\frac{1}{2}}[D(\tau)]}{D(\tau)}$	$\approx\tau^{-\frac{d}{4}}$, Eq. (26)	$\approx\frac{\ln^{\frac{1}{2}}\tau}{\tau^{\frac{d}{4}}}$, Eq. (27)	$\approx\tau^{-\frac{\beta}{4}}$, $d = 1$, Eq. (28) $\approx\tau^{-\frac{\beta}{2}}\ln^{\frac{1-\beta}{2}}\tau$, $d = 2$, Eq. (29) $\approx\tau^{-\frac{1+2\beta}{4}}$, $d = 3$, Eq. (30)	$\approx\ln^{-\frac{1}{2}}\tau$, $d = 1$, Eq. (32) $\approx\ln^{-1}\tau$, $d = 2$, Eq. (33) $\approx\tau^{-\frac{1}{4}}\ln^{-\frac{1}{4}}\tau$, $d = 3$, Eq. (34)	$\approx\tau^0$, $d = 1$, Eq. (38) $\approx\ln^{-\frac{1}{2}}\tau$, $d = 2$, Eq. (39) $\approx\tau^{-\frac{1-\alpha}{4}}$, $d = 3$, Eq. (40)	$\approx\tau^0$, Eq. (42)

$\mathrm{Var}^{1/2}[D(\tau)]/D(\tau)$ as a function of dimensionless time $\tau = w_0 t$. The long-time limit $\tau \gg 1$ is summarized in Table I.

The average value of the diffusion coefficient $D(\tau)$ diminishes with the increase of the disorder. It changes from a time-independent constant $\approx\tau^0$ through the logarithmic decay $\approx\ln^{-1}\tau$ and a faster power-law decay $\approx\tau^{-\alpha/(2-\alpha)}$, $\approx\tau^{-\alpha}\ln^{\alpha}\tau$, and $\approx\tau^{-\alpha}$ in 1D, 2D, and 3D, respectively, to $\approx\tau^{-1}$ for irreversible trapping. The latter corresponds to a limited mean-square displacement and forms, in fact, an intermediate-time asymptotic with the fluctuation tail left out. All these cases of the averaged evolution were traced in [21–24].

The main topic of the present study is self-averaging and non-self-averaging of the diffusion coefficient. At short time, the dispersion of the diffusion coefficient (24) is proportional to the degree of disorder and thus it is not small. In the intermediate-time domain the dispersion is not small either. Only at long time, the sample-to-sample fluctuations may start to decay; see the bottom row of Table I.

1. Regular self-averaging

Regular self-averaging at long time, Fig. 2, takes place in the cases of "relatively weak" disorder, starting with the regular case (3a), the column on the left. This "normal" self-averaging is, nevertheless, of a rather slow power-law-type $\approx\tau^{-d/4}$ [15,23]. With the increasing disorder (the columns to the right), the self-averaging slows down more for low-dimensional systems in the first place. In the subregular 2 case (3c) a logarithmic factor appears. In the subregular 3 case the exponent becomes β dependent (2). However, for all subregular cases, self-averaging remains of the power-law type. In 3D the regular power-law self-averaging persists even in the more strongly disordered subdispersive (3e) and dispersive (3f) cases. In the former, an additional logarithmic factor appears; in the latter, the exponent becomes α dependent.

2. Weak self-averaging

The weak (logarithmic) self-averaging appears in the subdispersive case (3e), Fig. 3, in one- and in two dimensions, $\approx\ln^{-1/2}\tau$ and $\approx\ln^{-1}\tau$, respectively. Weak self-averaging also persists in the stronger-disordered dispersive case in 2D $\approx\ln^{-1/2}\tau$. In practice, such logarithmic decay of fluctuations in time should hardly be observable.

3. Non-self-averaging

Non-self-averaging appears first in the dispersive case (3f) in 1D, Fig. 4. In the irreversible case (3g), the diffusion coefficient, calculated for all the particles, not the survivors only, is non-self-averaging in all dimensions. For both of these cases the variance of the diffusion coefficient is of the same order as its average value. Besides, we note that in the latter case, in fact, not the long-time asymptotics, but the intermediate-long-time asymptotics is implied, cf. [47].

4. General remarks

Within each case (column) the self-averaging gets worse with the diminishing dimension.

The crossover between all these regimes is traced qualitatively in Sec. V.

Weak self-averaging and, especially, non-self-averaging signify that the fluctuations of the measured diffusion coefficient are large. In the case of weak self-averaging, the tendency to the diminishing of these fluctuations will not be obvious. For non-self-averaging, the fluctuations remain of the same order as its average value. In experiments, this will be manifest as a huge dispersion of the measured quantities, in different samples and with different initial conditions (starting points). Not only the values, but also the shapes of the measured time-dependent curves may differ considerably in different samples. Single curves may deviate considerably from the calculated averages as well. In this case, the theoretical average can be practically restored only as a result of an averaging process over an anomalously large number of realizations or samples or measurements. The convergence of the averages in the measurements is expected to be anomalously slow.

Thus, all the regimes, starting with the subdispersive case (3e) are anomalous in terms of the average kinetics (the diffusion coefficient). Anomaly in the fluctuations decay starts with the subregular 2 case (3c). Non-self-averaging starts with the 1D dispersive (3f) case. The dispersion of the values of the diffusion coefficient in the irreversible case (3g) in the intermediate-long-time domain in all dimensions remains of the same order as its average value.

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