Random walks and anomalous diffusion in two-component random media

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The diffusion process in a random media consisting of two different components is studied by a random walk model. The latter is described by three parameters, namely, the fraction p of components, the ratio h of the diffusion coefficients in two components, and the parameter x defining a walker's jumps at the boundary. Depending on the values of these parameters the diffusion can be confined, normal, or anomalous (subdiffusion). The subdiffusion occurs, in particular, for $h=0$ (trapping model) and for $x=0$ (excluded volume model).

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I. INTRODUCTION

Random processes are of critical importance in all fields of nature [1]. There are two methods of approaching the problem of random transport. The microscopic method starts from the law of motion of an individual particle subjected to a random (and possible deterministic) force. The second, macroscopic, method treats an ensemble of particles and deals with such averaged concepts as the diffusion coefficients. These two methods are connected in the sense that the averaging over the random force in the microscopic equations gives the microscopic expression for the phenomenological coefficients in the macroscopic equations.

The Langevin equation and the random walk method are two common ways of treating the motion of a single particle. The Langevin equation is simply Newton's law for a Brownian particle of mass m subjected to the deterministic viscous force, $-\gamma(dx/dt)$, and random force $\xi(t)$

$$m\frac{d^2x}{dt^2}+\gamma\frac{dx}{dt}=\xi(t). \tag{1}$$

Instead of continuous variables x and t in Eq. (1), one can consider the discrete variables in the random walk of a particle on a periodic lattice with discrete jumps occurring at a regular discrete rate.

If the random force in Eq. (1) is the Gaussian white noise, so that

$$\langle\xi(t)\rangle=0, \quad \langle\xi(t)\xi(t_1)\rangle=2D\delta(t-t_1), \tag{2}$$

then the mean-square displacement $\overline{R^2(t)}\equiv\langle x^2-\langle x\rangle^2\rangle$ increases linearly with t for long times. The same limit law is obtained for a random walk of a particle executing equiprobable transitions to one of the nearest lattice sites in equal time intervals.

In the macroscopic approach the diffusion coefficient D enters the diffusion equation for the concentration $c(x,t)$

$$\frac{\partial c}{\partial t}=D\frac{\partial^2 c}{\partial x^2}. \tag{3}$$

However, it turns out that in many fields of natural science (dozens of examples can be found in the comprehensive reviews [2], [3]) diffusion is anomalous, namely, for large t

$$\overline{R^2(t)}\sim t^{\zeta}, \tag{4}$$

where the cases with $\zeta<1$ and $\zeta>1$ are called subdiffusion and superdiffusion, respectively, while $\zeta=1$ corresponds to normal diffusion.

The question arises as to whether the anomalous diffusion law (4) can be obtained from the foregoing Langevin equation or from the random walk approach. To this end, different generalizations of Eq. (1) have been proposed. These include: (a) the use of a power law correlation for the random force instead of Eq. (2); (b) the consideration of a power law time dependence of the viscosity $\gamma(t)$ [4]; and (c) the introduction of memory effects by replacing the viscous term in Eq. (1) by an integral operator with a special form of the kernel $\gamma(t-\tau)$ [5]. One can also obtain anomalous diffusion from a more complicated version of the random walk by assuming that a particle is able to execute jumps of very large distances (not only to nearest neighbors) or to wait for some time on a site before performing the next jump, being thereby temporarily immobilized. It is intuitively clear that the motion of a particle will be faster in the first case (superdiffusion) and slower in the second one (subdiffusion). It turns out [3] that the quantitative criteria for the appearance of anomalous diffusion are the divergence of the averaged square coordinates and of the averaged waiting time, respectively.

The possibility exists of anomalous diffusion in the random walk model not only by changing the rules of jumps of a particle, but also by changing the structure of the lattice on which a particle is moving. The best known example is that of random walks on a fractal self-similar structure [6]. Other more specific hierarchical structures are nested structures [7] or those with ultrametric topology [8]. In these cases the diffusion Eq. (3) has to be modified, e.g., by introducing fractional derivatives.

Anomalous diffusion occurs also in the so-called trapping problems, where a particle performs random walks in media with the overall fraction p covered by traps which are able to capture a particle [9]. In the trap model a system containing traps can be considered as a two-component system such that a particle moves in one of the components and becomes immobile in the second one. In our approach both components have nonzero diffusion coefficients. Although the diffusion in each component is normal, the effective diffusion coeffi-

cients become anomalous due to special anisotropic conditions at the boundary between two components.

II. LATTICE RANDOM WALK MODEL

We have considered [10] the generalized trapping problem where a lattice consists of two types of regions with different diffusion coefficients D_1 and D_2 for the moving particle with $h=D_2/D_1$. If $h=0$, the second region becomes a capturing one, and we come back to the trapping model. As in the trapping model, we assume that the two regions are randomly placed, with the overall fractions p and $1-p$. Hence, instead of one parameter p in the trapping problems, we have now two parameters p and h.

Since we are interested in the asymptotic behavior, the details at small distances are of no importance, and the random medium can be approximated by a lattice of units L_0. There are two types of bonds which, with probabilities p and $1-p$, defined by the concentrations of the two components. Accordingly, there are two characteristic times $\tau_1=L_0^2/D_1$ and $\tau_2=L_0^2/D_2$ with $h=\tau_1/\tau_2$.

In addition to two parameters p and h we introduce a third parameter x which plays a role of transmission factor, that determines how easily the random walker can pass to another domain. Although macroscopically the system remains isotropic, we introduce a local anisotropy by defining the direction of the next jump for a particle which reaches the boundary of two regions. If x is defined as the ratio of the probability to jump into the second region to that into the first one, then this parameter, by definition, equals unity for a locally isotropic medium, and equals zero when one of the components of the medium is completely nonpenetrable (excluded volume model).

The aim of this article is to show that the two-component disordered medium provides another microscopic model for anomalous diffusion. It turns out that there are at least two situations in which subdiffusion can take place. The first one corresponds to the excluded volume model with $x=0$, and the second one is the trapping model with $h=0$. These two models of random walks will be analyzed below. One can obtain anomalous diffusion in a more general case as well, by introducing correlations between successive jumps in the original lattice, but we leave this more complicated case for future investigations.

III. SCALING TRANSFORMATION

A. Original lattice

Our scaling analysis is quite similar to the Migdal-Kadanoff renormalization scheme used in the theory of critical phenomena [11]. However, we do not use this approach to calculate the exact values of the critical indices (for which there are more accurate methods), but rather to derive the very existence of the anomalous behavior of the diffusion coefficient.

To illustrate the scaling procedure let us consider the transition from the one-unit trajectories of random walks to the two-unit ones. As is shown in Fig. 1, there are three possible ways of continuation to the second jump after performing

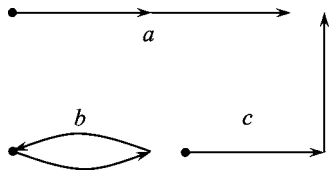

FIG. 1. The possible two-unit trajectories.

one of the $2d$ possible first jumps, where d is the dimension of space. One can continue in the same direction [Fig. 1(a)], or go back [Fig. 1(b)] or, finally, go in one of $(2d-2)$ perpendicular directions [Fig. 1(c)]. The total number of possible two-unit jumps is $2d+2d+2d(2d-2)=4d^2$. On the other hand, the distances covered are $2L_0$, zero, and $\sqrt{2}L_0$, respectively. Therefore, the averaged square distance $\tilde{L}^2$ will be $[2d(4L_0^2)+2d\times 0+2d(2d-2)(2L_0^2)]/4d^2=2L_0^2$, and $\tilde{L}=\sqrt{2}L_0$ independently of the dimension of space.

The presence of local anisotropy of particle jumps leads to the different probabilities to perform one step of random walk on bonds of the first or of the second types being

$$P_0=\frac{p_0}{p_0+x_0(1-p_0)},\quad 1-P_0=\frac{x_0(1-p_0)}{p_0+x_0(1-p_0)}. \tag{5}$$

Therefore, for the one-bond trajectories of random walks the mean square displacement independently of the time of the walk is

$$\overline{R_0^2}=P_0L_0^2+(1-P_0)L_0^2\equiv(\overline{R^2})_{01}+(\overline{R^2})_{02}. \tag{6}$$

But the mean square displacement for time τ_1 (the diffusive mean square displacement) is

$$\begin{aligned}\overline{R_d^2}&=P_0\frac{L_0^2}{\tau_1}\tau_1+(1-P_0)\frac{L_0^2}{\tau_2}\tau_1\\&=P_0L_0^2+(1-P_0)hL_0^2\\&\equiv(\overline{R_d^2})_{01}+(\overline{R_d^2})_{02},\end{aligned} \tag{7}$$

and the mean diffusion coefficient $\bar{D}_0$ is

$$\bar{D}_0=P_0D_1+(1-P_0)D_2\equiv D_{01}+D_{02}. \tag{8}$$

Here and in the following we denote all parameters for the initial lattice by subindex zero.

Taking into account the fact that

$$x_0=\left(\frac{p_0}{1-p_0}\right)\frac{(\overline{R^2})_{02}}{(\overline{R^2})_{01}}, \tag{9}$$

$$h_0=\frac{p_0}{x_0(1-p_0)}\frac{(\overline{R_d^2})_{02}}{(\overline{R_d^2})_{01}}=\frac{(\overline{R^2})_{01}}{(\overline{R^2})_{02}}\frac{(\overline{R_d^2})_{02}}{(\overline{R_d^2})_{01}}=\frac{(\overline{R^2})_{01}}{(\overline{R^2})_{02}}\frac{D_{02}}{D_{01}},$$

we can describe the system by Eqs. (6), (7), (8), and (9) which define the mean square displacement R_0^2, the mean square displacement for time τ_1, the mean diffusion coefficient $\bar{D}_0$, and the parameters x_0 and p_0. In the next section we find these parameters $(R_1^2,\bar{D}_1,x_1,p_1)$ for an enlarged lattice.

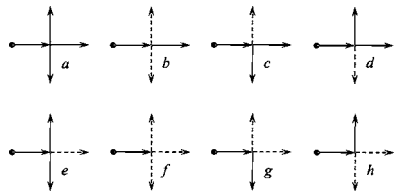

FIG. 2. The bonds of two-unit trajectories.

B. Two-unit lattice

For the enlarged two-unit lattice (two bonds of the original lattice), there are three types of new bonds shown in Fig. 1, where each one of them may contain two units of the first or of the second types and mixed bonds containing one unit of each type. While the new bonds of the first two groups clearly belong to the first and the second types, respectively, the new bonds of the third group have to be distributed among the bonds of two types in some proportion, since the enlarged lattices, as an initial one, has to contain only two types of bonds. The fact that each type of enlarged lattice bond contains the mixed bonds of the initial lattice results in the appearance of some correlation in bond location even if the initial bond location was non-correlated. So, we have to introduce the conventional probabilities for the second bonds in the two-unit trajectories. If the first bond is of the first type, let the conventional probabilities for the second bond $Q(p,x)$ and $Q(1-p,x)$ belong to the same or of the other type, respectively.

1. Mean square displacement

Let us illustrate the calculation of the mean square displacement by the example of a two-dimensional lattice of bond L_0, and an enlarged lattice composed of two-unit bonds of the original lattice. Of the three possible two-unit bonds shown in Fig. 1 only those shown in Figs. 1(a) and 1(c) contribute to the mean square displacement.

All possible two-unit bonds are shown in Fig. 2, where the bonds of the first and second types are depicted by solid and dotted lines, respectively, and the first step being performed in the horizontal direction on the bond of the first type with the probability P_0 (the bond coming from the left in Fig. 2). The next step in the same direction can be either on the bond of the first type with conventional probability $P_0Q(p_0,x_0)$ [Figs. 2(a)–2(d)] or on the bond of the second type with probability $P_0[1-Q(p_0,x_0)]$ [Figs. 2(e)–2(h)]. In both cases the vertical bonds will be of the first type with probability $Q(p_0,x_0)^2$ [Figs. 2(a), 2(e)], or of the second type with probability $[1-Q(p_0,x_0)]^2$ [Figs. 2(b), 2(f)], or of different types with probability $Q(p_0,x_0)[1-Q(p_0,x_0)]$ [Figs. 2(c)–2(d), 2(g)–2(h)]. The overall contribution to the mean square displacement on a distance $\sqrt{2}L_0$ will be

$$
\begin{aligned}
R_I^2 = P_0 Q(p_0,x_0) &\Bigg\{ Q(p_0,x_0)^2 + 2Q(p_0,x_0)[1-Q(p_0,x_0)] \\
&\times \left(\frac{4-1}{4-1+x_0} + \frac{x_0}{4-1+x_0} \right) \\
&+ [1-Q(p_0,x_0)]^2 \\
&\times \left(\frac{4-2}{4-2+2x_0} + \frac{2x_0}{4-2+2x_0} \right) \Bigg\} 2L_0^2 \\
&+ P_0[1-Q(p_0,x_0)] \\
&\times \Bigg\{ Q(p_0,x_0)^2 \left(\frac{4-2}{4-1+x_0} + \frac{2x_0}{4-1+x_0} \right) \\
&+ 2Q(p_0,x_0)[1-Q(p_0,x_0)] \left(\frac{4-3}{4-2+2x_0} + \frac{3x_0}{4-2+2x_0} \right) \\
&+ [1-Q(p_0,x_0)]^2 \left(\frac{4-4}{4-3+3x_0} + \frac{4x_0}{4-3+3x_0} \right) \Bigg\} 2L_0^2 .
\end{aligned}
\tag{10}
$$

Additional factors in Eq. (10) containing x_0, take into account the fact that each connection between bonds of different types brings an additional factor x_0. The form of these terms depends on the type of the bonds of the first type (n_1) and the second one (n_2) into which the particle can pass, which gives the factors $n_1/(n_1+x_0n_2)$ and $x_0n_2/(n_1+x_0n_2)$.

Equation (10) can be rewritten in the following form:

$$
R_I^2 = P_0\{Q(p_0,x_0)F_1(p_0,x_0) + x_0[1-Q(p_0,x_0)]F_2(p_0,x_0)\}2L_0^2, \tag{11}
$$

where

$$
F_1(p_0,x_0) = 1 + (1-x_0)\left\{ \frac{2Q(p_0,x_0)[1-Q(p_0,x_0)]}{4-1+x_0} + \frac{2[1-Q(p_0,x_0)]^2}{4-2+2x_0} \right\} \tag{12}
$$

and

$$
F_2(p_0,x_0) = 1 + (1-x_0)\left\{ \frac{Q(p_0,x_0)^2}{4-1+x_0} + \frac{4Q(p_0,x_0)[1-Q(p_0,x_0)]}{4-2+2x_0} + \frac{3[1-Q(p_0,x_0)]^2}{4-3+3x_0} \right\}. \tag{13}
$$

For an arbitrary number of dimensions d, Eq. (11) remains the same, but the functions $F_1(p_0,x_0)$ and $F_2(p_0,x_0)$ have the following form:

$$
F_1(p_0,x_0) = 1 + (1-x_0)\sum_{k=1}^{2d-2} \frac{kC_{2d-2}^k}{2d-k+kx_0} \times Q(p_0,x_0)^{2d-2-k}[1-Q(p_0,x_0)]^k, \tag{14}
$$

$$
F_2(p_0,x_0) = 1 + (1-x_0)\sum_{k=0}^{2d-2} \frac{(k+1)C_{2d-2}^k}{2d-(k+1)+(k+1)x_0} \times Q(p_0,x_0)^{2d-2-k}[1-Q(p_0,x_0)]^k, \tag{15}
$$

where C_n^k are the binomial coefficients. For $d=2$, Eqs. (14) and (15) reduce to Eqs. (12) and (13).

So far we considered the case where the first step was on the bond of the first type. Repeating the same calculation for the first bond of the second type, one gets for the contribution to the mean squared displacement,

$$R_{\mathrm{II}}^2 = (1-P_0)\{[1-Q(1-p_0,x_0)]\tilde{F}_1(p_0,x_0) + x_0 Q(1-p_0,x_0)\tilde{F}_2(p_0,x_0)\}2L_0^2, \tag{16}$$

where

$$\tilde{F}_1(p_0,x_0) = 1 + (1-x_0)\sum_{k=0}^{2d-2} \frac{(k+1)C_{2d-2}^k}{2d-(k+1)+(k+1)x_0} \times [1-Q(1-p_0,x_0)]^{2d-2-k} Q(1-p_0,x_0)^k, \tag{17}$$

and

$$\tilde{F}_2(p_0,x_0) = 1 + (1-x_0)\sum_{k=0}^{2d-2} \frac{(k+2)C_{2d-2}^k}{2d-(k+2)+(k+2)x_0} \times [1-Q(1-p_0,x_0)]^{2d-2-k} Q(1-p_0,x_0)^k. \tag{18}$$

Combining now Eqs. (11) and (16), one gets the final expression for the mean squared displacement of the enlarged lattice

$$\overline{R_1^2} = \{P_0 Q(p_0,x_0)F_1(p_0,x_0) + x_0(1-P_0)Q(1-p_0,x_0)\tilde{F}_2(p_0,x_0) + x_0 P_0[1-Q(p_0,x_0)]F_2(p_0,x_0) + (1-P_0)[1-Q(1-p_0,x_0)]\tilde{F}_1(p_0,x_0)\}. \tag{19}$$

2. Diffusion coefficient

Equation (19) contains three types of the two-units bond, namely, the first term in Eq. (19) corresponds to the two-unit bonds of the first type, the second term describes those of the second type, and the last two terms represent the mixed two-unit bonds composed from the single bonds of two different types. However, our original lattice contains only bonds of two types, and this main property must remain unchanged during the scaling transformations. Therefore, let us split the last two terms in Eq. (19) into two parts in ratio $\alpha(x_0,p_0,h_0)$ and $1-\alpha(x_0,p_0,h_0)$ belonging to the first and to the second type, respectively. Then the mean square displacement of the enlarged lattice (19) can be rewritten as

$$\overline{R_1^2} = \overline{R_{11}^2} + \overline{R_{12}^2}, \tag{20}$$

where

$$\overline{R_{11}^2} = \{P_0 Q(p_0,x_0)F_1(p_0,x_0) + [x_0 P_0[1-Q(p_0,x_0)]F_2(p_0,x_0) + (1-P_0)[1-Q(1-p_0,x_0)]\tilde{F}_1(p_0,x_0)] \times \alpha(p_0,h_0,x_0)\}2L_0^2, \tag{21}$$

and

$$\overline{R_{12}^2} = \{x_0(1-P_0)Q(1-p_0,x_0)\tilde{F}_2(p_0,x_0) + [x_0 P_0[1-Q(p_0,x_0)]F_2(p_0,x_0) + (1-P_0)[1-Q(1-p_0,x_0)]\tilde{F}_1(p_0,x_0)] \times [1-\alpha(p_0,h_0,x_0)]\}2L_0^2. \tag{22}$$

In order to find the mean square displacement for time $2\tau_1$ (the diffusion displacement in an enlarge lattice) one has to take into account that the characteristic time of a walk along the enlarged bond of the mixed type is $\tau_1+\tau_2$, and the characteristic time of a walk along the enlarged bond of the second type is $2\tau_2$. Therefore, one has to change the second terms in Eq. (21) and the first term in Eq. (22) in the ratio $2\tau_1/(\tau_1+\tau_2)=2h/(1+h)$, as well as the second terms in Eq. (22) in the ratio $2\tau_1/2\tau_2=h$.

Then, one gets for the diffusion coefficient

$$\overline{D_1} = \overline{D_{11}} + \overline{D_{12}}, \tag{23}$$

where

$$D_{11} = \left\{ P_0 Q(p_0,x_0)F_1(p_0,x_0) + \{x_0 P_0[1-Q(p_0,x_0)\}F_2(p_0,x_0) + (1-P_0)[1-Q(1-p_0,x_0)]\tilde{F}_1(p_0,x_0)] \times \frac{2h_0\alpha(p_0,h_0,x_0)}{1+h_0} \right\} D_1 \tag{24}$$

and

$$D_{12} = \left\{ x_0(1-P_0)Q(1-p_0,x_0)\tilde{F}_2(p_0,x_0) + \{x_0 P_0[1-Q(p_0,x_0)]F_2(p_0,x_0) + (1-P_0)[1-Q(1-p_0,x_0)]\tilde{F}_1(p_0,x_0)\} \times \frac{2[1-\alpha(p_0,h_0,x_0)]}{1+h_0} \right\} D_2. \tag{25}$$

3. Two types of enlarged bonds

The ratio of two types of bond changes during the scaling transformations reaching, after macroscopic average, one of the fix point values, $p=0$, $p=1$, or $p=1/2$. The ratio of the two-unit bonds of the first type p_1 is composed of those consisting two single bonds of the first type with probability $P_0Q(p_0)$, and those that appeared [in ratio $\alpha(p_0,x_0,h_0)$] from the mixed bonds, i.e.,

$$P_1 = P_0 Q(p_0,x_0) + \{P_0[1-Q(p_0,x_0)] + (1-P_0)[1-Q(1-p_0,x_0)]\}\alpha(p_0,h_0,x_0). \tag{26}$$

C. Connection with percolation theory

In order to find the function $\alpha(p_0,x_0,h_0)$, one can compare our diffusion problem with that of the percolation theory. There is no different interaction of a walking particle with two types of bonds in the percolation theory, i.e., x_0

$=1$. There are two types of bonds in a percolation problem (say, those with good and bad conductivity), and in the scaling transformation in the percolation problem [12], one also divides the mixed bonds into two types in ratio $\mu(p_0)$ and $1-\mu(p_0)$. Then, the averaging over the displacement (at specific time) in the percolation problem is equivalent to the average over times (at specific displacement) in our problem

$$\bar{D} = \alpha(p_0,h_0,x_0=1)\frac{L_0^2}{\tau_1} + [1-\alpha(p_0,h_0,x_0=1)]\frac{L_0^2}{\tau_2} = \frac{L_0^2}{\bar{\tau}}, \tag{27}$$

where the mean-time $\bar{\tau}$ is $\bar{\tau}=\mu(p_0)\tau_1+[1-\mu(p_0)]\tau_2$.

It follows from Eq. (27) that

$$\alpha(p_0,h_0,x_0,=1) = \frac{\mu(p_0)h_0}{\mu(p_0)h_0+[1-\mu(p_0)]}. \tag{28}$$

Assume that for $x_0 \neq 1$ the mean-time $\bar{\tau}$ can be generalized to the following form:

$$\bar{\tau} = \frac{\tau_1 f_1(p,h,x)+\tau_2 f_2(p,h,x)}{f_1(p,h,x)+f_2(p,h,x)} = \frac{\tau_1+\tau_2 F(p,h,x)}{1+F(p,h,x)}, \tag{29}$$

where $F(p,h,x)=f_2(p,h,x)/f_1(p,h,x)$.

Due to the arbitrary definition of the bonds of the first and the second type, there are the following symmetry properties of the function $F(p,h,x)$:

$$F(1-p,1/h,1/x) = 1/F(p,h,x). \tag{30}$$

By using Eqs. (27)–(29) one easily obtains that for $x=1$, $F(p,h,x=1)=[1-\mu(p)]/\mu(p)$. In addition, in two extreme cases, $x=0$ and $x=\infty$, the mixing parameter has to be the same as for the percolation problem, i.e., $F(p,h,x=0,\infty)=h[1-\mu(p)]/\mu(p)$.

The simplest form of the function $F(p,h,x)$ which meets these requirements is

$$F(p,h,x) = \frac{1-\mu(p)}{\mu(p)}\frac{hx^2+2x+h}{x^2+2xh+1}, \tag{31}$$

which gives

$$\alpha(p,h,x) = \frac{\mu(p)(x^2+2xh+1)h}{\mu(p)(x^2+2xh+1)h+[1-\mu(p)](hx^2+2x+h)}. \tag{32}$$

The function $\mu(p)$ in the percolation problem defines the separation of the mixed two units bonds into those of the first and the second types. To find the form of the function $\mu(p)$ in two dimension, let us consider the bonds shown in Fig. 3. The type of the new bond ac is determined by the properties of single bonds ab, bc, cd, and da of the original lattice. If all four bonds, or three of them [four possibilities with probability $p_0^3(1-p_0]$ belong to the first type, then the bond ac of the enlarged lattice belong to the same type. If, however, two single bonds belong to the first type and two bonds are of the second type (six possibilities with probability $p_0^2[1-p_0]^2$), only half of them result in the first type of bond of the enlarged lattice. Then, the ratio of the bonds of the first type in the enlarged lattice p_1 will be the following function of p_0:

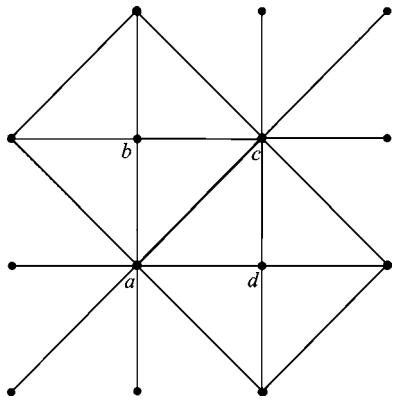

FIG. 3. The initial and enlarged lattices.

$$p_1 = p_0^4 + 4p_0^3(1-p_0) + \frac{1}{2}6p_0^2(1-p_0)^2$$
$$= p_0 - p_0(1-p_0)(1-2p_0). \tag{33}$$

Substituting into Eq. (26) the approximate value of $Q(p)$, $Q(p)=p$, as well as the expression (32) for $\alpha(p,x=1,h=1)$ and comparing the obtained equation with Eq. (33), one gets

$$\mu(p) = p \quad \text{for } d=2. \tag{34}$$

By similar arguments one can show that in three dimensions

$$\mu(p) = 0.5[1-(1-4p)(1-2p)(1-4p/3)] \quad \text{for } d=3. \tag{35}$$

D. Differential form of scaling transformations

Equation (33) defines the discrete transformation from the original lattice of size L_0 to the enlarged lattice of size $\sqrt{2}L_0$. One can pass from this discrete transformation to infinitesimal ones, changing thereby the difference equations into the differential ones. For two dimension, for example, one can rewrite Eq. (33) in the form

$$\frac{dp(n)}{dn} \approx \frac{p_1-p_0}{1} = -p(n)[1-p(n)][1-2p(n)]. \tag{36}$$

Equation (36) has two stable steady-states $p_0^*=0$, $p_1^*=1$, and one unstable steady-state $p^*=0.5$ which corresponds to the percolation threshold of a system.

One can write the differential form of other equations of the scaling transformations as well, but we prefer not to do it in the general case, but rather consider the special cases of the trapping model ($h=0$) and of the excluded volume model ($x=0$).

IV. TRAPPING MODEL

The special case of our model is one with $D_2=0$, and consequently $h=0$. It means that a walking particle is captured by the bonds of the second type, and remains immobilized (trapping model). We restrict ourselves to the simplified version of our model putting $x=1$, which corresponds to the

properties of most of the real systems and assumed in the well-known trapping model [9]. Then, our general formulas for the scaling transformation are substantially simplified leading to

$$P_0 = p_0, \quad F_1 = F_2 = 1, \quad \alpha = 0, \quad \bar{D}_1 = p_0 Q(p_0) D_1, \tag{37}$$

$$p_1 = P_1 = p_0 Q(p_0).$$

All relations in Eq. (37) are readily obtained from Eqs. (5), (11)–(13), (23), (26), and (32), respectively by substituting $h=0$ and $x=1$. Here and later on we omit the argument $x=1$ in function $Q(p,x)$.

From the last equation in Eq. (37) one gets on the nth step of the scaling transformations

$$p_{n+1} - p_n = -p_n[1 - Q(p_n)]. \tag{38}$$

The standard way of analysis of the scaling transformations involves the transition from the discrete n transformation (38) to the continuous dependence on n, i.e., on time of walk t, $dp/dn=(dp/dt)(dt/dn)=t(dp/dt)$. Then, Eq. (38) becomes

$$t\frac{dp}{dt} = -p(t)[1 - Q(p)]. \tag{39}$$

Due to the traps, the correct asymptotic solution of Eq. (39) which vanishes at $t \to \infty$, has the following form:

$$\frac{p(t)}{p_0} \sim \left(\frac{t}{\tau_1}\right)^{-[1-Q(p=0)]}. \tag{40}$$

The concentration of the walking particles will decrease with time due to their capture by the trapping centers. The rate of this decrease on the nth step dC/dn is proportional to the overall concentration of the walking particles in the regions in which there are no traps C/p and the probability $1-Q(p)$ to meet a trap

$$\frac{dC}{dn} \equiv t\frac{dC}{dt} = -\frac{[1 - Q(p)]}{p}C. \tag{41}$$

Division of Eq. (41) by Eq. (39) gives $dC(p)/dp=-C(p)/p^2$ with the asymptotic solution for the so-called survival probability, $C[p(t)]$

$$C(t) = C_0 \exp\left[-A\left(\frac{t}{\tau_1}\right)^{1-Q(p=0)}\right]. \tag{42}$$

One can compare the last equation with the general result for the survival probability in a d-dimensional trapping system obtained by different methods [9,13,14]

$$C(t) = \exp\left[-A\left(\frac{t}{t_0}\right)^{d/(d+2)}\right]. \tag{43}$$

Comparison of Eqs. (42) and (43) shows that

$$1 - Q(p=0) = \frac{d}{d+2}. \tag{44}$$

From the two last equations in Eq. (37), one gets for the diffusion coefficient

$$\frac{dD_1}{dp} = \frac{D_1}{p}, \tag{45}$$

which gives $D_1(t)/D_0=p(t)/p_0$, and using Eq. (40) we finally obtain

$$\overline{R^2(t)} = D_1(t)t \approx t^{2/(d+2)}. \tag{46}$$

Hence, our method shows anomalous (subdiffusive) behavior of a system with trapping centers in all dimensions.

V. EXCLUDED VOLUME MODEL

Another limit case that results in an essential simplification of the equations of scaling transformation is that of the excluded volume, i.e., the bonds of the second type are completely impenetrable for a walking particle. Then, all the properties of the second type of bonds cannot influence the diffusion of a walking particle. Indeed, in our formalism the excluded volume corresponds to the special value of parameter x, namely, $x=0$. Then, as follows from Eq. (5), $1-P_0=0$, which, in turn, means that parameters h and D_2 drop out from Eqs. (23), (26), and (28), leading to

$$\bar{D}_1 - D_1 = [Q(p_0)F_1(p_0, x_0 = 0) - 1]D_1, \quad \alpha = \mu(p),$$
$$p_1 - p_0 = -p_0[1 - Q(p_0)][1 - 2\mu(p_0)]. \tag{47}$$

From three parameters of our theory, p, h, and x, only parameter p is imporant for the considered case of the excluded volume since h becomes nonrelevant, and x is fixed $x=0$. Accordingly, the symmetry property $p \rightleftarrows 1-p$ can be expressed as

$$p[1 - Q(p)] = (1 - p)[1 - Q(1 - p)]. \tag{48}$$

Since obviously $Q(p=1)=1$, it follows from Eq. (48) that $Q(p=0)=0$ in contrast to the trapping models. As in the previous section, the argument $x=0$ in function $Q(p,x)$ is omitted.

One can transfer the difference equations in Eq. (47) into differential equations, as was done in Eqs. (38) and (39), leading to

$$t\frac{dD(t)}{dt} = -[1 - Q(p)][1 - W(p)]D(t),$$

$$t\frac{dp(t)}{dt} = -p(t)[1 - Q(p)][1 - 2\mu(p)], \tag{49}$$

where $W(p)=Q(p)/1-Q(p)[F_1(p_0,x_0=0)-1]=1-1/2d-1\Sigma_{k=0}^{2d-2}[1-Q(p)]^k$.

Combining the two Eqs. (49), one obtains

$$\frac{dD}{dp} = \frac{D[1 - W(p)]}{p[1 - 2\mu(p)]}. \tag{50}$$

Let us consider separately the two- and three-dimensional cases.

A. Two dimensions

According to Eq. (34), $\mu(p)=p$ for $d=2$, and the second equation in Eq. (49) has two stable fixed points $p_0^*=0$ and

$p_1^*=1$ [since $Q(p=1)=1$], and one unstable fix point $p^* \approx 0.5$ (the exact value of the unstable fixed point p^* is not important for our goals).

Therefore, for $t\to\infty$, one gets

$$p(t) \sim \begin{cases} p_0(1-2p_0)^{-1/\alpha}(t/\tau_1)^{-1}, & p_0 < 0.5, \\ 0.5, & p_0 = 0.5, \\ 1-(1-p_0)[p_0(2p_0-1)^{-1/\alpha}(t/\tau_1)^{-1}]^{\beta}, & p_0 > 0.5, \end{cases} \tag{51}$$

where $\alpha=1-Q(p=0.5)>0$, $\beta=dQ(p)/dp|_{p=1}$.

Using Eq. (51) and the two-dimensional form of the function $W(p)$, $W(p)=1-1/3\{[1-Q(p)]^2+[1-Q(p)]+1\}$, one can easily find from Eq. (50) the diffusion coefficient D and the mean square displacement $R^2=Dt$ which gives

$$\overline{R^2(t)} = D(t)t \sim \begin{cases} (1-2p_0)^{-\nu}D_1\tau_1, & p_0 < 0.5, \\ \frac{1}{2}D_1\tau_1(t/\tau_1)^{\alpha\nu}, & p_0 = 0.5, \\ (2p_0-1)^{(1/\alpha)-\nu}D_1 t, & p_0 > 0.5. \end{cases} \tag{52}$$

here $\nu=\alpha^{-1}-\frac{1}{3}(\alpha^2+\alpha+1)>0$, $\alpha\nu<1$.

This result means that if the fraction of the excluded volume in a system is too high $(1-p_0>0.5)$, the diffusion is confined so that a walking particle remains in a restricted region. When passing from the confined diffusion at $p_0<0.5$ to the normal diffusion at $p_0>0.5$, the localization radius is increasing as $(1-2p_0)^{-\nu}$ and at a special point $p_0=0.5$ (percolation threshold in two dimension) the diffusion is anomalous (subdiffusion).

B. Three dimension

Substituting expression (35) for $\mu(p)$ in the second equation in Eq. (49), one finds that the latter equation has three stable fixed points: $p_0^*=0$, $p^*=0.5$, and $p_1^*=1$, and two nonstable fix points: $p_2^*=0.25$ and $p_3^*=0.75$. Taking into account the three-dimensional form of the function $W(p)$, $W(p)=1-\frac{1}{5}\{[1-Q(p)]^4+[1-Q(p)]^3+[1-Q(p)]^2+[1-Q(p)]+1\}$ one finds, analogously Eq. (52), the following asymptotic dependence of the mean square displacement in three dimension:

$$\overline{R^2(t)} \propto \begin{cases} (1-4p_0)^{-3\nu_1}D_1\tau_1, & p_0 < 1/4, \\ D_1\tau_1(t/\tau_1)^{\gamma\nu_1}, & p_0 = 1/4, \\ (4p_0-1)^{-3(\nu_1-\alpha\tilde{\nu}/\gamma)}(3-4p_0)^{-(\nu_2-\alpha\tilde{\nu}/\delta)}D_1\tau_1(t/\tau_1)^{\alpha\tilde{\nu}}, & 1/4 < p_0 < 3/4, \\ D_1\tau_1(t/\tau_1)^{\delta\nu_2}, & p_0 = 3/4, \\ (4p_0-3)^{(1/\delta)-\nu_2}D_1 t, & p_0 > 3/4, \end{cases} \tag{53}$$

here $\alpha=1-Q(p_0=0.5)$, $\gamma=1-Q(p_0=0.25)$, $\delta=1-Q(p_0=0.75)$, $\tilde{\nu}=\alpha^{-1}-\frac{1}{5}(\alpha^4+\alpha^3+\alpha^2+\alpha+1)>0(\alpha\tilde{\nu}<1)$, $\nu_1=\gamma^{-1}-\frac{1}{5}(\gamma^4+\gamma^3+\gamma^2+\gamma+1)>0(\gamma\nu_1<1)$, $\nu_2=\delta^{-1}-\frac{1}{5}(\delta^4+\delta^3+\delta^2+\delta+1)>0$, $(\delta\nu_2<1)$.

Thus, for a three-dimensional lattice, just as in the case of a two-dimensional lattice, the confined diffusion occurs for a large concentration of the excluded volume $(1-p_0>0.75)$, while for a low concentration of the excluded volume $(1-p_0<0.25)$ the normal diffusion takes place. However, in the three-dimensional case these two regions of concentrations are separated not by an isolated point (as $p_0=0.5$ in the two-dimensional case), but rather by the region $(0.25<p_0<0.75)$. In line with this, the anomalous diffusion in three dimensions occurs in a whole region of concentrations, and not at the special concentration as it was in the two-dimensional case.

Note, that the indices introduced in Eqs. (51)–(53) are not independent. Substituting $p=1/4$ in Eq. (48), one finds that $\delta=\gamma/3$. Moreover, the simplest form of function $Q(p)$ satisfying the symmetry conditions (48) is

$$Q(p) = p[1+a(1-p)^2]. \tag{54}$$

Then, one has only one independent index in Eqs. (51)–(53). The rough estimate of the single unknown index can be performed under the assumption that in the regime of confined diffusion $(p<0.25)$ the mean square displacement $\overline{R^2(t)} \approx |p-p_0|^{-3\nu_1}$ is defined by the square of the mean cluster size $\xi^2 \approx |p-p_0|^{-2\beta}$ where $\beta \approx 0.8-0.9$ near $p_0=0.25$ [15], i.e., $\nu_1 \approx 0.53-0.6$. Then, as follows from the formulas for $\nu_1(\gamma)$, $\gamma[Q(p_0)]$ and $\tilde{\nu}(\alpha)$ written after Eq. (53), $\gamma \approx 0.81-0.79$; $Q(p=0.25)=1-\gamma \approx 0.19-0.21$; $\alpha=1-Q(p=0.5) \approx 0.44-0.47$; $\tilde{\nu} \approx 1.9-1.8$, and, finally, $\alpha\tilde{\nu} \equiv \zeta \approx 0.84-0.83$. Hence, for $p \gtrsim 0.25$

$$\overline{R^2(t)} \approx t^{\zeta} \quad \zeta \simeq 0.83-0.84, \tag{55}$$

i.e., the diffusion in this region is anomalous (subdiffusion). This result has been checked by numerical simulations.

C. Numerical analysis

We have generated a sample of about 10 000 free random walks of 1000 steps on a cubic lattice of $350\times350\times350$ sites with periodic boundary conditions. The rules for the random walks were as follows. At each step the walker may move with equal probability 1/6 to any of the six nearest neighbors of the lattice site he is at. A fraction $1-p$ of the bonds is lacking, and when the cast indicates to go to this direction, the die is cast again without any correlations with

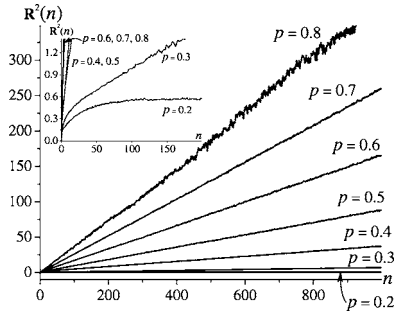

FIG. 4. The mean square displacement $\overline{R^2(t)}$ as a function of the number of steps (time) for different fractions of bonds: $p=0.2$ (confined diffusion), $p=0.3$, $p=0.4$, $p=0.5$, $p=0.6$, $p=0.7$ (anomalous diffusion), and $p=0.8$ (normal diffusion). The inset clearly shows the confined diffusion for $p=0.2$.

the previous cast. The results of calculations show that after 1000 steps the asymptotic behavior is certainly reached. The calculations were performed for $p=0.2-0.8$, where, according to Eq. (53), the diffusion should be confined, anomalous, and normal, respectively. The results of the calculations shown in Figs. 4 and 5 support this prediction. In Fig. 4 we show the mean square displacements as a function of the number of steps (time). Since for $p=0.2$ a walker is very restricted in its motion, $\overline{R^2(t)}$ is very small. However, as is shown in the inset in Fig. 4, the appropriate graph shows saturation, which denotes confined diffusion. On the other hand, the plots for $p=0.4$ and $p=0.8$ show a diffusion behavior of the form $\overline{R^2(t)} \approx t^{\zeta}$ with $\zeta_{p=0.8} > \zeta_{p=0.4}$. In order to arrive at a better approximation for index ζ, the data shown in Fig. 4 are displayed on a logarithmic plot in Fig. 5. Since the indices $\zeta_{p=0.8}$ and $\zeta_{p=0.4}$ are very close, the inset in Fig. 5 shows that these indices are different, namely, $\zeta_{p=0.8}=1$ (normal diffusion), and $\zeta_{p=0.4}=0.86$ (subdiffusion). The agreement between the numerical $\zeta_{p=0.4}=0.86$ and the theoretical results (55) $\zeta_{p=0.4}=0.84$ seems to be quite reasonable. It must be emphasized, that due to the approximations made, both the renormalization group theoretical estimates and the numerical calculations on the finite sample are quite approximate. However, our contention that subdiffusion occurs for $0.25 < p < 0.75$ seems to be correct. In order to show the

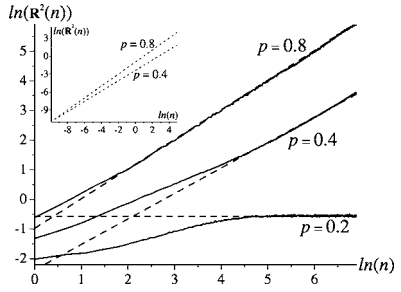

FIG. 5. The same data as in Fig. 4 for two fractions of bonds: $p=0.2$ (confined diffusion), $p=0.4$ (anomalous diffusion), and $p=0.8$ (normal diffusion) shown in the logarithmic plot. Since the indices $\zeta_{p=0.8}$ and $\zeta_{p=0.4}$ are very close, the inset shows that these indices are different, namely, $\zeta_{p=0.8}=1$ (normal diffusion), and $\zeta_{p=0.4}=0.86$ (subdiffusion).

TABLE I. Index ζ defining the anomalous diffusion $[R^2(t) \approx t^{\zeta}]$ for different fractions of bonds p.

p	0.2	0.3	0.4	0.5	0.6	0.7	0.8
ζ	0	0.84	0.86	0.94	0.96	0.99	1

transition from the confined diffusion at $p<0.25$ to the normal diffusion ($\zeta=1$) for $p>0.75$, we bring in Table I the change of index ζ with p, deduced from the numerical calculations.

VI. CONCLUSION

A random walk on the lattice forms the microscopic basis for the diffusive process. Brownian motion is the well-known phenomenon leading to normal diffusion, when the mean-square displacement increases linearly with time for long times. The nonlinearity of this dependence defines anomalous diffusion. There are various ways of providing a microscopic explanation of anomalous diffusion by changing the rules of jumps of a walking particle. Here we use a different approach, changing the structure of the lattice on which a particle is moving. We assume that a disordered medium consists of two randomly distributed components with different diffusion coefficients. In the lattice description, this means that there are two types of bonds randomly distributed over the lattice, and a random walker interacts differently with these two components. We describe a system by three parameters which define the fractions p and $1-p$ of the two components, the ratio h of time scales (or diffusion coefficients) for a random walker on each of the two components, and parameter x which describes a local anisotropy, being the ratio of the probability to jump into second region to that into first region.

Our aim was to find the asymptotic value of the mean square displacement and the effective diffusion coefficient of a two-component random medium when the diffusion is anomalous. To this end, we apply the idea of scaling widely used in the theory of phase transitions. The scaling invariance means that the overall properties of a system, such as the diffusion coefficient, does not depend on the details at small distances, so that the functional dependence on our parameters will be the same for the original lattice and a series of enlarged lattices. We found the scaling transformations which give the connection between parameters in the original and enlarged lattice. These difference equations are transformed into differential equations with a set of fixed points which define the behavior of a system being discussed.

Note, that our approach does not deal with critical phenomena. Anomalous diffusion can appear in the latter case as well (in the framework of percolation theory such calculations have been performed, for example, in Ref. [16]), but there it is always restricted to the close vicinity of the critical point. In our case anomalous diffusion occurs in a wide region of values of the parameter p between two percolation points $p_0 \approx 0.25$ and 0.75. In some sense, the situation is

similar to self-organized criticality in nonequilibrium systems [17], where the "criticality" occurs in a wide region of parameter values and not just near the critical point.

The appearance of anomalous diffusion is not surprising since in our model the motion of a walker is essentially hindered and leads to subdiffusion like in similar problems of diffusion on fractals, self-avoiding walks, long-range correlated walks, porous media, etc.

The general equations have been analyzed for the two limit cases of trapping systems ($h=0$), and the excluded volume system ($x=0$). In the former case anomalous diffusion occurs in all dimensions. For the latter case, in two dimension anomalous diffusion takes place only for a special value of the parameter p while in three dimension anomalous diffusion holds in the whole region of this parameter.

For arbitrary values of the parameters the analysis is much more cumbersome. Moreover, one can obtain anomalous diffusion by introducing correlations between successive jumps in the original lattice. Another way of generalization of our model is to take into account an existence of energy barriers on the boundary between regions of different types, which will define the probabilities of the appropriate jumps.

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