Random walk of particles interacting differently with the components of a two-dimensional two-component disordered media

A. E. Arinshteĭn and A. P. Moroz

N. N. Semenov Institute of Chemical Physics 117977 Moscow, Russia
(Submitted 22 February 1994)
Zh. Eksp. Teor. Fiz. **106**, 315–334 (July 1994)

The scaling approach previously suggested by the present authors[1,2] [Adv. Phys. **36**, 695 (1987) and Phys. Rep. **150**, 265 (1987)] in order to describe the diffusive processes in disordered systems has been generalized to the case in which the random-walking particles interact differently with the different components of the medium. A procedure is described for coarsening the lattice and a system of renormalization-group equations is introduced to describe the infinitesimal scale transformation in the system, taking into account the differences in probabilities for the direct and reverse passages of a wandering particle through the boundary separating the components of the disordered medium. The effective diffusion coefficients of the medium are calculated, along with the time dependence of the mean square displacement of a particle when the components are in various proportions, and also for different probabilities of direct and return crossings of the separation boundary. In the case in which one of the components of the medium is absolutely impenetrable for the particles a regime is observed in which the diffusion is bounded and the effective diffusion coefficient exhibits critical behavior as a function of the density.

1. INTRODUCTION

The study of random-walk processes in disordered systems is currently an actively pursued and complicated problem, attracting the interest of many investigators.[3–6] This interest is occasioned by the fact that many physical processes in actual condensed media have a diffusive nature or are related to diffusive processes, and in a number of cases the diffusive stage is the limiting one. As examples we can cite diffusion in amorphous systems and polymeric solutions,[7] the kinetics of diffusively controlled chemical reactions,[8,9] dispersive transport,[10] the description of the properties of polymeric macromolecules[11,12] using the language of nonintersecting random walks, etc.

Despite the seeming simplicity of the problem, the mathematical difficulties that arise, related to the non-Markovian nature of random-walk processes in disordered media, often make it impossible to find an exact solution for the problems of interest. Usually random-walk processes in disordered media are studied in the simple lattice models either by mathematical modeling techniques[13] or by analytical techniques using various approximations.[3–6,14–16] The most widely used methods are the mean-field approximation[5,14] and expansion in the density of impurities[15] using the generating functional.[16]

The scaling approach[17] has been used to describe the process of random walks in a special case, namely over fractals; this success seems to us very promising. Note that real systems have actual fractal dimensions only over a narrow range of scales, and on the whole real systems must be regarded as fractals with variable dimensionality. However, using the ideas formulated by Kadanoff[18] and Kirkpatrick[19] to describe scale transformations (the lattice-coarsening procedure) in lattice statistical models, one can also find it possible to employ the scaling approach to describe random walks in a two-component disordered medium. Thus, in our previous work we constructed a scaling description of particle random walk in two-dimensional[1] and three-dimensional[2] two-component disordered media whose components differ in their diffusion coefficients (for the one-dimensional case see also Ref. 6).

In the present work we generalize the technique proposed in Refs. 1 and 2, including the difference in the interaction of the random-walking particles with the components of the medium. It is clear that by virtue of this difference the probability for a particle to pass through the interface separating the components depends on direction (inward or outward). Consequently, the system develops local anisotropy when the direction of particle motion is specified, although macroscopically the system remains isotropic. In the limiting case when one of the components of the medium is completely impenetrable (when the probability for the particle to penetrate into the region occupied by this component goes to zero) we have a model of an excluded region, which was treated, e.g., in the mean-field approximation by Harrison and Zwanzig.[14]

In Secs. 2–4, using the model of hopping diffusion on a square lattice, we derived a system of equations describing the infinitesimal scale transformation including both local anisotropy in the choice of the direction of motion and the difference in the diffusion coefficients of the components of the medium.

The procedure described in Sec. 2 for coarsening the lattice is based on a widely known fact: in the hopping-

 1063-7761/94/070175-11$10.00

diffusion model there exists a certain arbitrariness in the choice of the characteristic spatial and temporal scales. Changing one of these gives rise to a corresponding alteration in the other, so as to leave the properties of the system unchanged. If we treat the original (seed) square lattice with a characteristic hopping scale (segment) L_0, consisting randomly of two kinds of segments ("good," type I and "bad," type II) with time scales (temporal jumps) τ_0^{I} and τ_0^{II}, corresponding to the different components of the medium, we arrive at a new coarsened lattice, whose spatial scale corresponds to a mean-square displacement of two hops. Thus, the procedure of scale transformation is derived from comparing the results of particle random walk over one- and two-segment trajectories. A detailed description and justification for this procedure is given in our previous work (Refs. 1 and 2).

Then, in Sec. 3 a system of equations is derived describing the discrete scale transformation of the system, and in Sec. 4 the infinitesimal scale transformation. However, since this system of equations is excessively complicated, in Secs. 5–8 we restrict consideration just to local anisotropy in the choice of the direction of the hop in order to simplify the problem, with the same particle diffusion coefficients in both components of the medium. (These diffusion coefficients, which we will call "intrinsic," are determined by $D_{c0}^{\mathrm{I}} = L_0^2/\tau_0^{\mathrm{I}}$ and $D_{c0}^{\mathrm{II}} = L_0^2/\tau_0^{\mathrm{II}}$. The model in which they were assumed to be different, but without local anisotropy, was studied previously in Refs. 1 and 2.

2. LATTICE-COARSENING PROCEDURE

We will evaluate the magnitude of the mean diffusion coefficient D_n of the medium (lattice) on the spatial scale L_n corresponding to the mean square displacement of a particle over 2^n hops (for the detailed determination of D_n see Refs. 1 and 2).

In order to quantitatively characterize the local anisotropy in the choice of the direction of the next hop, we define the preference factor x_0 as the ratio of the probabilities for a particle to jump through one of the two adjacent segments, bad or good. To be specific we will assume that good segments attract the particle and bad ones repel it. Thus we have $0 \leqslant x_0 \leqslant 1$. In evaluating the contributions to the diffusion coefficient from one-segment trajectories (taking into account their probabilities) we must keep in mind the fact that if at the start of observation the particle distribution over the sites of the initial lattice has already reached equilibrium, then the probability that a particle will be found at this initial time in a particular site depends on the relative number of good and bad segments connecting with this site, as well as the preference factor x_0. While this is taken into account automatically on the second and subsequent steps of the trajectory, at the first step of the random walk it is necessary to treat this dependence, introducing into the formula for the probability of the corresponding single-segment trajectory an additional factor that takes into account the probability that the particle will initially be at a site with the specified environment.

Simple calculations show that the probabilities for achieving single-segment random-walk trajectories consisting, respectively, of good and bad segments are equal to

$$\hat{P}_0^{\mathrm{I}} = \frac{p_0}{p_0 + x_0(1-p_0)}, \tag{1a}$$

$$\hat{P}_0^{\mathrm{II}} \equiv 1 - \hat{P}_0^{\mathrm{I}} = \frac{x_0(1-p_0)}{p_0 + x_0(1-p_0)}, \tag{1b}$$

here p_0 and $1-p_0$ are the respective fractions of good and bad segments; the subscript 0 signifies that these quantities belong to the initial lattice.

Using Eqs. (1) we find that the effective diffusion coefficient averaged over single-segment trajectories on the initial lattice is equal to

$$D_0 = \frac{p_0}{p_0 + x_0(1-p_0)} D_{c0}^{\mathrm{I}} + \frac{x_0(1-p_0)}{p_0 + x_0(1-p_0)} D_{c0}^{\mathrm{II}}$$

$$= D_0^{\mathrm{I}} + D_0^{\mathrm{II}} = \frac{p_0 + h_0 x_0(1-p_0)}{p_0 + x_0(1-p_0)} D_{c0}^{\mathrm{I}}, \tag{2}$$

where we have written $h_0 = D_{c0}^{\mathrm{II}}/D_{c0}^{\mathrm{I}}$.

To introduce the coarsened lattice it is necessary to treat all possible two-segment trajectories, the mean-square displacement over which determines the new coarsened segment. Altogether, three types of two-segment trajectories are possible: "good," "bad," and "mixed." If both of the consecutive steps of the random walk on the original lattice are performed on good segments, then the segments of the coarsened lattice corresponding to these two-segment trajectories will be called good. If both steps of the random walk on the original lattice are performed over bad segments, then the segments of the coarsened lattice corresponding to these two-segment trajectories will be called bad. And finally, on mixed trajectories the particle executes a jump through both a good and a bad segment of the original lattice, where we must treat trajectories on which the first step is performed on the good segment and the second on the bad separately from those in which the order is reversed.

Since in the process of a systematic classification of trajectories it is found that a particular segment of the initial lattice contributes to trajectories corresponding to adjacent (emerging from a single site) segments of the new coarsened lattice, the properties of these adjacent segments are found to be correlated. As in our previous work,[1,2] we take into account this effect by introducing new probabilities for the properties of segments that meet in the second step. Thus, $Q(p)$ is the probability that a segment adjacent to a good segment is also good, while $1-Q(p)$ is the probability that it is found to be bad. Similarly, we introduce the probabilities $W(p)$ and $1-W(p)$ such that a segment adjacent to a bad segment will turn out to be, respectively, bad or good. (We will make the simplifying assumption that the correlation, i.e., the conditional probability Q or W, is the same for all segments of a single type that can be met by the particle in the second step.) The functions $Q(p)$ and $W(p)$ that prescribe the initial probabilities must satisfy the following obvious requirements:

$$W(p)=Q(1-p), \tag{3a}$$

$$p[1-Q(p)]=(1-p)[1-W(p)]. \tag{3b}$$

Property (3a) corresponds to symmetry of the system in question with respect to simultaneous interchange of good and bad segments and p and $1-p$. Property (3b) is a reflection of the fact that the probability of a mixed trajectory should not depend on the order in which the segments of different types are traversed: first good and then bad or vice versa. Note that with this way of including correlations expressions (1) and (2) do not change. We also note that the correlation should decrease as the scale increases, when the medium becomes macroscopically uniform (p approaches either zero or unity). Hence for p sufficiently close to zero or unity it is necessary that $Q(p)\approx p$ and $W(p)\approx 1-p$ hold.

In analytical calculations we do not need the specific form of the functions $Q(p)$ and $W(p)$ (it suffices to determine the values of these functions at the characteristic percolation point $p=1/2$). For numerical calculations we limit ourselves to polynomial functions of the lowest order sufficient to satisfy the requirements given above:

$$Q(p)=p[1+ap(1-p)^3],$$

$$W(p)=(1-p)[1+a(1-p)p^3], \tag{4}$$

with the parameter a determined from the value of the function $Q(1/2)=W(1/2)\equiv\varkappa$: $a=16(2\varkappa-1)$, $0<\varkappa<1$.

By going through all possible two-segment trajectories for all possible configurations of good and bad segments we can calculate the contributions of the corresponding trajectories to the diffusion coefficient.

For a good trajectory the geometrical probability of which (i.e., the fraction of all possible combinations of two adjacent segments) is equal to $p_0Q(p_0)$, we find that the contribution to the diffusion coefficient is equal to

$$\tilde{D}^{\mathrm{I}}=\frac{p_0Q_0}{p_0+x_0(1-p_0)}\left\{1+(1-x_0)(1-Q_0)\times\left[\frac{2Q_0}{3+x_0}+\frac{1-Q_0}{1+x_0}\right]\right\}D^{\mathrm{I}}_{c0}, \tag{5}$$

for a bad trajectory, the geometrical probability of which equals $(1-p_0)W(p_0)$, the contribution to the diffusion coefficient is equal to

$$\tilde{D}^{\mathrm{II}}=\frac{x_0(1-p_0)W_0}{p_0+x_0(1-p_0)}\left\{1-(1-x_0)(1-W_0)\times\left[\frac{2W_0}{1+3x_0}+\frac{1-W_0}{1+x_0}\right]\right\}D^{\mathrm{II}}_{c0}, \tag{6}$$

for mixed trajectories in which the order is first a good segment and then a bad one, for which the geometric probability is $p_0[1-Q(p_0)]$, the contribution to the diffusion coefficient is equal to

$$\begin{aligned}\tilde{D}^{\mathrm{I,II}}&=\frac{2x_0p_0(1-Q_0)}{p_0+x_0(1-p_0)}\left\{1+(1-x_0)\left[\frac{Q_0^2}{3+x_0}+\frac{2Q_0(1-Q_0)}{1+x_0}+\frac{3(1-Q_0)^2}{1+3x_0}\right]\right\}\frac{D^{\mathrm{II}}_{c0}}{1+h_0}\\&=\frac{2x_0p_0(1-Q_0)}{p_0+x_0(1-p_0)}\left\{1-(1-x_0)\left[\frac{3Q_0^2}{3+x_0}+\frac{2Q_0(1-Q_0)}{1+x_0}+\frac{(1-Q_0)^2}{1+3x_0}\right]\right\}\frac{h_0D^{\mathrm{I}}_{c0}}{1+h_0},\end{aligned} \tag{7}$$

for mixed trajectories in which the order is first a bad segment and then a good one, the geometrical probability of which equals $(1-p_0)[1-W(p_0)]$ [by virtue of condition (4) this probability also equals $p_0[1-Q(p_0)]$], the contribution to the diffusion coefficient is equal to

$$\begin{aligned}\tilde{D}^{\mathrm{II,I}}&=\frac{2x_0(1-p_0)(1-W_0)}{p_0+x_0(1-p_0)}\left\{1+(1-x_0)\left[\frac{(1-W_0)^2}{3+x_0}+\frac{2W_0(1-W_0)}{1+x_0}+\frac{3W_0^2}{1+3x_0}\right]\right\}\frac{D^{\mathrm{II}}_{c0}}{1+h_0}\\&=\frac{2x_0(1-p_0)(1-W_0)}{p_0+x_0(1-p_0)}\times\left\{1-(1-x_0)\times\left[\frac{3(1-W_0)^2}{3+x_0}+\frac{2W_0(1-W_0)}{1+x_0}+\frac{W_0^2}{1+3x_0}\right]\right\}\frac{h_0D^{\mathrm{I}}_{c0}}{1+h_0}.\end{aligned} \tag{8}$$

Note that under the simultaneous interchange $p\to 1-p$, $x\to 1/x$, $h\to 1/h$ expressions (5), (6) and (7), (8) transform pairwise into one another, which corresponds to the symmetry of this system with respect to interchange of good and bad segments.

The diffusion coefficient, averaged over all possible two-segment trajectories, is equal to

$$D_1=\tilde{D}^{\mathrm{I}}+\tilde{D}^{\mathrm{I,II}}+\tilde{D}^{\mathrm{II,I}}+\tilde{D}^{\mathrm{II}}. \tag{9}$$

In order to construct a coarsened lattice consisting, like the original one, of segments of both types, we must write the expression for the mean diffusion coefficient (9) in the form of two terms, analogous to (2):

$$D_1=D_1^{\mathrm{I}}+D_1^{\mathrm{II}}, \tag{10}$$

here D_1^{I} corresponds to diffusion over the good segments of the new coarsened lattice and D_1^{II} to diffusion over the bad ones, and the subscript 1 indicates the first step in the coarsening procedure.

Since in the coarsening process segments have appeared on the new lattice not of two but of three types (good, bad, and mixed), with respective fractions

$$P_1^{\mathrm{I}}=p_0Q(p_0); \tag{11a}$$

$$P_1^{\mathrm{II}}=(1-p_0)W(p_0); \tag{11b}$$

$$P_1^{\mathrm{m}}=p_0[1-Q(p_0)]+(1-p_0)[1-W(p_0)]$$
$$=2p_0[1-Q(p_0)]$$
$$=2(1-p_0)[1-W(p_0)], \tag{11c}$$

we can divide all mixed segments into two kinds:

$$P_1^{\mathrm{m}}=\alpha_0 P_1^{\mathrm{m}}+(1-\alpha_0)P_1^{\mathrm{m}}, \quad |0\leqslant\alpha_0\equiv\alpha(x_0,h_0,p_0)\leqslant 1, \tag{12}$$

and combine one part (the fraction proportional to the subdivision parameter α_0) with good segments of the coarsened lattice and the other mixed segments of the new lattice with bad ones.

Then the fractions of good and bad segments of the new lattice, which agree to within geometrical probabilities with the corresponding two-segment trajectories, are equal to

$$p_1^{\mathrm{I}}\equiv p_1=P_1^{\mathrm{I}}+\alpha_0 P_1^{\mathrm{m}}, \tag{13a}$$

$$p_1^{\mathrm{II}}\equiv 1-p_1=P_1^{\mathrm{II}}+(1-\alpha_0)P_1^{\mathrm{m}}. \tag{13b}$$

3. DISCRETE SCALING TRANSFORMATION

In accordance with the division of the mixed trajectories (12) we determine D_1^{I} and D_1^{II} from (10) using Eq. (9) as follows:

$$D_1^{\mathrm{I}}=\tilde{D}^{\mathrm{I}}+\alpha_0(\tilde{D}^{\mathrm{I,II}}+\tilde{D}^{\mathrm{II,I}}), \tag{14a}$$

$$D_1^{\mathrm{II}}=\tilde{D}^{\mathrm{II}}+(1-\alpha_0)(\tilde{D}^{\mathrm{I,II}}+\tilde{D}^{\mathrm{II,I}}), \tag{14b}$$

here the quantities $\tilde{D}^{\mathrm{I}}$, $\tilde{D}^{\mathrm{I,II}}$, $\tilde{D}^{\mathrm{II,I}}$, and D^{II} are defined by expressions (5)–(8).

In what follows, along with the quantities D_1^{I} and D_1^{II} which characterize the contributions of the good and bad segments of the new coarsened lattice to the average diffusion coefficient D_1, we will use D_{c1}^{I} and D_{c1}^{II} (the intrinsic diffusion coefficients corresponding to segments of the new lattice, which we define in terms of D_1^{I} and D_1^{II}) and the fractions (13a) and (13b) by analogy with (2):

$$D_1^{\mathrm{I}}=\frac{p_1}{p_1+x_1(1-p_1)}D_{c1}^{\mathrm{I}}\equiv\hat{P}_1^{\mathrm{I}}D_{c1}^{\mathrm{I}}, \tag{15a}$$

$$D_1^{\mathrm{II}}=\frac{x_1(1-p_1)}{p_1+x_1(1-p_1)}D_{c1}^{\mathrm{II}}\equiv\hat{P}_1^{\mathrm{II}}D_{c1}^{\mathrm{II}}. \tag{15b}$$

Here $\hat{P}_1^{\mathrm{I}}$ and $\hat{P}_1^{\mathrm{II}}\equiv 1-\hat{P}_1^{\mathrm{I}}$ are the probabilities for realizing single-segment trajectories consisting, respectively, of good and bad segments of the coarsened lattice [cf. Eq. (1)]. Straightforward calculation shows that the probabilities $\hat{P}_1^{\mathrm{I}}$ and $\hat{P}_1^{\mathrm{II}}$, which coincide with the probabilities of realizing the corresponding two-segment trajectories on the initial lattice, are given to within an overall factor by the expressions

$$\hat{P}_1^{\mathrm{I}}=\hat{D}^{\mathrm{I}}+\alpha_0(p_0,x_0,h_0)(\hat{D}^{\mathrm{I,II}}+\hat{D}^{\mathrm{II,I}}), \tag{16a}$$

$$\hat{P}_1^{\mathrm{II}}=\hat{D}^{\mathrm{II}}+[1-\alpha_0(p_0,x_0,h_0)](\hat{D}^{\mathrm{I,II}}+\hat{D}^{\mathrm{II,I}}). \tag{16b}$$

The quantities $\hat{D}^{\mathrm{I}}$, $\hat{D}^{\mathrm{II}}$, $\hat{D}^{\mathrm{I,II}}$, and $\hat{D}^{\mathrm{II,I}}$ are given, respectively, by relations (5), (6), (7), and (8), in which we set $D_{c0}^{\mathrm{I}}=D_{c0}^{\mathrm{II}}=h_0=1$.

From (15) it follows that the preference factor x_1 of the coarsened lattice is defined analogous to x_0 as the ratio of the probabilities for jumps on the bad and good segments when they are equal in number:

$$x_1=\frac{\hat{P}_1^{\mathrm{II}}/(1-p_1)}{\hat{P}_1^{\mathrm{I}}/p_1}. \tag{17}$$

In exactly the same way, in analogy with the definition of h_0 and using Eq. (15), we give for h_1

$$h_1=D_{c1}^{\mathrm{II}}/D_{c1}^{\mathrm{I}}=(D_1^{\mathrm{II}}/D_1^{\mathrm{I}})(\hat{P}_1^{\mathrm{I}}/\hat{P}_1^{\mathrm{II}}). \tag{18}$$

In order to complete the definition of the procedure for passing to a coarsened lattice we have only to prescribe the form of the subdivision parameter $\alpha_0(p_0,x_0,h_0)$ of the mixed trajectories into two groups. There is no compact recipe for determining the form of $\alpha_0(p_0,x_0,h_0)$, and we can only indicate some ideas which underlie our choice.

First, for $x_0\equiv 0$, when a particle undergoing random walk is totally excluded from the bad regions, macroscopic diffusion in this system is possible only for values of p_0 above the percolation threshold for the problem of links on a two-dimensional square lattice [i.e., $D_{\mathrm{eff}}>0$ only for $p_0>1/2$; see Eq. (36) below]. In order to satisfy this requirement, conditions (40) must be satisfied at $x\equiv 0$ (see Sec. 5), and for this it is necessary that Eq. (30) take the form (38) at $x\equiv 0$; consequently we must have $\alpha_0(p_0,x_0\equiv 0,h_0)=p_0$.

Secondly, at $x_0=1$, when the direction of the random walk does not depend on the environment of the particle, the problem reduces to that which we treated earlier:[1] the problem of random walks in a heterogeneous medium whose components differ in their diffusion coefficients, while the interaction of the diffusing particle with the different components in the medium is the same and $\alpha_0(p_0,x=1,h_0)=h_0p_0/[h_0p_0+1-p_0]$ holds.

In order to satisfy these requirements we choose $\alpha_0(p,x,h)$ in the form

$$\alpha_0(p,x,h)=\frac{pf_1(x,h)}{pf_1(x,h)+(1-p)f_2(x,h)}, \tag{19}$$

and

$$1-\alpha_0(p,x,h)=\frac{(1-p)f_2(x,h)}{pf_1(x,h)+(1-p)f_2(x,h)}. \tag{20}$$

By virtue of the symmetry in our problem, i.e., the invariance under the interchange $p\to 1-p$, $x\to 1/x$, $h\to 1/h$, the function $f_{1,2}$ satisfies the relation

$$f_2(x,h)=f_1(1/x,1/h). \tag{21}$$

Let us consider the ratio

$$\frac{\alpha(p,x,h)/p}{[1-\alpha(p,x,h)]/(1-p)}=\frac{f_1(x,h)}{f_2(x,h)}\equiv F(x,h) \tag{22}$$

(here and below we omit the subscript 0 from the subdivision parameter α); by virtue of the conditions given above the function $F(x,h)$ should have the following properties:

$$F(1/x,1/h)=1/F(x,h), \tag{23a}$$

$$F(x=0,h)=F(x=\infty,h)=1, \tag{23b}$$

$$F(x=1,h)=h. \tag{23c}$$

We look for $F(x,h)$ in the form of a ratio of polynomials. By virtue of property (23a) the polynomials of the numerator and denominator in Eq. (22) should be of the same degree. The lowest degree of these polynomials which enables us to satisfy the above requirements is found to be two, so the function $F(x,h)$ using (23) can be represented in the form

$$F(x,h)=\frac{x^2+\beta_1(h)x+\gamma(h)}{x^2+\beta_2(h)x+\gamma(h)}. \tag{24}$$

Using the property (23a), we find for $\gamma(h)$ the functional equation

$$\gamma(h)=1/\gamma(1/h), \tag{25a}$$

whence we have

$$\gamma(h)=h^{\lambda}, \tag{25b}$$

and the function $\beta_2(h)$ is expressed in terms of $\beta_1(h)$ and $\gamma(h)$ by

$$\beta_2(h)=\gamma(h)\beta_1(1/h). \tag{26}$$

Using the ratio (26), from (23a) we find for the function $\beta_1(h)$ the functional equation

$$\beta_1(h)=h^{\lambda+1}\beta_1(1/h)-(1-h)(1+h^{\lambda}), \tag{27a}$$

whose solution takes the form

$$\beta_1(h)=h(1+h^{\lambda}). \tag{27b}$$

The parameter λ can be evaluated from the natural requirement that the extremum of the function $F(x,h)$ with respect to x should coincide with the distinctive point $x=1$, the inversion point. The parameter λ is found to equal zero, and finally we obtain

$$F(x,h)=\frac{x^2+2xh+1}{x^2+2x/h+1} \tag{28}$$

[so that condition (23b) is satisfied automatically].

Using (22) and (28) we find an expression for the function $\alpha(p,x,h)$:

$$\alpha(p,x,h)=\frac{ph(x^2+2hx+1)}{hx^2+2[1-(1-h^2)p]x+h}, \tag{29a}$$

and

$$1-\alpha(p,x,h)=\frac{(1-p)h(x^2+2x/h+1)}{hx^2+2[1-(1-h^2)p]x+h}. \tag{29b}$$

The above sequence of relations (2), (5)–(8), (10), (11), (13)–(18) and (29) completely specify the transition from the initial lattice to the new coarsened one. Taking the new coarsened lattice as the starting one, but with the new parameters derived in the above procedure and repeating this procedure we can pass to a still larger scale. Repeating this procedure as many times as necessary, we ultimately arrive at a scale on which the system becomes uniform and the diffusive properties evaluated on each step of the coarsening are found to be effective macroscopic diffusive properties of the original nonuniform medium.

4. INFINITESIMAL SCALE TRANSFORMATION: THE SYSTEM OF RENORMALIZATION-GROUP EQUATIONS

On the $(n+1)$th step of the above procedure for coarsening we obtain recurrence relations which connect the parameters pD^{I}, D^{II}, h, and x of the lattice with the scales corresponding to the $(n+1)$th and nth steps of the coarsening. Using these recurrence relations we can easily derive the renormalization-group equations for the infinitesimal scale transformation:

$$\frac{dp(n)}{dn}=p(n)[1-Q(p)][2\alpha(p,x,h)-1]$$
$$=[1-p(n)][1-W(p)][2\alpha(p,x,h)-1], \tag{30}$$

$$\frac{dD^{\mathrm{I}}(n)}{dn}=-[1-Q(p)]\left\{1-\frac{4\alpha(p,x,h)h(n)}{1+h(n)}-[1-x(n)]\right.$$
$$\left.\times\left[F_1^{\mathrm{I}}-\frac{2\alpha(p,x,h)h(n)}{1+h(n)}F_2^{\mathrm{I}}\right]\right\}D^{\mathrm{I}}(n), \tag{31}$$

$$\frac{dD^{\mathrm{II}}(n)}{dn}=-[1-W(p)]\left\{1-\frac{4[1-\alpha(p,x,h)]}{1+h(n)}+[1-x(n)]\right.$$
$$\left.\times\left[F_1^{\mathrm{II}}-\frac{2[1-\alpha(p,x,h)]}{1+h(n)}F_2^{\mathrm{II}}\right]\right\}D^{\mathrm{II}}(n), \tag{32}$$

$$\frac{dh(n)}{dn}=\frac{2h(n)[1-h(n)]}{1+h(n)}\left\{\alpha(p,x,h)[1-Q(p)]\right.$$
$$\times\left[1-\frac{[1-x(n)]}{2}F_2^{\mathrm{I}}\right]+[1-\alpha(p,x,h)]$$
$$\left.\times[1-W(p)]\left[1+\frac{[1-x(n)]}{2}F_2^{\mathrm{II}}\right]\right\}, \tag{33}$$

$$\frac{dx(n)}{dn}=-x(n)[1-x(n)]\{[1-Q(p)]$$
$$[F_1^{\mathrm{I}}-\alpha(p,x,h)F_2^{\mathrm{I}}]+[1-W(p)]$$
$$\times[F_1^{\mathrm{II}}-[1-\alpha(p,x,h)]F_2^{\mathrm{II}}]\}. \tag{34}$$

$$F_1^{\mathrm{I}}\equiv Q(p)\left[\frac{2Q(p)}{3+x(n)}+\frac{1-Q(p)}{1+x(n)}\right],$$

$$F_1^{\mathrm{II}}\equiv W(p)\left[\frac{2W(p)}{1+3x(n)}+\frac{1-W(p)}{1+x(n)}\right],$$

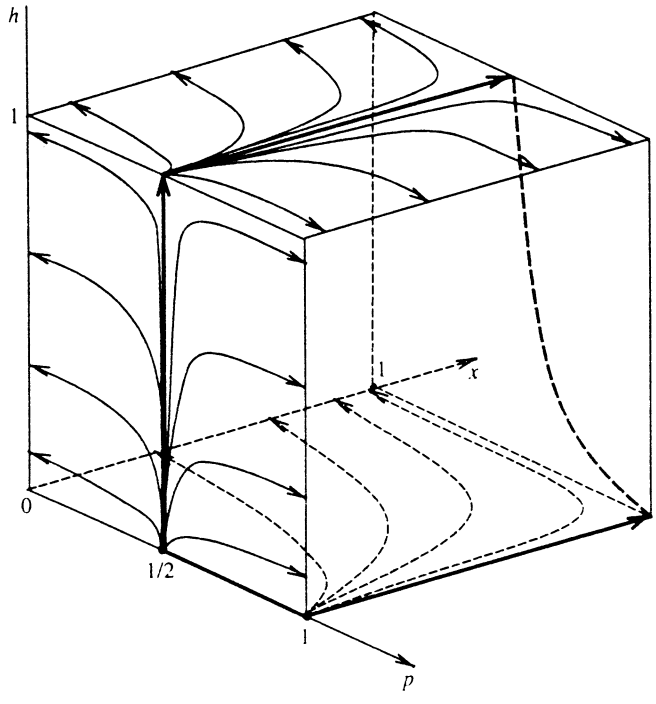

FIG. 1. The most interesting cross sections of the phase portrait of the system of kinetic equations (30)–(34). The heavy lines indicate the trajectories on which the separatrix surface passing through the unstable site ($p=1$, $x=0$, $h=0$) and the saddle points ($p=1$, $x=1$, $h=0$), ($p=1/2$, $x=1$, $h=1$) and ($p=1/2$, $x=0$, $h=1$), intersects the phase planes $x=0$, $x=1$, $h=0$, and $h=1$. The planes $p=0$ and $p=1$ are attractive and correspond to a macroscopic uniform medium with infinitely large scale. The phase portrait lying on the separatrix of the surface with $x_0\neq 0$ end at a saddle point ($p=1/2$, $x=1$, $h=1$), which also corresponds to a macroscopically uniform medium. The medium remains nonuniform on any scale in one case, for $x\equiv 0$, $p\equiv 1/2$. The phase portrait of the $x=1$ plane was studied in detail in Ref. 1.

$$F_2^{\mathrm{I}}\equiv 3\frac{Q^2(p)+[1-W(p)]^2}{3+x(n)}+2\frac{Q(p)[1-Q(p)]+W(p)[1-W(p)]}{1+x(n)}+\frac{[1-Q(p)]^2+W^2(p)}{1+3x(n)},$$

$$F_2^{\mathrm{II}}\equiv\frac{Q^2(p)+[1-W(p)]^2}{3+x(n)}+2\frac{Q(p)[1-Q(p)]+W(p)[1-W(p)]}{1+x(n)}+3\frac{[1-Q(p)^2+W^2(p)}{1+3x(n)}.$$

The phase portrait (more precisely, its most interesting cross sections) of this kinetic system is shown in Fig. 1.

The initial conditions for the system of kinetic equations (30)–(34) are determined by the properties of this system on the original scale:

$$\begin{aligned} &p(n=0)=p_0,\quad h(n=0)=h_0\equiv D_{c0}^{\mathrm{II}}/D_{c0}^{\mathrm{I}},\\ &x(n=0)=x_0,\\ &D^{\mathrm{I}}(n=0)=\frac{p_0D_{c0}^{\mathrm{I}}}{p_0+x_0(1-p_0)},\\ &D^{\mathrm{II}}(n=0)=\frac{x_0(1-p_0)}{p_0+x_0(1-p_0)}D_{c0}^{\mathrm{II}}. \end{aligned}\tag{35}$$

The system of kinetic equations (30)–(34) with the initial conditions (35) completely describe the properties of the system of interest and enable us to calculate the effective diffusion coefficient of the disordered medium:

$$D_{\mathrm{eff}}=\lim_{n\to\infty}[D^{\mathrm{I}}(n)+D^{\mathrm{II}}(n)].\tag{36}$$

The solution of the system of kinetic equations (30)–(34) also enables us to determine how the mean square displacement of a particle undergoing random walk depends on time, using the relations which we derived previously in Refs. 1 and 2:

$$R_{\mathrm{ms}}^2(t)=t\{D^{\mathrm{I}}[n(t)]+D^{\mathrm{II}}[n(t)]\},\tag{37}$$

here the coarsening parameter n and the random-walk time t are related simply by

$$n(t)=\ln(t/\tau_0^{\mathrm{I}}),$$

where τ_0^{I} is the characteristic hopping time over a good segment of the original lattice.

In this case, when complete averaging is performed in the system and it becomes macroscopic on large scales, the dependence (37) after long times becomes linear and random walks through the disordered medium enter the diffusive regime.

5. THE CASE IN WHICH ONE OF THE COMPONENTS OF THE MEDIUM IS TOTALLY IMPENETRABLE ($x_0\equiv 0$); THE EXCLUDED-REGION MODEL

In this section we consider the simplest special case in which one of the components of the medium is completely impenetrable to the particle undergoing random walk, i.e., in the initial condition (35) we set $x_0\equiv 0$. Despite its simplicity, this limiting case turns out to be very interesting: even for $x_0\equiv 0$ we can observe a regime in which the diffusion is bounded, and the effective diffusion coefficient behaves critically as a function of the fraction of the impenetrable component.

From the definition of the quantity x_0 and Eqs. (1) it follows that if at $x_0\equiv 0$ the fraction p_0 of the good component in the medium is nonzero, then the probability for a particle to penetrate into the bad region (segment) is equal to zero. Moreover, the random walk of particles in a uniform medium consisting only of bad regions ($p_0=0$) is not restricted at all even for $x_0\equiv 0$, while the diffusion coefficient D_{eff} in this case is equal to D_{c0}^{II}. Consequently, at $x_0\equiv 0$ the bad regions are excluded for the particle only for $p_0>0$.

At $x_0 \equiv 0$ the system of equations (30)–(34) simplifies considerably. First, Eq. (34) for the quantity $x(n)$ has the trivial solution $x(n) \equiv 0$, where the right-hand sides of (30) and (31) do not depend on h. Furthermore, by virtue of the initial condition (35) for $p_0 \neq 0$ we have $D^{II}(n) \equiv 0$, and hence Eqs. (32) and (33) for the quantities $D^{II}(n)$ and $h(n)$ can be disregarded. The explanation for this fact is obvious: since the trajectories of particles undergoing random walk cannot pass through the impenetrable component of the medium, its properties (which we label by the superscript II) cannot influence the diffusion coefficient of the medium.

The remaining equations (30) and (31) assume the form

$$dp(n)/dn = p(n)[1-Q(p)](2p-1), \tag{38}$$

$$dD^{I}(n)/dn = -[1-Q(p)]\{1-Q(p) \times [1-Q(p)/3]\}D^{I}(n), \tag{39}$$

and the initial conditions (35) are $D^{I}(n=0) = D^{I}_{c0}$, $p(n=0) = p_0$. Here we have assumed that, in accordance with (29), we have $\alpha(p,x,h) \equiv p$ at $x_0 \equiv 0$.

Note that Eq. (38) does not depend on the solution of Eq. (39), and its roots ($p=0$, $p=1/2$, $p=1$) exactly coincide with the roots of the equation for the conductivity in the percolation model with respect to coupling.[19] Its solution has a critical behavior with critical density (percolation threshold) $p_{crit} = 1/2$, where

$$\lim_{n\to\infty}[p(n)] = \begin{cases} 0, & p_0 < 1/2, \\ 1, & p_0 > 1/2. \end{cases} \tag{40}$$

Dividing Eq. (39) by (38), we obtain an ordinary differential equation which can easily be integrated:

$$\ln \frac{D^{I}(p)}{D^{I}_0} = -\int_{p_0}^{p(n)} \frac{1-Q(p)[1-Q(p)/3]}{2p(p-1/2)}\,dp. \tag{41}$$

Retaining only the principal terms in the integral, we finally find

$$D^{I}[p(n)] \approx D^{I}_{C0} \exp\{-c[p(n) - p_0]\} \frac{p(n)}{p_0} \left|\frac{p_0 - 1/2}{p(n) - 1/2}\right|^{\delta}, \tag{42}$$

where $c = 2/3 + \varkappa(1-\varkappa/3)$, $\delta = 1 - \varkappa(1-\varkappa/3)$, $\varkappa = Q \times (p = 1/2)$.

Since in the present case $x_0 \equiv 0$ the effective diffusion coefficient of the medium is equal to the value $D_{eff} = \lim_{n\to\infty}\{D^{I}[p(n)]\}$, given by (36), from (42) using (40) we find

$$D_{eff} = \begin{cases} 0, & 0 < p_0 \leqslant 1/2, \\ (1/p_0)\,|2p_0 - 1|^{\delta} \exp[-c(1-p_0)]\,D^{I}_{c0}, & p_0 \geqslant 1/2. \end{cases} \tag{43}$$

Note that for $0 < \varkappa < 1$ the inequality $0 < \delta < 1$ applies to the exponent $0 < \delta < 1$.

The value of the parameter $\varkappa$ which determines the scaling index δ in the critical dependence (43) can be evaluated by comparing the radius within which the random-walking particle is localized in the regime where the diffusion is bounded for $p_0 < p_{crit}$ with the correlation radius, which is the average size of the bound cluster in the percolation problem also for $p_0 < p_{crit}$.

Taking into account (37) we determine the particle localization radius as follows:

$$R_{loc} = \sqrt{\lim_{n\to\infty} t(n)\,D^{I}[p(n)]}, \tag{44}$$

where $t(n) = \tau^{I}_0 e^{n}$.

Using Eq. (39) we can find a relation between the quantities t and p:

$$\frac{tp}{p_0} \approx \tau^{I}_0 \frac{1-p_0}{1-p} \left|\frac{1/2-p}{1/2-p_0}\right|^{1/(1-\varkappa)}, \tag{45}$$

and using (40) in the expression (44) we can pass from the coarsening limit $n \to \infty$ to the limit $p \to 0$:

$$\begin{aligned} R_{loc} &= \sqrt{\lim_{p\to 0} t(p)\,D^{I}(p)} \\ &\approx \sqrt{\lim_{p\to 0}\left[\frac{tp}{p_0}\left|\frac{1/2-p_0}{1/2-p(n)}\right|^{\delta}\right] D^{I}_{c0}} \\ &\approx L_0\sqrt{1-p_0}\,(1-2p_0)^{-\varkappa[1-\varkappa/3+1/(1-\varkappa)]/2}. \end{aligned} \tag{46}$$

Note that as the density p_0 approaches the percolation threshold 1/2 the size of the localization region for the random-walking particle diverges, since the exponent in (46) is negative for $0 < \varkappa < 1$.

The resolving localization radius is comparable to the correlation radius of this system, which can easily be estimated by using Eq. (39) and the equation for the transformation of the spatial scale,

$$dL(n)/dn = (\sqrt{2}-1)L, \tag{47}$$

which follows from the discrete transition to diagonal coarsening of the lattice: $L^2_{n+1} = 2L^2_n$. Integrating (39) using (47) we find that the correlation radius depends on the density of the conducting component as follows:

$$L_g \approx L_0(1-2p_0)^{-[(\sqrt{2}-1)/(1-\varkappa)]}. \tag{48}$$

Equating the exponents in expressions (46) and (48) we find $\varkappa \approx 0.65$. This value of $\varkappa$ yields something of an underestimate for the critical index of the correlation radius, which is well known from percolation theory:[20] 1.19 compared with 1.33. This discrepancy, which in our opinion is unimportant, can be explained by the errors which entered in the transition from the discrete scaling transformation to the infinitesimal one.

To conclude this section we briefly summarize the results.

The dependence of the effective diffusion coefficient on the density $1-p_0$ of the "impenetrable" component behaves critically, since its derivative near the percolation point $p_{crit} = 1/2$ has a square-root singularity [see Eq. (43), where $\delta = 0.49$ and $c = 1.18$].

This result agrees qualitatively with the results of Ref. 14, where particles undergoing random walk in a medium with an excluded region were studied using the mean-field

approximation. The reduced value of the critical density obtained in Ref. 14 ($p_{crit}\approx 0.3$) is explained by the error of the mean-field approximation used in Ref. 14, whereas in the present method the critical value of the density coincides with the percolation point of the system. On the other hand, since the error in the scaling approach increases with distance from the percolation point, the value of the derivative of the effective diffusion coefficient with respect to p_0 in the limit $p_0 \to 1$ is slightly underestimated, and in the region $1-p_0 \ll 1$ the results obtained in Ref. 14 are more trustworthy.

Using relations (37), (42), and (45), we can estimate the way the mean square of the displacement depends on time. In the initial stage of the process, where $|p(t)-1/2| \ll 1$ holds for arbitrary values of the density p_0 near 1/2, the function $R^2_{ms}(t)$ is nonlinear:

$$R^2_{ms}(t) \sim t^{(\varkappa/3)(\varkappa^2-4\varkappa+6)} \approx t^{0.83}. \tag{49}$$

However, subsequently, depending on the value of the density p_0, the particle is either localized for $p_0 < 1/2$ or for $p_0 > 1/2$ its random walk at late times carries it into the diffusive regime and the function $R^2_{ms}(t)$ becomes linear:

$$R^2_{ms}(t) = \begin{cases} R^2_{loc} \approx (1-2p_0)^{-2.36} L_0^2, & 0 < p_0 < 1/2, \quad p(t) \ll 1, \\ (t/p_0)\,|2p_0-1|^{0.49} \exp[-1{,}18(1-p_0)]\, D^{I}_{C0}, & p_0 > 1/2, \quad [1-p(t)] \ll 1. \end{cases} \tag{50}$$

It would seem that this result contradicts the conclusions of Ref. 12, in which the conformation of the phantom polymer chains in a random potential was studied both numerically and analytically. In that work it was shown that a phantom polymer chain undergoes localization in the presence of any arbitrarily small quantity of impenetrable impurity. However, in the same work the question arises about the rigor of the description of phantom polymer chain statistics in the general case using a hopping diffusion model. Our result shows that despite the successful application of the hopping diffusion model to describe the statistics of a polymer chain,[11] this approach is impossible in the presence of an external random walk.

6. CASES OF STRONG REPULSION OF PARTICLES OF THE COMPONENTS OF THE MEDIUM ($x_0 \ll 1$) HAVE THE SAME DIFFUSION COEFFICIENT

The components of the medium have identical intrinsic diffusion coefficients, and in accordance with Eq. (33) this identity is preserved in the process of coarsening the lattice, $h(n) \equiv h_0 = 1$. Dividing Eqs. (31), (32), and (34) by Eq. (30) and integrating with respect to p, Eqs. (31) and (32), using the initial condition (35), we find the following relations describing the effective diffusion coefficient:

$$D^{I}(p) = \frac{p(n)\, D^{I}_{c0}}{p_0 + x_0(1-p_0)} \times \exp\left[\int_{p_0}^{p(n)} \frac{[1-x(p)](F^{I}_1 - pF^{I}_2)}{2p(p-1/2)}\, dp \right], \tag{51}$$

$$D^{II}(p) = \frac{[1-p(n)]\, x_0 D^{I}_{c0}}{p_0 + x_0(1-p_0)} \exp \times \left[- \int_{p_0}^{p(n)} \frac{[1-x(p)][F^{II}_1 - (1-p)F^{II}_2]}{2p(p-1/2)}\, dp \right], \tag{52}$$

$$\frac{dx(p)}{dp} = \frac{x(p)[1-x(p)]}{2(p-1/2)} \left[F^{I}_2 + F^{II}_2 - \left(\frac{F^{I}_1}{p} + \frac{F^{II}_1}{1-p} \right) \right]. \tag{53}$$

Here we have assumed that $D^{I}_{c0} = D^{II}_{c0}$ and [in accordance with Eq. (29)] $\alpha(p,x,h\equiv 1) \equiv p$ hold. Since for $h \equiv 1$ Eq. (30) assumes the form (38), the limiting relations (40) also apply. Consequently, Eq. (36) together with (51) and (52) yields

$$D_{eff} = \begin{cases} \lim\limits_{n\to\infty} [D^{I}\{p(n)\}] = D^{I}(1), & p_0 > 1/2; \\ \lim\limits_{n\to\infty} [D^{II}\{p(n)\}] = D^{II}(0), & p_0 < 1/2. \end{cases}$$

Assuming that $x(p) \ll 1$ holds for all p, and retaining in what follows only the leading terms in the expansion in powers of x_0, we find the solution of Eq. (53):

$$x(p) \approx x_0 |(p-1/2)/(p_0-1/2)|^{0.78}, \tag{54}$$

from the form of which the restriction on the initial conditions for which it is valid is easily found: $x_0 \ll |p_0-1/2|^{0.78}$.

Then for $p_0 \ll 1/2 - x_0^{1.28}$ we have $p_\infty = 0$ and the effective diffusion coefficient is determined from (52) for $p=0$. For $p_0 \gg 1/2 + x_0^{1.28}$ the limiting value is $p_\infty = 1$ and the effective diffusion coefficient is determined for $p=1$ from (51).

If the initial value p_0 is close to the percolation point $p_{crit} = 1/2$, i.e., $|p_0 - 1/2| \ll x_0^{1.28}$, then the range of integration in (51) or in (52) is broken into two integrals from p_0 to p_1, where $x(p)$ increases rapidly from x_0 almost to unity, and from p_1 to unity or zero, from which we can assume $x(p) \approx 1$. The value of the parameter p_1 is determined from the conditions

$$p_1 \approx \tfrac{1}{2}(1 \pm x_0^{1.28}), \tag{55}$$

here the sign $+(-)$ is taken in accordance with that in $p_0 > (<) 1/2$.

Integrating (51) and (52), assuming that we have $x(p) \approx 0$ or $x(p) \approx 1$ depending on the range of integration, using the condition (55) we finally obtain

$$D_{\text{eff}}(p_0) \approx D_{c0}^{\text{I}} \begin{cases} \dfrac{x_0 D_{c0}^{\text{I}}}{p_0 + x_0(1-p_0)} (1-2p_0)^{-\nu}, & p_0 < \dfrac{1}{2}(1-x_0^{1.28}), \\ 2x_0^{0.63}, & |p_0 - \dfrac{1}{2}| < \dfrac{1}{2} x_0^{1.28}, \\ \dfrac{1}{p_0} |2p_0 - 1|^{\delta} \exp[-c(1-p_0)], & p_0 > \dfrac{1}{2}(1+x_0^{1.28}). \end{cases} \tag{56}$$

Here $\nu = (\varkappa^2 - 7\varkappa + 5)/3 \approx 0.29$, holds and δ and c are defined in (43) to be $\delta = 0.49$, $c = 1.18$. [The accuracy of Eqs. (56) decreases as the value of the density p_0 moves further away from 1/2.]

Note that in contrast to the case $x_0 \equiv 0$, for small but nonvanishing x_0 the function $D_{\text{eff}}(p_0)$ has a minimum which, as follows from (56), is attained at the value $p_0 \approx 0.39$. A numerical calculation based on relation (52) for $x(p) \ll 1$ yields a more precise value for the position where the function $D_{\text{eff}}(p_0)$ has a minimum, $p_0 \approx 0.25$. As x_0 increases the location of the minimum moves to the right, and for x_0 close to unity it coincides with the point $p_0 = 1/2$ (see Fig. 2).

This behavior of the effective diffusion coefficient is completely natural. If almost the entire medium consists of the second component ($p_0 \ll 1$), then a particle undergoing random walk rarely needs to pass through the interface between the components, and the quantity D_{eff} is close to $D_{c0}^{\text{II}} = D_{c0}^{\text{I}}$, the diffusion coefficient in a uniform medium. As the fraction of the medium consisting of the first component increases, attracting the random-walking particle to itself, trapping regions arise in the medium and the effective diffusion coefficient sharply decreases. As the fraction of the first component increases further the volumes of the regions where the probability for particles to penetrate is small begin to overlap, and for $p_0 \geqslant 1/2$ these regions form a continuous cluster. As a result, the effective diffusion coefficient increases abruptly and ultimately for some small fraction of the repulsive impurity ($1 - p_0 \ll 1$) the medium again becomes almost uniform, and D_{eff} reaches its original value D_{c0}^{I}.

7. CASES IN WHICH THE PARTICLES ARE WEAKLY REPELLED FROM ONE OF THE COMPONENTS OF THE MEDIUM ($1 - x_0 \ll 1$) AND THE DIFFUSION COEFFICIENTS OF THE COMPONENTS ARE IDENTICAL

When the particles are weakly repelled from the bad component the magnitude $x(p)$ remains close to unity for all values of p, i.e., the local anisotropy of the system in the process of the scale transformation remains weak. It is found that in order to take into account the affect of this weak local anisotropy of the system, the linear approximation is inadequate. Specifically, if we linearize Eq. (53) then it acquires the form

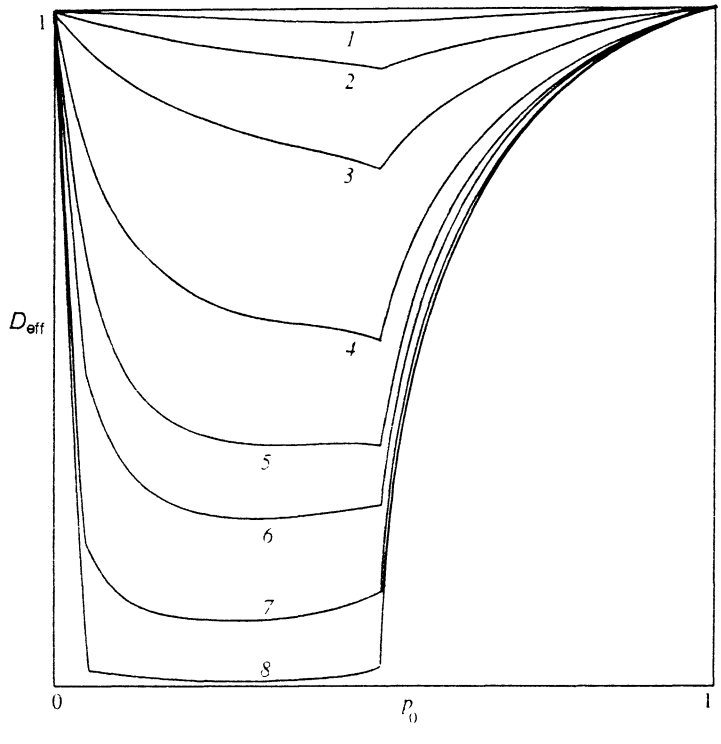

FIG. 2. Results of the numerical calculation of the effective diffusion coefficient $D_{\text{eff}}(p_0)$ at $h \equiv 1$ for different values of x_0: *1*—0.7; *2*—0.45; *3*—0.25; *4*—0.1; *5*—0.05; *6*—0.03; *7*—0.01; *8*—0.001.

$$\frac{d\varepsilon(p)}{dp}=-\frac{\varepsilon(p)}{p-1/2}\left\{1-\frac{1}{4}\left[\frac{Q(p)}{p}+\frac{W(p)}{1-p}\right]\right\}, \quad (57)$$

where we have $\varepsilon(p)=1-x(p)\ll 1$, with $\varepsilon(p_0)\equiv\varepsilon_0=1-x_0\ll 1$.

From Eqs. (51) and (52), retaining only terms to first order in ε_0, we find

$$\ln\frac{D^{\mathrm{I}}(1)}{D^{\mathrm{I}}_{c0}}=\varepsilon_0(1-p_0)-\int_{p_0}^{1}\frac{dp\varepsilon(p)}{2(p-1/2)}\times\left[1-\frac{Q(p)}{2p}+\frac{Q(p)-W(p)}{2}\right], \quad (58)$$

$$\ln\frac{D^{\mathrm{II}}(0)}{D^{\mathrm{I}}_{c0}}=-\varepsilon_0 p_0-\int_{0}^{p_0}\frac{dp\varepsilon(p)}{2(p-1/2)}\times\left[1-\frac{W(p)}{2(1-p)}-\frac{Q(p)-W(p)}{2}\right]. \quad (59)$$

Integrating (57), we can represent $\varepsilon(p)$ in the form

$$\varepsilon(p)=\varepsilon_0\exp[f(p_0)-f(p)], \quad (60)$$

where

$$\frac{df(p)}{dp}=\frac{1}{p-1/2}\left\{1-\frac{1}{4}\left[\frac{Q(p)}{p}+\frac{W(p)}{1-p}\right]\right\}. \quad (61)$$

Using Eqs. (60) and (61) we can easily show that, e.g., the integrand in (58) is a total derivative of the expression $-(1-p)\exp[-f(p)]$, and hence

$$\ln\frac{D^{\mathrm{I}}(1)}{D^{\mathrm{I}}_{c0}}=\varepsilon_0(1-p_0)+\varepsilon_0\exp[f(p_0)]\times\int_{p_0}^{1}\frac{d(1-p)\exp[-f(p)]}{dp}dp\equiv 0. \quad (62)$$

Similarly it can be shown that to within terms $o(\varepsilon_0)$ we also have $o(\varepsilon_0)$ and $\ln[D^{\mathrm{II}}(0)/D^{\mathrm{I}}_{c0}]\equiv 0$. Consequently, to first order in ε_0 we have $D_{\mathrm{eff}}(p_0)\equiv D^{\mathrm{I}}_{c0}$. Including second-order corrections does not present any problem in principle, although the resulting expressions are quite lengthy. For this reason we will not report them here. We note only that $D_{\mathrm{eff}}(p_0)$ is a symmetric function about the point $p_0=1/2$ to second order in ε_0, which is a consequence of the symmetry of the problem for $h\equiv 1$ and $\varepsilon_0\ll 1$ with respect to the interchange $p_0\to 1-p_0$, $\varepsilon_0\to-\varepsilon_0$.

Since for arbitrary initial conditions x_0 and p_0 it is impossible to find an analytical solution for $h_0=1$, we have integrated the corresponding equations numerically for several values of x. The results of the calculation are shown in Fig. 2.

8. RANDOM WALK IN A PERCOLATION STRUCTURE

If the fractions of the components in the system are the same, i.e., $p_0=1/2$, then on large scales there is no absorption of one component by the other [in Eq. (30) the point $p_0=1/2$ is an unstable fixed point, $p(n)\equiv 1/2$]. Such systems are called percolative, and one of the notable properties of such systems is the infinitely large correlation radius. The description of random walks over the structures of such systems is of unquestionable interest.

As before we assume $h_0=1$ and write down equations for the quantities $x(n)$ and $D^{\mathrm{I,II}}(n)$ at $p_0=1/2$:

$$\frac{dD^{\mathrm{I}}(n)}{dn}=(1-\varkappa)[1-x(n)]\left[G^{\mathrm{I}}_1-\frac{1}{2}G^{\mathrm{I}}_2\right]D^{\mathrm{I}}(n), \quad (63)$$

$$\frac{dD^{\mathrm{II}}(n)}{dn}=(1-\varkappa)[1-x(n)]\left[G^{\mathrm{II}}_1-\frac{1}{2}G^{\mathrm{II}}_2\right]D^{\mathrm{II}}(n), \quad (64)$$

$$\frac{dx(n)}{dn}=(1-\varkappa)x(n)[1-x(n)]\times\left[\frac{1}{2}(G^{\mathrm{I}}_2+G^{\mathrm{II}}_2)-(G^{\mathrm{I}}_1+G^{\mathrm{II}}_1)\right]. \quad (65)$$

Here we have written

$$G^{\mathrm{I}}_1=\varkappa\left(\frac{2\varkappa}{3+x}+\frac{1-\varkappa}{1+x}\right),\quad G^{\mathrm{II}}_1=\varkappa\left(\frac{2\varkappa}{1+3x}+\frac{1-\varkappa}{1+x}\right),$$

$$G^{\mathrm{I}}_2=3\frac{\varkappa^2+(1-\varkappa)^2}{3+x}+4\frac{\varkappa(1-\varkappa)}{1+x}+\frac{\varkappa^2+(1-\varkappa)^2}{1+3x},$$

$$G^{\mathrm{II}}_2=\frac{\varkappa^2+(1-\varkappa)^2}{3+x}+4\frac{\varkappa(1-\varkappa)}{1+x}+3\frac{\varkappa^2+(1-\varkappa)^2}{1+3x},$$

and the initial conditions for Eqs. (63)–(65) assume the form

$$x(n=0)=x_0,\quad D^{\mathrm{I}}(n=0)=(1+x_0)^{-1}D^{\mathrm{I}}_{c0},$$

$$D^{\mathrm{II}}(n=0)=x_0(1+x_0)^{-1}D^{\mathrm{I}}_{c0}.$$

It can easily be shown that Eq. (65) in the physical region has only two fixed points, an unstable one at $x=0$ and a stable one at $x=1$. Consequently, we have $x(n)\to 1$ asymptotically for $n\to\infty$.

By integrating the expressions (63) and (64) and using (65) to transform from integration with respect to n to integration with respect to x, we can determine the effective diffusion coefficient over a percolation structure:

$$D_{\mathrm{eff}}=\frac{2D^{\mathrm{I}}_{c0}}{1+x_0}\times\exp\left\{\int_{x_0}^{1}\frac{\left(G^{\mathrm{I}}_1-\frac{1}{2}G^{\mathrm{I}}_2\right)dx}{\left[\frac{1}{2}(G^{\mathrm{I}}_2+G^{\mathrm{II}}_2)-(G^{\mathrm{I}}_1+G^{\mathrm{II}}_1)\right]x}\right\}$$

$$=\frac{2x_0D^{\mathrm{I}}_{c0}}{1+x_0}\times\exp\left\{-\int_{x_0}^{1}\frac{\left(G^{\mathrm{II}}_1-\frac{1}{2}G^{\mathrm{II}}_2\right)dx}{\left[\frac{1}{2}(G^{\mathrm{I}}_2+G^{\mathrm{II}}_2)-(G^{\mathrm{I}}_1+G^{\mathrm{II}}_1)\right]x}\right\}. \quad (66)$$

The relation (66) is a reflection of the fact that for

$h_0=1$ and $p_0=1/2$ we have $D_{\text{eff}} = 2\lim_{n\to\infty} D^{\text{I}}(n) = 2\lim_{n\to\infty} D^{\text{II}}(n)$, which is a consequence of the symmetry in the problem with respect to interchange of the good and bad segments, noted previously.

The integral in (66) can be carried out analytically, and we finally obtain

$$D_{\text{eff}}=\frac{2D^{\text{I}}_{c0}}{1+x_0}\,x_0^{\sigma}\left(\frac{4.78}{x_0^2+2.78x_0+1}\right)^{0.128}, \qquad (67)$$

where $\sigma=(\varkappa^2-3\varkappa+3)/2(1-\varkappa)(4-\varkappa)\approx 0.63$.

Note that these values of D_{eff} for difference values of x_0 agree well with the results of the numerical calculation of $D_{\text{eff}}(p_0)$ at $p_0=1/2$.

Using Eqs. (63)–(65) and relations (37) we can also determine how the mean square displacement depends on time for random walks in a percolative structure. Elementary calculations yield the following imperfect dependence:

$$R^2_{\text{ms}}(t)=D^{\text{I}}_{c0}t\,\frac{1+x(t)}{1+x_0}\left(\frac{x_0}{x(t)}\right)^{\sigma}\left(\frac{x(t)^2+2.78x(t)+1}{x_0^2+2.78x_0+1}\right)^{0.128}, \qquad (68)$$

where $x(t)$ is given to good accuracy by the inverse of the function

$$t\approx\tau_0^{\text{I}}\left(\frac{1-x_0}{1-x(t)}\right)^{8.16}\left(\frac{x(t)}{x_0}\right)^{3.66}. \qquad (69)$$

The behavior of Eqs. (68) and (69) in the nonlinear stage of the process is nonlinear, but at late times the random walk enters the diffusive regime and the function $R^2_{\text{ms}}(t)$ becomes essentially linear. The explanation for this behavior of particles undergoing random walk, as in the case of their localization, is obvious. At early times the fluctuations play a major role, since the particles themselves have still not managed to enter many regions of space, while at late times, although the space itself remains nonuniform, the average reflects the fact the particle has managed to pass through many regions and the local nonuniformity no longer affects it seriously.

It is especially worthwhile to consider the case in which we have $p_0=1/2$ and $x_0\equiv 0$ simultaneously, i.e., the fractions of the two components are equal and the bad regions are absolutely impenetrable to the particle. In this case, after carrying out the limit $x_0\to 0$ we find that expression (68) reduces to

$$R^2_{\text{ms}}(t)=L_0^2(t/\tau_0^{\text{I}})^{(\varkappa/3)(\varkappa^2-4\varkappa+6)}\approx L_0^2(t/\tau_0^{\text{I}})^{0.83}, \qquad (70)$$

which agrees with (49); the latter holds for $p_0=1/2$ not only at early times but also at late times. The function $R^2_{\text{ms}}(t)$ given by (70) remains nonlinear at all times, i.e., it does not approach a diffusive regime. The exponent in (70) is positive for any value of x, so in the limit $t\to\infty$ we have $R^2_{\text{ms}}(t)\to\infty$, which agrees with (46) for $p_0\to 1/2$.

This work was supported by a grant from the Soros Fund, awarded by the American Physical Society.

[1] A. E. Arinshtein and A. P. Moroz, Zh. Eksp. Teor. Fiz. **102**, 221 (1992) [Sov. Phys. JETP **75**, 117 (1992)].
[2] A. E. Arinshtein and A. P. Moroz, Zh. Eksp. Teor. Fiz. **102**, 1921 (1992) [Sov. Phys. JETP **75**, 1033 (1992)].
[3] S. Havlin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987).
[4] J. W. Haus and K. W. Kehr, Phys. Rep. **150**, 265 (1987).
[5] W. Schirmacher, Int. J. Phys. Chem. **95**, 386 (1991).
[6] C. Van den Broeck and V. Balakrishnan, Int. J. Phys. Chem. **95**, 342 (1991).
[7] A. I. Maklakov, V. D. Skrida, and N. F. Fatkullin, *Self-Diffusion in Solutions and Polymer Melts* [in Russian], Kazan State University, Kazan (1987).
[8] M. V. Smoluchovsky, Z. Phys. Chem. **28**, 113 (1924).
[9] V. A. Bagryanskiĭ, Khim. Fiz. **6**, 1429 (1987).
[10] V. I. Gol'danskiĭ, L. I. Trakhtenberg, and V. N. Flerov, *Tunnel Phenomena in Chemical Physics* [in Russian], Nauka, Moscow (1986).
[11] J. M. Zimann, *Models of Disorder: The Theoretical Physics of Homogeneously Disordered Systems*, Cambridge University Press, Cambridge (1979).
[12] A. Baumgärtner and M. Muthukumar, J. Chem. Phys. **89**, 3082 (1987); S. F. Edwards and M. Muthukumar, *ibid.*, 2435 (1988).
[13] K. W. Kehr, P. Kutner, and J. K. Binder, Phys. Rev. B **23**, 4931 (1981).
[14] A. K. Harrison and R. Zwanzig, Chem. Phys. Lett. **164**, 639 (1989).
[15] V. Ya. Balagurov and V. T. Vaks, Zh. Eksp. Teor. Fiz. **65**, 1939 (1973) [Sov. Phys. JETP **38**, 968 (1974)].
[16] I. M. Lifshits, S. A. Gradeskul, and L. A. Pastur, *Introduction to the Theory of Disordered Systems* [in Russian], Nauka, Moscow (1982), Ch. 1.
[17] S. Alexander and R. Orbach, J. de Phys. Lett. **43**, L625 (1982).
[18] L. P. Kadanoff, Physics **2**, 263 (1966).
[19] S. Kirkpatrick, Rev. Mod. Phys. **45**, 574 (1973).
[20] B. I. Shklovskiĭ and A. L. Efros, Usp. Fiz. Nauk **117**, 401 (1975) [Sov. Phys. Usp. **18**, 845 (1975)].

Translated by David L. Book