Diffusion in a continuous medium with space-correlated disorder

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(Received 24 April 1990)

We analyze the effect of space-correlated disorder on diffusion in a one-dimensional continuous disordered medium. We calculate the frequency-dependent diffusion coefficient using a method based on a perturbative treatment around an effective homogeneous medium. Exact results for disorder modeled by a two-level process and by a generalized Poisson process are obtained. We show that, in the Poisson case, changes in the correlation length can induce essential changes in the diffusive behavior of the medium, from strong to weak disorder or vice versa.

I. INTRODUCTION

Diffusion in disordered media is a subject of increasing interest.[1] Main topics of this subject are diffusion through porous media, diffusion in fractal structures, and, in general, phenomena related to anomalous diffusion.

The analysis of diffusion in random media has been mainly developed with the use of discrete models. A standard model can be a random walk, with random transition probabilities. Since these transition probabilities are usually assumed to be independent, the effect of correlated disorder has been scarcely studied. Some aspects of correlated disorder in a discrete medium have been recently discussed.[2] It would seem appropriate to obtain a model for disorder in a continuous medium from a certain limit of a standard discrete model, but, as we show elsewhere[3] the continuum limit of a disordered random walk does not lead to a proper case of diffusion in a standard random field. On the other hand, continuous models of disorder are scarce, and they usually consider Gaussian noise, leading to negative values for the diffusion coefficient.[4] We shall see in this paper that the positivity of the random diffusion coefficient is essential to obtain results with a clear physical meaning. This positivity leads to the necessity of dealing with random processes bounded from below. Then, Gaussian noises are not allowed.

In this paper we analyze the problem of diffusion through a one-dimensional continuous medium. Mathematically, the model consists of a diffusion equation with a random coefficient. Our aim is to calculate averaged transport coefficients for several classes of disorder, and then to analyze the effect of the correlation length. The average of the probability density is not influenced by rare fluctuations, i.e., transport quantities are typical, since the positivity of the random diffusion coefficient prevents nondiffusive behavior. Negative values of the diffusion coefficient, even with very small probability, could influence the value of the averages leading, in some cases, to ballistic behavior. In our case, this is not possible, and we always obtain diffusive or subdiffusive behavior. We use a method based on projection techniques and ordered cumulants. We have applied this method to discrete models[5] and here we adapt it to the continuous case. Essentially, the method is a perturbative calculation around an effective medium. This effective medium seems to be the continuum version of the one found in the effective-medium approximation (EMA) in discrete models.

Our results show that the averaged transport coefficients are very sensitive to the behavior of the probability distribution of the random diffusion coefficient for values close to zero. The effect of the correlation length on the transport coefficients can be understood through the behavior of the probability density.

In order to illustrate this point, we consider two kinds of disorder: one with a two-level process, and the other with a generalized Poisson process. Both are exponentially correlated. We obtain exactly the effective diffusion coefficient and compare the results in both situations. Since, in the first case, the probability density of the diffusion coefficient is independent of the correlation length, likewise is the effective diffusion coefficient. In the second case, we obtain a coefficient strongly dependent of the correlation length, also related to the behavior of the probability density of the random diffusion coefficient. This dependence is so strong that, in some situations, a change of the correlation length implies a change from strong to weak disorder or vice versa.

The paper is organized as follows. In Sec. II we give a sketch of the method and obtain an averaged diffusion equation, in terms of cumulants and the Green's function. From this equation, we obtain an exact expression for the generalized frequency-dependent diffusion coefficient. In Sec. III we take a two-level process as a model of disorder, and we evaluate the generalized diffusion coefficient up to the first order in the frequency, analyzing the effect of the correlation length. A similar analysis, but restricted to the effective diffusion coefficient, is done in Sec. IV, taking a generalized Poisson process as a model of disorder.

II. AVERAGED DIFFUSION EQUATION AND EFFECTIVE-MEDIUM APPROXIMATION

Let us consider our model of diffusion in a one-dimensional disordered medium, by means of the following equation:

$$\frac{\partial P(x,t)}{\partial t}=D\frac{\partial^2 P(x,t)}{\partial x^2}+\frac{\partial}{\partial x}\xi(x)\frac{\partial}{\partial x}P(x,t) , \tag{1}$$

where $P(x,t)$ is the probability density of the diffusing particle, and $D+\xi(x)$ is the random diffusion coefficient. We take $\xi(x)$ with zero mean value, $\langle \xi \rangle=0$, and bounded from below $\xi(x)\geq -D$. In this way, the positivity of the diffusion coefficient, $D+\xi(x)$, is always guaranteed.

To average Eq. (1), we follow the method of Ref. 5. This method has been successfully used in discrete models, and we adapt it to work in the continuum. We start defining two operators, O_ξ and M, as

$$O_\xi=\frac{\partial}{\partial x}\xi(x)\frac{\partial}{\partial x} ,$$

$$Mf(x,t)=\int_{-\infty}^{\infty}dx'\int_0^t dt' G(x,t|x',t')f(x',t') ,$$

where $G(x,t|x',t')$ is the Green's function associated to the diffusion without disorder. In terms of these operators, the random diffusion equation (1) can be written as

$$P(x,t)=M\delta(t-t_0)P(x,t_0)+MO_\xi P(x,t) . \tag{2}$$

We define a projection operator $\mathcal{P}$, which averages over any random function, i.e., $\mathcal{P}F(\xi_1,\dots,\xi_n)=<F(\xi_1,\dots,\xi_n)>$. Applying $\mathcal{P}$ and $(1-\mathcal{P})$ to Eq. (1), we get two coupled equations for $\bar{P}=\mathcal{P}P$ and $(1-\mathcal{P})P$. Formally solving the second equation and substituting into the first one, we obtain

$$\frac{\partial \bar{P}}{\partial t}=D\frac{\partial^2 P}{\partial x^2}+\mathcal{P}O_\xi\bar{P}+\mathcal{P}O_\xi M(1-\mathcal{P})O_\xi\bar{P} +\mathcal{P}O_\xi M(1-\mathcal{P})O_\xi M(1-\mathcal{P})O_\xi\bar{P}+\cdots , \tag{3}$$

and after integrating by parts and rearranging, it reads as

$$\frac{\partial \bar{P}}{\partial t}=D\frac{\partial^2 \bar{P}}{\partial x^2}+\frac{\partial}{\partial x}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}dx_1\dots\int_{-\infty}^{\infty}dx_n\int_0^t dt_1\dots\int_0^{t_{n-1}}dt_n<\xi(x)\xi(x_1)\dots\xi(x_n)>_T \times\frac{\partial^2 G(x-x_1,t-t_1)}{\partial x_1^2}\dots\frac{\partial^2 G(x_{n-1}-x_n,t_{n-1}-t_n)}{\partial x_n^2}\frac{\partial \bar{P}(x_n,t_n)}{\partial x_n} , \tag{4}$$

where $\langle \xi_1,\dots,\xi_n\rangle_T$ denotes the Terwiel cumulants[6] defined as

$$\langle \xi_1\xi_2\cdots\xi_n\rangle_T=\mathcal{P}\xi_1(1-\mathcal{P})\xi_2\cdots(1-\mathcal{P})\xi_n .$$

This equation is our starting point. When cumulants depend on the difference of arguments,

$$\langle \xi_1\xi_2\cdots\xi_n\rangle_T=\theta(x-x_1,x_1-x_2,\dots,x_{n-1}-x_n) , \tag{5}$$

transport coefficients can be straightforwardly obtained from (4). For the generalized diffusion coefficient $D(k,s)$, defined through the expression

$$\bar{P}(k,s)=\frac{1}{s+k^2D(k,s)} ,$$

where $\bar{P}(k,s)$ is the Fourier-Laplace transformation of $\bar{P}(x,t)$, we obtain

$$D(k,s)=D+\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}dy_1\cdots\int_{-\infty}^{\infty}dy_n e^{ik(y_1+\cdots y_n)}\theta(y_1\cdots y_n)\frac{\partial^2 G(y_1,s)}{\partial y_1^2}\cdots\frac{\partial^2 G(y_n,s)}{\partial y_n^2} . \tag{6}$$

The frequency-dependent diffusion coefficient is given by $D(s)=D(k=0,s)$. In this paper we restrict ourselves to the calculation of this coefficient for long times (small s). A direct calculation of this coefficient from Eq. (6) involves an infinite number of terms, even for the lowest order in s given by s^0. A rearrangement of (6) thus becomes necessary. The method consists of two steps. The first one is the summation of terms containing δ functions. In the second step, an effective medium is introduced.

The Laplace transformed Green's function is given by

$$G(x,s)=\frac{1}{2(Ds)^{1/2}}e^{-(s/D)^{1/2}|x|} . \tag{7}$$

Then we get the following relation:

$$\frac{\partial^2 G(x,s)}{\partial x^2}=\frac{1}{D}[sG(x,s)-\delta(x)] . \tag{8}$$

Substituting (8) in (6), integrating the δ terms, and resumming, we obtain

$$D(k,s)=D+\langle\psi\rangle+\sum_{i=1}^{\infty}D_i(k,s)$$
$$=D+\langle\psi\rangle+\sum_{n=1}^{\infty}\left[\frac{s}{D}\right]^n\int_{-\infty}^{\infty}dx_1\cdots\int_{-\infty}^{\infty}dx_n e^{-ikx_n}\langle\psi(0)\psi(x_1)\cdots\psi(x_n)\rangle_T G(-x_1,s)\cdots G(x_{n-1}-x_n,s)\,, \tag{9}$$

with

$$\psi(x)=\frac{\xi(x)}{1+(1-\mathcal{P})\xi(x)/D}\,.$$

This summation seems to be equivalent to the sum of the contributions of neighbors in a discrete case.[4] With the same criterion, the term ψ can be thought of as equivalent to the connective term appearing in the single-site approximation in discrete models.

Since $\langle\psi\rangle\neq 0$, the cumulants do not vanish in all the intervals of integration. As a consequence, all of the terms in the series (9) are of the order of s^0, and expression (9) is not useful to obtain the low-frequency behavior of $D(k,s)$. Things would be very different if $\langle\psi\rangle=0$, because a cumulant with only one argument x_i far enough from the other points $\{x_1,x_2,\ldots,x_i,x_{i+1},\ldots,x_n\}$ vanishes. Then, the order of each term would be $D_n(s)\sim s^{(n+2)/4}$ (n even), $D_n(s)\sim s^{(n+1)/4}$ (n odd), and this is our desired expansion. As a conclusion, we must get a transformation $\psi\to\tilde{\psi}$, where $D(s)$ is given by an expansion similar to (9), but with $\langle\tilde{\psi}\rangle=0$. This is possible by our introducing from the beginning an effective medium, adding and subtracting a quantity Γ in (1),

$$\frac{\partial P}{\partial t}=(D+\Gamma)\frac{\partial^2 P}{\partial x^2}+\frac{\partial}{\partial x}(\xi-\Gamma)\frac{\partial}{\partial x}P\,, \tag{10}$$

and following, step by step, exactly the same calculation. For the generalized diffusion coefficient, we obtain

$$D(k,s)=D+\Gamma+\sum_{n=1}^{\infty}D_i(k,s)=D+\Gamma+\sum_{n=1}^{\infty}\left[\frac{s}{D+\Gamma}\right]^n\int_{-\infty}^{\infty}dx_1\cdots\int_{-\infty}^{\infty}dx_n e^{-ikx_n}$$
$$\times\langle\tilde{\psi}(0)\tilde{\psi}(x_1)\cdots\tilde{\psi}(x_n)\rangle_T\tilde{G}(-x_1,s)\tilde{G}(x_1-x_2,s)\cdots\tilde{G}(x_{n-1}-x_n,s)\,, \tag{11}$$

where $\tilde{G}$ is the Green's function, associated to the diffusion equation with coefficient $\tilde{D}=D+\Gamma$, and

$$\tilde{\psi}=\frac{\xi-\Gamma}{1+(1-\mathcal{P})(\xi-\Gamma)/(D+\Gamma)}\,.$$

The precise value of Γ will be fixed by the condition $\langle\tilde{\psi}\rangle=0$. In such a case,

$$\Gamma=\left\langle\frac{\xi}{D+\xi}\right\rangle\Big/\left\langle\frac{1}{D+\xi}\right\rangle\,. \tag{12}$$

This condition is equivalent to the self-consistency condition of the EMA found in discrete models. Now, the expansion (11) is appropriate to obtain the behavior in the limit $s\to 0$. The order of $D_i(s)$ is as expected, $s^{(i+2)/4}$ (i even) and $s^{(i+1)/4}$ (i odd). We remark that this method only permits us to calculate transport coefficients in the case of weak disorder. With strong disorder, we obtain a zero diffusion coefficient, i.e., $\Gamma=-D$. Then, expression (11) is not well defined, and it is necessary to introduce a frequency-dependent effective medium $\Gamma(s)$. This problem will be treated elsewhere. In this paper we calculate diffusion coefficients in the weak disorder case. We are also able to analyze the transition from weak to strong disorder when changing parameters as the correlation length. This change is detected when the diffusion coefficient $\tilde{D}=D+\Gamma$ vanishes.

III. EXACT RESULTS FOR A TWO-LEVEL PROCESS

Our first example is a disordered medium, such that the diffusion coefficient $D+\xi(x)$ has two possible states, $D+\Delta$ and $D-\Delta$, with the same probability; that is, $\langle\xi(x)\rangle=0$. For the sake of simplicity, we assume $\xi(x)$ to be an exponential correlated process, so that its correlation function has the form

$$\langle\xi(x)\xi(x')\rangle=\Delta^2 e^{-|x-x'|/l} \tag{13}$$

with l being the correlation length. In order to keep the positivity of the diffusion coefficient, the amplitude of the process ξ must be smaller than D, $\Delta<D$. The limiting case, $D=\Delta$, leads to strong disorder, and it will not be treated in this paper.

The application of Eq. (12) to this example immediately gives an exact effective diffusion coefficient $\tilde{D}$ as

$$\tilde{D}=D+\Gamma=\frac{D^2-\Delta^2}{D}\,. \tag{14}$$

From this formula, we see that the disorder acts to reduce the diffusion of the particle. An interesting thing appearing in this model is that the effective diffusion coefficient D is only dependent on the intensity Δ. This is not surprising, because the probability density of the two-level process is only dependent on the intensity Δ, so that

$$P(\xi)=\delta(\xi-\Delta)/2+\delta(\xi+\Delta)/2\ ,$$

and the diffusion coefficient $\tilde{D}$ only depends on this probability.

The frequency-dependent terms $D_i(s)$ can be obtained from expression (11). In the case of a process with fixed levels, it is not difficult to obtain directly $\tilde{\psi}$ in terms of ξ. In our case, this expression is

$$\tilde{\psi}=\frac{D^2-\Delta^2}{D^2}\xi+\frac{D^2-\Delta^2}{D^3}\xi\mathcal{P}\xi\ . \tag{15}$$

Substituting $\tilde{\psi}$ in (11) and operating, one can easily check that the order in s of $D_i(s)$ is in agreement with the one derived in Sec. II. The three first terms are given by

$$D_1(s)=\frac{D^2-\Delta^2}{D^3}\left[\frac{sD}{D^2-\Delta^2}\right]^{1/2}\times\frac{\Delta^2}{1/l+[sD/(D^2-\Delta^2)]^{1/2}}+O(s)\ , \tag{16}$$

$$D_2(s)=\frac{\Delta^4 s}{D^4\{1/l+[sD/(D^2-\Delta^2)]^{1/2}\}^2}+O(s^{3/2})\ , \tag{17}$$

$$D_3(s)=\frac{5\Delta^4}{6D^4}sl^2+O(s^{3/2})\ , \tag{18}$$

where the expression for $D_3(s)$ is valid only for finite l. The term $D_3(s)$ has a structure similar to $D_1(s)$ and $D_2(s)$, but due to its size, we write only the leading term in s and l. The effect of the correlation length can now be analyzed with these exact expressions. We first note that for times large enough, such that $l \ll (D/s)^{1/2}$, the coefficients $D_1(s)$, $D_2(s)$,. . . are proportional to the relation between l and the length diffused by the system with the effective diffusion coefficient. Then for large times, the system sees the random diffusion coefficient as uncorrelated, and the diffusion has no dynamic components.

The effective diffusion coefficient is independent of l when l is finite [see (14)]. However, in the limit $l\to\infty$, the coefficients $D_1(s)$, $D_2(s)$, etc. become static. Then, they contribute to the effective diffusion coefficient. Since in this limit the diffusion coefficient is given by $D(0,s)=D$, this value must be recovered from the sum of all the terms in (11). On the other hand, when l decreases, the $D_i(s)$ also decrease, going to zero in the limit $l\to 0$. In this limit, the diffusion has no dynamic components; that is, it is a pure diffusion with a coefficient $\tilde{D}=D+\Gamma$. This is a rather surprising fact, because it means that a process with a δ Kronecker correlation, $\langle\xi(x)\xi(x')\rangle=\Delta^2\delta_{x,x'}$ has an important effect on the diffusive properties of a disordered medium. This kind of δ Kronecker correlated noise also appears in the continuum limit of disordered random walk.[3]

Finally, we remark the necessity of taking a positive random diffusion process, $D+\xi>0$, in order to obtain results with a physical meaning. A violation of this rule, $\Delta>D$, would lead to a negative diffusion coefficient in (14) and imaginary coefficients in $D_i(s)$. We note that in the limit of Gaussian white noise ($l\to 0$), $\Delta^2 l=D$ implies an unbounded noise, and it has no physical consistency.

IV. EFFECTIVE DIFFUSION COEFFICIENT FOR A GENERALIZED POISSON PROCESS

We consider now a disordered medium with a generalized Poisson process as diffusion coefficient. This process can be thought of as composed of elementary functions located at points x_i The x_i points follow a Poisson distribution of parameter λ. The magnitude of the elementary functions depends of a random parameter. In this example, we have chosen exponential functions with a height ω and decay parameter $1/l$, with ω being a random variable exponentially distributed and with mean value ω_0. With this choice we obtain a process $\theta(x)$ exponentially correlated with $\lambda\omega_0$ as mean value. The Poisson process, with zero mean value, is then $\xi(x)=\theta(x)-\lambda\omega_0$. Now the correlation function for the process $\xi(x)$ is given by

$$\langle\xi(x)\xi(x')\rangle=\frac{\lambda\omega_0^2}{l}e^{-|x-x'|/l}\ , \tag{19}$$

and its probability distribution is[7]

$$P(\xi)=\frac{e^{-\lambda l}}{(\omega_0/l)^{\lambda l}\Gamma(\lambda l)}e^{-l\xi/\omega_0}(\xi+\lambda\omega_0)^{\lambda l-1}\ . \tag{20}$$

The positivity of the stochastic diffusion coefficient $D+\xi(x)$ is guaranteed, if the condition $D>\lambda\omega_0$ holds.

The effective diffusion coefficient $D+\Gamma$ can be calculated from (12) and (20), giving

$$\tilde{D}=D+\Gamma=(D-\lambda\omega_0)\left[\frac{(al)^{-\lambda l}e^{-al}}{\Gamma(1-\lambda l,al)}\right]\ , \tag{21}$$

where $a=(D-\lambda\omega_0)/\omega_0$ and $\Gamma(\alpha,x)=\int_x^\infty e^{-t}t^{\alpha-1}dt$.

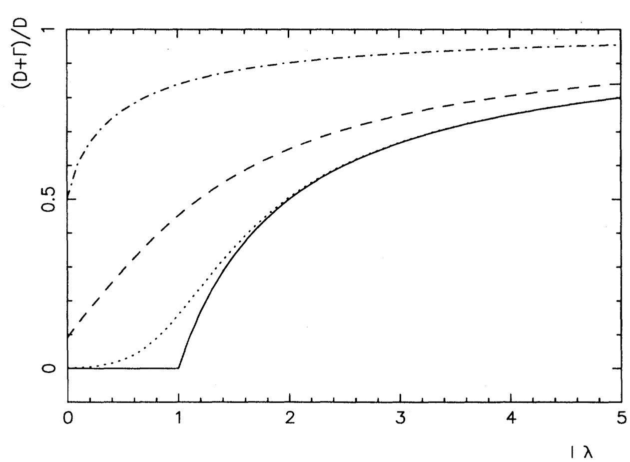

FIG. 1. Effective diffusion coefficient for a generalized Poisson process $(D+\Gamma)/D$ vs correlation length, in units of λ^{-1} for different values of D: solid line, $D=1$; dotted line, $D=1.001$; dashed line, $D=1.1$; dot-dashed line, $D=2$. The parameters taken are $\lambda=1$, and $\omega_0=1$.

In this case, the coefficient $\tilde{D}$ depends strongly on the correlation length. A plot of the relative change of the diffusion coefficient $\tilde{D}/D$ versus the correlation length in units of λ^{-1} is given in Fig. 1 for different values of $\lambda\omega_0/D$. In all cases, the disorder reduces the diffusion coefficient as in our preceding example. However, the correlation length plays an important role in the determination of the diffusive properties. The effective diffusion coefficient grows with an increase of the correlation length.

It can be shown that $\tilde{D}\to D$ when $l\to\infty$. In the opposite limit, $l\to 0$, we get $\tilde{D}\to D-\lambda\omega_0$. In the limiting case, $\lambda\omega_0/D=1$ (solid curve), we can see a transition from weak disorder ($\lambda l>1$) to strong disorder ($\lambda l<1$). In this case, we get from (21) that $\tilde{D}=D-\omega_0/l$ for $\lambda l>1$, and $\tilde{D}=0$ for $\lambda l<1$. This transition is also observable at the level of the probability density $P(\xi)$ in (20), as a change from finite to infinite of inverse moments. The transition from weak to strong disorder can be understood in the following way. When $\lambda\omega_0=D$, the random diffusion coefficient is not zero due to the spatial pulses. The mean distance between pulses is larger than the width of the pulses when $l<\lambda^{-1}$. In this case, there is no overlapping of the pulses, and the effective diffusion coefficient $\tilde{D}$ vanishes. On the contrary, when $l>\lambda^{-1}$, the pulses overlap, and $\tilde{D}>0$.

V. CONCLUSIONS

In this paper we have analyzed the effect of the correlation length on the diffusive properties of a disordered medium. We deal with a one-dimensional continuous medium, so that our starting point is a simple diffusion equation with a random coefficient. Despite its simplicity, there are no exact results for this model, even in the case of a two-level process. Most studies have been devoted to discrete models. On the other hand, these models usually consider independent random probabilities from site to site. As a consequence, the effect of correlation has been scarcely analyzed.

Our analysis is valid for a general process with the physical constraint imposed by considering positive diffusion coefficients. This restriction implies a bounded process and, hence, prevents the use of Gaussian noise. Concerning this, our exact results indicate that this restriction is essential in order to obtain real and positive diffusion coefficients.

We use a perturbative method around a continuous effective medium, which is the equivalent to the effective medium found in discrete models when using the EMA. This method permits us to establish a parallelism between the discrete model and the continuous one. In this way, we can do a resummation similar to the single-site approximation and find a relation equivalent to the autoconsistency relation of the EMA.

Finally, we analyze two different cases of disorder. The first case is a medium modeled by a two-level process. We get the frequency-dependent diffusion coefficient $D(s)$ up to order s. The static diffusion coefficient $D(0)$ is only dependent of the probability distribution of the process and, consequently, is independent of the correlation length.

The second case analyzed is a disordered medium modeled by a generalized Poisson process. We calculate the exact expression of the static diffusion coefficient $D(0)$. The correlation length has, in this case, a strong influence. In some situations, a change of the correlation length can induce a transition from weak to strong disorder or vice versa.

As a general conclusion, we note that the diffusive properties, obtained, for example, from the effective diffusion coefficient $D(0)$, depend on the disorder only through the probability distribution of the process. This dependence appearing explicitly in (21) is very sensitive to the value of the inverse moments, which explains our first conclusion about the impossibility of using Gaussian noise (with infinite inverse moments). This conclusion is known to be valid also in discrete models. As a consequence, the effect of correlated disorder can be analyzed through the behavior of the one-point probability distribution of the process, with respect to the correlation length.

ACKNOWLEDGMENTS

Financial support from Dirección General de Investigación Científica y Técnica, Project No. PB-87-0014 is acknowledged.

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