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Diffusion in a random multiplying medium: Exact bounds and simulations

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We analyze the problem of diffusion in a one-dimensional random multiplying medium. We consider the case of a Gaussian δ-correlated field. Exact bounds, valid for any time, are obtained for the averaged concentration. Results of simulations are explained by considering the contribution of random-walk realizations with small spans.

The problem of diffusion in random multiplying media has attracted considerable attention in recent literature.[1-5] This problem appears in several physical and biological systems and has been treated with different techniques.

Diffusion in random multiplying media is equivalent to a polymer in a random potential, so it has been analyzed with Flory theory and the replica trick.[1,3] Also, it models chemical reactions, biological multiplication, and the evolution of species.[6] Then, random-walk techniques are more convenient. By considering imaginary time, the diffusion equation transforms to a Schrödinger equation with a random potential and then techniques for the calculation of the density of states also become useful.[5] Finally, when the multiplicative factor is imaginary the problem is reduced to that of transverse spin depolarization of a diffusing particle.[7]

The basic equation governing the evolution of such models is a diffusion equation with a random multiplicative factor:

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

where $n(x,t)$ can be either a concentration of particles or other magnitudes related with polymer chains, electronic density, etc. For the sake of concreteness we take $n(x,t)$ to be a concentration of diffusive particles in a multiplicative medium. In this paper we only deal with one-dimensional problems. The random multiplicative field $\xi(x)$ is taken to be Gaussian with a zero mean and correlation given by

$$\langle \xi(x)\xi(x')\rangle=\theta\delta(x-x')\,. \tag{2}$$

Other cases with a correlation length different from zero have a more regular behavior[5] and will not be treated in this paper.

The quantities of interest are either the averaged Green function taken in the initial point $\langle G(x,t/x,0)\rangle$ (Refs. 1 and 3) or the total contribution $\overline{n(t)}=\int\langle G(x,t)\rangle dx$.[2,4,5] Both quantities have the same exponential behavior and only differ in factor. We take $\overline{n(t)}$ as the object of our calculations. By now two kinds of analyses have been done on such quantities: one investigating the asymptotic time behavior[1-5] and the other obtaining bounds valid for any time.[8]

After some confusing results the asymptotic form of $\overline{n(t)}$ or $\langle G(x,t/x,0)\rangle$ seems to be established as $\exp(\gamma t^3)$, where the constant γ is $\frac{1}{48}$.[1-5,8] Bounds for any time are surer quantities but apparently more difficult to calculate. On the other hand, simulations are scarce and do not reproduce the exact behavior.[1,3] The disagreement between simulations and the analytic result has been partially explained by Guyer and Machta[3] using a Flory theory and taking into account the effect of a finite number of configurations (realizations of the random field).

The aim of this Rapid Communication is to study the complementary effect due to a finite number of random-walk realizations and to explain simulation results with the calculation of bounds valid for any time. This effect can be analyzed in a separate way by averaging exactly over all possible configurations of the field. Our simulations of diffusive trajectories over this averaged field give an asymptotic behavior as $\overline{n(t)}_s\approx\exp(\gamma_0\theta/D^{1/2}t^{3/2})$ where γ_0 depends slowly on the number of realizations but is independent of the spatial step. In the following, we use the lower index s to denote simulation results. This behavior is different from the exact asymptotic form $\exp(\gamma t^3)$ because, as we will see, the exact $\overline{n(t)}$ is dominated by the contribution of nontypical realizations of very low probability which cannot be reproduced in the computer. So, in our analysis of the simulations we only take into account realizations with a probability large enough to be reproduced in the computer. In this form we obtain analytical results in agreement with simulations. We remark that our simulations are affected only by finite-random-walk realization effects and not by finite configuration effects. We then conclude that the behavior $\exp(\gamma_0 t^{3/2})$ is due to finite-random-walk realization effects. Furthermore, if one considers a finite number of field configurations, we show that the behavior should be exponential, $\exp(at)$, as t becomes large, in agreement with a previous analysis.[3]

From Eq. (1) it is easy to obtain an exact solution in the form of series. We take $n(x,t)$ in powers of ξ:

$$\begin{aligned}n(x,t|x_0)=&\,G(x,t|x_0,0)\\&+\sum_{n=1}^{\infty}\int_0^t dt_1\cdots\int_0^{t_{n-1}}dt_n\int_{-\infty}^{\infty}dx_1\cdots\int_{-\infty}^{\infty}dx_n G(x,t|x_1,t_1)\\&\times G(x_1,t_1|x_2,t_2)\cdots G(x_n,t_n|x_0,0)\xi(x_1)\cdots\xi(x_n)\,,\end{aligned} \tag{3}$$

where $G(x,t/x',t')$ is the Green function of the diffusion equation. Now we average over field configurations, take the Laplace transform in time, and change integration variables, obtaining

$$\langle n(x,s|x_0)\rangle=\tilde{G}(x-x_0,s)+\sum_{n=1}^{\infty}\left[\frac{\theta}{4(Ds^3)^{1/2}}\right]^n\frac{1}{2\sqrt{Ds}}\int dz_1\cdots\int dz_{2n}\exp[-|(x-x_0)(s/D)^{1/2}-z_1|]$$
$$\times e^{-|z_1-z_2|}\cdots e^{-|z_{2n}|}\sum_p\delta(z_{i_1}-z_{j_1})\cdots\delta(z_{i_n}-z_{j_n})\,. \tag{4}$$

Here $\tilde{G}$ is the Laplace transform of G given by

$$\tilde{G}(x-x_0,s)=\frac{1}{2\sqrt{Ds}}\exp\left[-\frac{|x-x_0|}{\sqrt{D/s}}\right] \tag{5}$$

and $\sum_p$ indicates a summation over all possible partitions of $(1,2,\ldots,2n)$ in pairs $(i_1,j_1)\cdots(i_n,j_n)$. Note that we have used the Gaussian property of $\xi(x)$. Integrating in (4) and antitransforming we finally obtain

$$\overline{n(t)}=1+\sum_{n=1}^{\infty}\left[\frac{\theta t^{3/2}}{2\sqrt{D}}\right]^n\frac{\gamma_{n\nu}}{\Gamma[(3n/2)+1]}\,, \tag{6}$$

where Γ is the gamma function and γ_n is given by

$$\gamma_n=\int dy_1\cdots\int dy_{2n}\,e^{-|y_1|\cdots-|y_{2n}|}\sum_p\delta\left[\sum_{i_1}^{2n}y_k-\sum_{j_1}^{2n}y_k\right]\cdots\delta\left[\sum_{i_n}^{2n}y_k-\sum_{j_n}^{2n}y_k\right]. \tag{7}$$

From (6) it is difficult to obtain the time behavior but it is easy to have an upper bound. Taking into account the inequality $\gamma_n<2^n(2n-1)!!$ in (6) we get the following bound valid for any time:

$$\overline{n(t)}\le\left[1+\frac{9\theta t^{3/2}}{\sqrt{\pi D}}\right]\exp\left[\frac{4\theta^2t^3}{27D}\right]. \tag{8}$$

It is also possible to obtain lower bounds from (6) and (7) but we will obtain a better bound using a different method in the following section.

Since simulations must be performed in a discrete space we analyze the corresponding discrete equation and its continuous limit. We take the following discrete version of (1):

$$\frac{\partial N_i(t)}{\partial t}=\frac{\lambda}{2}[N_{i+1}(t)+N_{i-1}(t)-2N_i(t)]+\omega_iN_i(t)\,, \tag{9}$$

where $N_i(t)$ is the number of particles in site i at time t and ω_i is the multiplication factor in site i. ω_i must be a random Gaussian variable with a zero mean and correlation given by

$$\langle\omega_i\omega_j\rangle=\frac{\theta}{L}\delta_{i,j}\,, \tag{10}$$

L being the spatial step. Equation (9) represents a random walk in a chain with a random multiplicative factor. The continuous limit from (9) and (10) is obviously defined through a simultaneous limit of $L\to 0$ and $\lambda\to\infty$ as

$$n(x,t)=\lim_{L\to 0}\frac{1}{L}N_{x/L}(t)\,, \tag{11}$$

$$D=\tfrac{1}{2}\lim_{\substack{\lambda\to\infty\\ L\to 0}}\lambda L^2. \tag{12}$$

Taking D and θ as constants, the limit process can be characterized by only the parameter L.

Let us consider realizations of the random walk with span s. In terms of such realizations we can calculate $\overline{N(t)}$ as

$$\overline{N(t)}=\left\{\left\langle\exp\left[\sum_{i=1}^{s}\omega_iz_i\right]\right\rangle\right\}, \tag{13}$$

$1,2,3,\ldots,s$ being the distant sites visited and $z_1,z_2,z_3,\ldots,z_s$ the occupation time of each site during a total time $t=\sum z_i$. The curly brackets indicate an average over all possible random walks, and as before the angular brackets average over field realizations. The last averaging can be immediately performed taking into account the Gaussian nature and independence of ω_i obtaining

$$\overline{N(t)}=\left\{\exp\left[\frac{\theta}{2L}\sum_{i=1}^{s}z_i^2\right]\right\}. \tag{14}$$

By considering the trivial inequalities $(\sum z_i=t)$

$$t^2\ge\sum_{i=1}^{s}z_i^2\ge\frac{t^2}{s}\,,$$

in (14) we have two bounds for $\overline{N(t)}$:

$$\sum_s e^{\theta t^2/2Ls}P_s(t)\le\overline{N(t)}\le e^{\theta t^2/2L}\,, \tag{15}$$

where $P_s(t)$ is the probability of having a span s in time t. For large t it is given by[9]

$$P_s(t)\approx\frac{8t\lambda}{s^3}\sum_{j=0}^{\infty}\left[\frac{\pi^2(2j+1)^2t\lambda}{s^2}-1\right]\times\exp\left[-\frac{\pi^2(2j+1)^2t\lambda}{2s^2}\right]. \tag{16}$$

From (15) and taking only the contribution of $s=1$ we can deduce the asymptotic form of $\overline{N(t)}$ as $\exp(\theta t^2/2L)$. This is the original result of Zeldovich[10] which is valid in discrete space and asymptotic time.

The continuous limit of (15) provides a lower bound for $\overline{n(t)}$ in the form

$$\overline{n(t)}>\int_0^{\infty}e^{\theta t^2/2x}P(x,t)dx\,, \tag{17}$$

where now $P(x,t)$, the probability of a span x, is given for any time by

$$P(x,t)=\frac{16Dt}{x^3}\sum_{j=0}^{\infty}\left[\frac{\pi^2(2j+1)^2 2Dt}{x^2}-1\right]\times\exp\left[-\frac{\pi^2Dt(2j+1)^2}{x^2}\right]. \tag{18}$$

Integration of (17) with (18) gives, for any time

$$\overline{n(t)}>\sum_{j=0}^{\infty}\left[\frac{4\theta t^{3/2}}{\pi^{5/2}\sqrt{D}(2j+1)^3}+\frac{\theta^3 t^{9/2}}{4\pi^{9/2}D^{3/2}(2j+1)^5}\right]\times\exp\left[\frac{\theta^2t^3}{16\pi^2(2j+1)^2D}\right], \tag{19}$$

where as in the discrete case the contribution of spans close to zero is dominant.

The lower bound in (15) has been used as an approximation in the calculation of spin depolarization.[7] Physically the bound represents the case in which all sites are occupied during the same time (t/s). When the contribution of small spans is dominant the equal-time occupancy seems to be a good approximation.[5] Then the asymptotic behavior must be well approximated by this lower bound. So we are going to consider (15) and (19) not only as strict lower bounds but also as approximations able to explain qualitatively results of simulations. We note that bounds for $\langle G(x,t/x,0)\rangle$ can be immediately obtained translating known results from the equivalent problem of the density of states of a particle in a Gaussian potential.[8] It is a remarkable fact that there is a lower bound that gives the exact asymptotic behavior.[8]

It is possible to perform simulations of this problem, among other ways, from expressions (13) or (14). The first case includes random-walk and random-field simulations, so that two effects due to a finite number of both random-walk realizations and field configurations affect the final result. In expression (14) one of the averages has been exactly performed and only the effect of a finite number of random-walk realizations remains. This last method obviously is less time consuming and only presents one kind of uncertainty. A similar method has been used to simulate spin depolarization of a diffusing particle in Ref. 7. Here we consider this method and for the sake of comparison with other simulations we discuss finite field-configuration effects at the end of this paper. So, in what follows, we shall refer only to realizations of the random walk.

The contribution of $s=1$ in (15) is dominant in the asymptotic value of $\overline{N(t)}$ and it has an exponentially small probability. Realizations corresponding to such small spans cannot be reproduced in a simulation of great but finite realizations. Hence, in a simulation we expect to have the contribution of realizations with small span but with significant probability. A rough estimation of simulation results can be obtained by substituting in (15) s by the smallest span obtained in simulations $s^-=\gamma_0(M)(Dt)^{1/2}/L$,

$$\overline{N(t)}s\approx\exp[\gamma_0(M)\theta t^{3/2}/D^{1/2}], \tag{20}$$

where $\gamma_o(M)$ is a factor depending on the number of realizations M, and $(Dt)^{1/2}/L$ is proportional to the asymptotic mean value of s. This behavior differs from the one obtained when considering a finite number of field configurations.[3] In this case a slower time dependence $\exp(\alpha t)$ was derived by using the Flory theory.[3] In our case (a finite number of random-walk realizations) it is easy to see from (15) that $\exp(\beta t^{3/2})$ is strictly a lower bound when taking the contributions close to $s=(Dt/L)^{1/2}$. Such contributions have enough significance to be simulated in the computer. The exponential growth $\exp[L\theta t/(2D)]$ can be produced by taking contributions close to $s\approx\lambda t$. This is obviously a bound lower than (20) and with a small probability of occurrence.

We show in Table I our results of simulations made from expression (14). In order to analyze the time behavior we have compared the quantities $\ln\overline{N(t)}_s/(t^2\theta/2L)$, $\ln\overline{N(t)}_s/(t^{3/2}\theta/D^{1/2})$, and $\ln\overline{N(t)}_s/[(\theta/L)^{1/2}t]$ related, respectively, with the Zeldovich result or a case with infinite random-walk realizations, the estimation of the smallest span and the exponential growth due to finite field configurations. This last effect is analyzed at the end of the paper [see (26)]. As time increases the first quantity decreases, the second fluctuates, and the third increases. We have obtained similar results for several values of D and θ so that we conclude that (20) is a correct estimation. Moreover, we have confirmed that the value of $\overline{N(t)}_s$ for large enough (t) is independent of L. This can be seen in Fig. 1 where we have plotted $\overline{N(t)}_s$ for different values of L. Since we are mostly interested in the continuous limit $L\to 0$ we analyze this case in detail. From (17) and (18) we can write $\overline{n(t)}$ in a form more adequate for our analysis:

$$\overline{n(t)}\geq\int_0^{\infty}\exp\left[\frac{\theta t^{3/2}}{2\sqrt{2D}y}\right]P(y)dy, \tag{21}$$

where now $P(y)$ is independent of time,

$$P(y)=\frac{8}{y^3}\sum_{j=0}^{\infty}\left[\frac{\pi^2(2j+1)^2}{y^2}-1\right]\exp\left[-\frac{\pi^2(2j+1)^2}{2y^2}\right]. \tag{22}$$

A plot of $P(y)$ can be found on page 423 of Ref. 9. As

TABLE I. Evolution of the quantities $A=2L\ln\overline{N}_s/\theta t^2$, $B=D^{1/2}\ln\overline{N}_s/\theta t^{3/2}$, and $C=\ln\overline{N}_s/[(\theta/L)^{1/2}t]$ with time. The parameters of the simulation are $\theta=2\times10^{-3}$, $D=1$, $L=4.47$, and $M=70000$.

t	A	B	C
900	6.73×10^{-2}	0.226	0.641
1800	1.30×10^{-1}	0.617	2.475
2700	1.30×10^{-1}	0.756	3.717
3600	1.25×10^{-1}	0.841	4.772
4500	1.16×10^{-1}	0.867	5.501
5400	1.12×10^{-1}	0.920	6.395
6300	1.03×10^{-1}	0.910	6.834
7200	9.26×10^{-2}	0.878	7.053
8100	9.09×10^{-2}	0.915	7.792
9000	8.66×10^{-2}	0.918	8.245

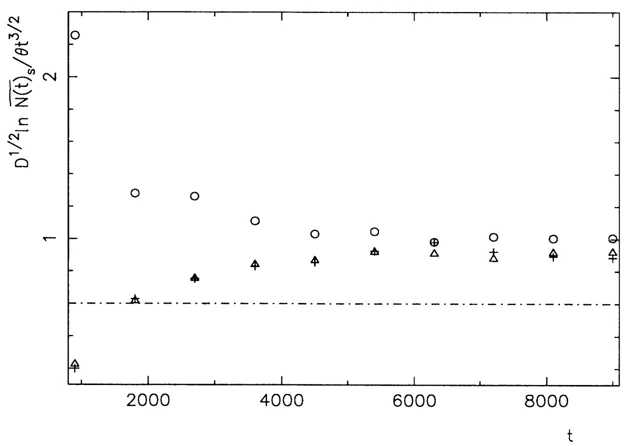

FIG. 1. Time evolution of $D^{1/2}\ln\overline{N(t)}_s/\theta t^{3/2}$ for three values of the step L. Circles correspond to $L=14.14$, triangles to $L=4.47$, and crosses to $L=1.414$. The dot-dashed line is the lower bound estimated from (23). Other parameters are $D=1$, $\theta=2\times10^{-3}$, and $M=70000$.

representative parameters of this curve we take the mean value $y=(8/\pi)^{1/2}$ and variance $\sigma_y=2(\ln2-2/\pi)^{1/2}$. In a simulation only realizations corresponding to values of $y\in(y_0,y_1)$ such that $p(y)$ has a significant value are possible. Then for large enough t $[t\gg t_a=(\pi^2 2(2D)^{1/2}/y_0\theta)^{2/3}]$, $\overline{n(t)}_s$ has a lower bound given by

$$\overline{n(t)}_s \geq \int_{y_0}^{y_1}\exp\left[\frac{\theta t^{3/2}}{2\sqrt{2D}y}\right]P(y)dy \approx \exp\left[\frac{\theta t^{3/2}}{2\sqrt{2D}y_0}\right]. \tag{23}$$

Here t_a is the time such that the integrand in (23) is much greater than unity when $P(y)$ is estimated by the term $j=0$ in (22). In Table II we show the influence of the number of realizations. The parameter $y_0(M)$ can be calculated as

$$\frac{1}{M}=\int_0^{y_0}P(y)dy. \tag{24}$$

As expected, (23) is a lower bound of $\overline{n(t)}_s$ and also gives a good estimation of the variation due to the number of realizations. The relation between $\gamma_0(M)$ and the estimation given by (23), $1/(8^{1/2}y_0)$, is nearly constant. From simulations we have observed that the asymptotic regime appears in a time between $4t_a$ and $5t_a$.

TABLE II. Values of y_0, t_a, $(8^{1/2}y_0)^{-1}$, and $\gamma_0(M)$ for different M. Parameters of simulation are $L=1.4142$, $D=1$, and $\theta=2\times10^{-3}$.

M	y_0	t_a	$(8^{1/2}y_0)^{-1}$	$\gamma_0(M)$
20	0.974	590.0	0.363	0.60 ± 0.1
1000	0.715	725.0	0.494	0.78 ± 0.05
5000	0.658	766.3	0.537	0.79 ± 0.05
70000	0.589	825.0	0.600	0.91 ± 0.08

Finally, the effect of a finite number of configurations (field realizations) can be analyzed from (13) by considering the value obtained for $\overline{N(t)}$. For N realizations of the Gaussian variable ω_i we can estimate $\overline{N(t)}$ by

$$\overline{N(t)}\approx\left[\frac{2\pi\theta}{L}\right]^{-1/2}\left\{\prod_{i=1}^{s}\left[\int_{-x_0}^{x_0}dx \times\exp\left[-\frac{1}{2\theta}x^2+xz_i\right]\right]\right\}, \tag{25}$$

where the curly brackets indicate an average over random-walk realizations and x_0 is such that $\mathrm{erfc}[x_0(L/\theta)^{1/2}]\approx1/N$, that is, $x_0\approx(\theta\ln N/L)^{1/2}$. The effect of a finite number N of field configurations is important in (25) when $z_i\gg(L\ln N/\theta)^{1/2}$. Using the uniform occupation time approximation, $z_i\approx t/s\approx(t/D)^{1/2}$, we obtain $t\gg DL\ln N/\theta$. Therefore, as t becomes large we get, from (25),

$$\overline{N(t)}\approx\exp[(\theta\ln N/L)^{1/2}t]. \tag{26}$$

This result is in agreement with previous analysis.[3] However, when $z_i<(L\ln N/\theta)^{1/2}$, the value for $\overline{N(t)}$ obtained from (25) can be approximated by the averaged value over all field realizations given by (14). In this case we can apply our analysis to study finite-random-walk realization effects. It is then possible that for certain values of the parameters an intermediate time scale exists such that simulation results for $\overline{N(t)}$ show the behavior $\exp(t^{3/2})$. This kind of behavior has been obtained in simulations performed with a finite number of field realizations.[1,3]

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