Exact Solution for Diffusion in a Random Potential

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An analytical solution for one-dimensional diffusion in a Gaussian random potential is presented. In the long-time limit, the logarithm of the average population at the center, $\ln(\langle P\rangle)$, grows as fast as $t^{3/2}$, disproving some former estimates that $\ln(\langle P\rangle)$ increases at the rate of t^2. Numerical simulations have confirmed the theoretical solution.

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Diffusion in random media has attracted a great deal of attention.[1] Zhang[2] and Ebeling and co-workers[3] recently related the diffusion process of the equation

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

to the localization in quantum mechanics, and studied the behavior of $P(\mathbf{x},t)$ in individual potentials, where $V(\mathbf{x})$ has a Gaussian distribution, and D and λ are constants. In the long-time limit, they found that diffusion in random media is related to hopping from one localized center to another.

Physical quantities averaged over the random potentials are of great importance in the study of random systems. This issue, which was not addressed by the above authors, will be explored in detail in this Letter. If, for example, Eq. (1) describes a biological model, $P(\mathbf{x},t)\,d\mathbf{x}$ is the population of the bacteria at position $\mathbf{x}$ in region $d\mathbf{x}$ at time t. The average $\langle P(\mathbf{x},t)\rangle$ would provide an expectation value for experiments.

In a previous work by Zel'dovich *et al.*,[4] it was argued that $\langle P(x,t)\rangle$, the average over a Gaussian random potential, has the behavior

$$\lim_{t\to\infty}\frac{\ln\langle P(\mathbf{x},t)\rangle}{t^2}=\frac{\sigma^2}{2}, \tag{2}$$

where the angular brackets represent the average; $\sigma^2=\langle[\lambda V(\mathbf{x})]^2\rangle$, the variance of the potential which has zero mean $\langle V\rangle=0$. According to them, the above result is not affected by the diffusion constant D, the initial condition $P(\mathbf{x},0)$, or the dimensionality. Their prediction also says that the fluctuation[4] in P is even bigger than the average $\langle P(\mathbf{x},t)\rangle$,

$$\ln\langle[P(\mathbf{x},t)-\langle P(\mathbf{x},t)\rangle]^2\rangle\sim 2\sigma^2t^2. \tag{3}$$

Then it is difficult to check the above result by numerical calculations.

This issue has recently received a lot of attention and has become somewhat controversial. Contradictory conclusions have been obtained by different methods.[5,6] It is clear that an exact analytical result can shed light on the problem. In order to clarify the issue, we shall investigate the one-dimensional version of the above model and present its analytical solution in this Letter. $V(x)$ is Gaussian, namely,

$$\langle V(\mathbf{x})\rangle=0,\quad \langle V(x_1)V(x_2)\rangle=\delta(x_1-x_2). \tag{4}$$

The initial condition is $P(\mathbf{x},0)=\delta(\mathbf{x})$. In such a case, the result of Zel'dovich *et al.* reads

$$\lim_{t\to\infty}\frac{\ln\langle P(\mathbf{x},t)\rangle}{t^2}=\frac{\lambda^2}{2}\delta(0), \tag{5}$$

which is the same as obtained by Heinrichs and Kumar.[6]

Our analytical solution for this problem gives a different answer,

$$\lim_{t\to\infty}\frac{\ln\langle P(0,t)\rangle}{t^{3/2}}=\frac{\lambda^2}{4}\left(\frac{\pi}{D}\right)^{1/2}, \tag{6}$$

which grows slower than the result in Eq. (5). Since the growth rate of $\ln\langle P\rangle$ as $t^{3/2}$ is first reported, extensive numerical simulations have also been performed. As shown in Fig. 1, the numerical results confirm the above solution quite well. It is easy to understand that when $t\gg 1$, $\langle P(\mathbf{x},t)\rangle$ is of the same order as $\langle P(0,t)\rangle$, if $x<\sqrt{Dt}$. A careful reexamination of the approach by Zel'dovich *et al.* reveals that their original argument is flawed, i.e., Eq.

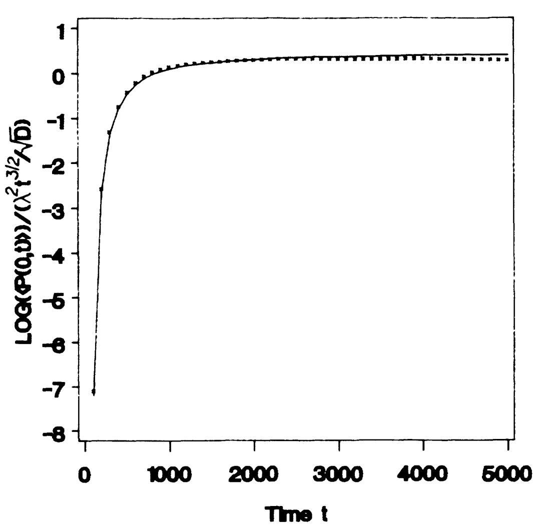

FIG. 1. $\ln\langle P(0,t)\rangle/(\lambda^2t^{3/2}/\sqrt{D})$ vs time t. The theoretical curve is $\sqrt{\pi}/4-\ln[2(\pi Dt)^{1/2}]/(\lambda^2t^{3/2}/\sqrt{D})$. The lattice size is 2000, $\lambda=0.01$, and $D=0.1$.

(5) is invalid. In Fig. 2 the numerical results $\ln\langle P(0,t)\rangle/t^2$ are decreasing instead of tending to a constant as $t\to\infty$, which implies that $\ln\langle P(\mathbf{x},t)\rangle$ cannot grow as fast as t^2.

The method[7] employed here was developed by the present author and Luttinger, a combination of Feynman path integral[8] and replica trick.[9] Mathematically, $P(x,t)$ is the solution of Eq. (1). If $P(\mathbf{x},t)$ grows faster than the exponential growth,[4] its Laplace transform may not be convergent. As a standard mathematical measure, we turn t to the imaginary axis, $t=i\tau$. Then Eq. (1) reads

$$i\frac{\partial P(x,i\tau)}{\partial\tau}=-D\frac{\partial^2P(x,i\tau)}{\partial x^2}-\lambda V(x)P(x,i\tau)\,,\tag{7}$$

with the initial condition $P(x,0)=\delta(x)$. The Fourier transform of $P(x,i\tau)$, $\psi(x,s)=\int_0^\infty e^{-is\tau}P(x,i\tau)d\tau$, satisfies the equation $H\psi(x,s)=-i\delta(x)$, where $H=-D\nabla^2-\lambda V(x)+s$. The solution is $\psi(x,s)=-i\langle x\,|\,1/H\,|\,0\rangle$. After using a path integral,[7] we write $\psi(x,s)$ in the form

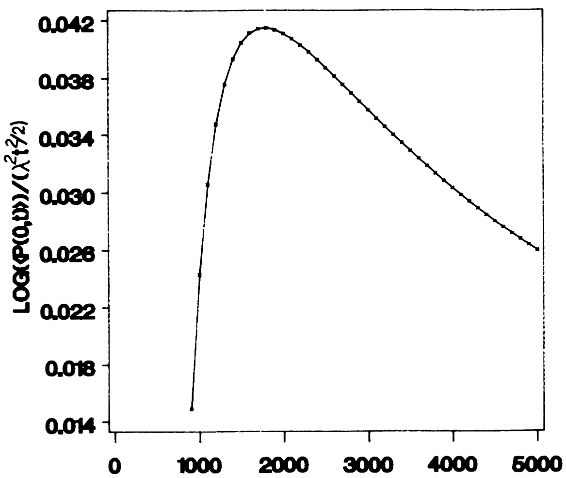

FIG. 2. The same numerical results plotted in $\ln\langle P(0,t)\rangle/(\lambda^2t^2/2)$ vs time t. As t increases, the curve decreases instead of tending to a constant.

$$\psi(x,s)=-\frac{2}{D}\lim_{n\to 0}\int d\boldsymbol{\varphi}\,\varphi_1(0)\varphi_1(x)\exp\left[-i\int_{-\infty}^{\infty}dz\,\boldsymbol{\varphi}\left(\frac{d^2}{dz^2}+\frac{\lambda}{D}V(z)-\frac{s}{D}\right)\boldsymbol{\varphi}\right],\tag{8}$$

where $\boldsymbol{\varphi}=(\varphi_1,\ldots,\varphi_n)$ is an n-dimensional vector.

Equation (8) enables us to carry out the average over the potential V in a simple manner. Denoting this average by $\langle\psi(x,s)\rangle$, we have $\langle\psi(x,s)\rangle$ in the form

$$\langle\psi(x,s)\rangle=\frac{-2}{D}\lim_{n\to 0}\int d\boldsymbol{\varphi}\,\varphi_1(0)\varphi_1(x)\exp\left\{-i\int_{-\infty}^{\infty}dz\left[\boldsymbol{\varphi}\left(\frac{d^2}{dz^2}-\frac{s}{D}\right)\boldsymbol{\varphi}-\frac{i\lambda^2}{2D^2}(\boldsymbol{\varphi}^2)^2\right]\right\},\tag{9}$$

where we have used the formula

$$\left\langle\exp\left[-i\int_{-\infty}^{\infty}\frac{\lambda}{D}V(z)\boldsymbol{\varphi}^2dz\right]\right\rangle=\exp\left[-\frac{\lambda^2}{2D^2}\int_{-\infty}^{\infty}(\boldsymbol{\varphi}^2)^2dz\right].\tag{10}$$

Following the same procedure as in Ref. 7, we get the solution for $\langle\psi(x,s)\rangle$,

$$\langle\psi(x,s)\rangle=-\frac{2}{D}\int_0^\infty dr\int_0^\infty dr_1\,\phi_0(r)\phi_0(r_1)g(r,r_1,|x|)\,,\tag{11}$$

where $g(r,r_1,t)$ is a Green's function, satisfying the equation

$$i\frac{\partial g}{\partial t}=\left[-\frac{1}{4}\left(\frac{\partial^2}{\partial r'}-\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\right)-\frac{s}{D}r^2-i\frac{\lambda^2}{2D^2}r^4\right]g\,,\tag{12}$$

and the boundary conditions $g(r,r_1,0)=r\delta(r-r_1)$; ϕ_0 is the solution of the equation

$$-\frac{1}{4}\left(\frac{d^2\phi_0}{dr^2}-\frac{1}{r}\frac{d\phi_0}{dr}\right)-\left(\frac{s}{D}r^2+\frac{\lambda^2}{2D^2}ir^4\right)\phi_0=0\,,\tag{13}$$

with the boundary conditions $\phi_0(0)=1$, $\phi_0(\infty)=0$. The differential Eq. (13) can be solved exactly. Using $u=r^2/2$, we transform it to the form

$$\frac{d^2\phi_0}{du^2}+4\left(\frac{s}{D}+i\frac{\lambda^2}{D^2}u\right)\phi_0=0\,,\tag{14}$$

which implies that ϕ_0 is an Airy function. After taking the boundary conditions into account, we represent it in the form

$$\phi_0=\left(1+\frac{i\lambda^2}{Ds}u\right)^{1/2}H_{1/3}^{(1)}\left[\frac{4(sD+i\lambda^2u)^{3/2}}{3i\lambda^2D}\right]\Bigg/H_{1/3}^{(1)}\left[\frac{4(s^3D)^{1/2}}{3i\lambda^2}\right],\tag{15}$$

where $H_{1/3}^{(1)}$ is the Hankel function of the first kind.

As $t\to\infty$, $\langle P(x,t)\rangle$ should be little different from $\langle P(0,t)\rangle$, if x is not too far from the center. We thus consider $\langle P(0,t)\rangle$, which has a simpler analytical expression. From Eq. (11), at $x=0$, we have

$$\langle \psi(0,s)\rangle = -\frac{2}{D}\int_0^\infty [\phi_0(r)]^2 r\,dr = -\frac{2}{D}\int_0^\infty [\phi_0]^2 du\,. \tag{16}$$

Here again $u=r^2/2$. Differentiating Eq. (14) with s, we get

$$\frac{d^2}{du^2}\left[\frac{\partial\phi_0}{\partial s}\right] + 4\left[\frac{s}{D}+i\frac{\lambda^2}{D^2}u\right]\frac{\partial\phi_0}{\partial s} + \frac{4}{D}\phi_0 = 0\,. \tag{17}$$

Multiplying Eq. (17) by ϕ_0, Eq. (14) by $\partial\phi_0/\partial s$, and subtracting and integrating over u, we find

$$\langle \psi(0,s)\rangle = \frac{1}{2}\left[\phi_0\frac{d}{du}\left[\frac{\partial\phi_0}{\partial s}\right] - \frac{d\phi_0}{du}\frac{\partial\phi_0}{\partial s}\right]_{u=0}^{u=\infty} = -\frac{1}{2}\frac{\partial}{\partial s}\left[\left.\frac{d\phi_0}{du}\right|_{u=0}\right], \tag{18}$$

where we have used $\phi_0(0)=1$, $\phi_0(\infty)=0$, $\partial\phi_0(u)/\partial s\,|_{u=0}=0$, and $\partial\phi_0(u)/\partial s\,|_{u=\infty}=0$ in the derivation. From Eq. (15), we have

$$\left.\frac{d\phi_0}{du}\right|_{u=0} = i\left[\frac{\lambda^2}{D}\right]\left[\frac{Z'(s)}{Z(s)}\right], \tag{19}$$

where $Z(s)=s^{1/2}H_{1/3}^{(1)}[4(s^3D)^{1/2}/3i\lambda^2]$. $\langle P(0,i\tau)\rangle$ is then given by

$$\langle P(0,i\tau)\rangle = -\frac{i\lambda^2}{4\pi D}\int_{-\infty}^{\infty} ds\,\frac{\partial}{\partial s}\left[\frac{Z'(s)}{Z(s)}\right]e^{is\tau}. \tag{20}$$

The solution of $\langle P(0,t)\rangle$ is obtained by replacing $i\tau$ with t.

Now let us examine the result of Eq. (20). As $\lambda\to 0$, from Eq. (19), $\psi(0,s)=-(i/2\sqrt{sD})$, which yields the exact result for diffusion without a potential, $P(0,t)=1/2(\pi Dt)^{1/2}$. A variable transform $\eta=s(D/\lambda^4)^{1/3}$ in Eq. (20) concludes that $\langle P(0,t)\rangle$ must have the form

$$\langle P(0,t)\rangle = (\lambda/D)^{2/3} f(t(\lambda^4/D)^{1/3})\,, \tag{21}$$

where the function f is given by

$$f(iy) = -\frac{i}{4\pi}\int_{-\infty}^{\infty} d\eta\left\{\frac{\partial^2}{\partial\eta^2}\ln\left[\eta^{1/2}H_{1/3}^{(1)}\left[\frac{4}{3i}\eta^{3/2}\right]\right]\right\}e^{iy\eta}. \tag{22}$$

Using the formula for a Hankel function,[10]

$$H_\nu^{(1)}(x) = \left[\frac{2}{\pi x}\right]^{1/2}\exp\left[i\left[x-\frac{\nu}{2}\pi-\tfrac{1}{4}\pi\right]\right]\sum_{m=0}^{\infty}\frac{1}{m!}\frac{\Gamma(\nu+m+\frac{1}{2})}{\Gamma(\nu-m+\frac{1}{2})}\frac{1}{(2ix)^m}, \tag{23}$$

we can expand $f(iy)$ in the form

$$f(iy) = \frac{1}{2(\pi iy)^{1/2}}\left[\sum_{l=0}^{\infty} c_l (iy)^{3l/2}\right]. \tag{24}$$

Coefficients c_l can be derived from Eq. (23). For example, $c_0=1$, $c_1=\sqrt{\pi}/4$, etc. Comparing these coefficients, we find that as $t\to\infty$,

$$\langle P(0,t)\rangle \to \frac{1}{2(\pi DT)^{1/2}}\exp\left[\frac{\sqrt{\pi}}{4}\frac{\lambda^2}{\sqrt{D}}t^{3/2}\right]. \tag{25}$$

In order to further clarify the issue, we have reexamined the approach used by Zel'dovich *et al.* From Eq. (1), $P(x,t)$ can be expressed as

$$P(x,t) = \frac{1}{A}\int [dx]\exp\left\{-\int_0^t\left[\frac{1}{4D}\left[\frac{\partial x}{\partial\tau}\right]^2 + \lambda V(x(\tau))\right]d\tau\right\}, \tag{26}$$

where A is the normalization factor. The integration is over all paths between $x(0)=0$ and $x(t)=x$. The property of

V in Eq. (4) enables us to find the average

$$\langle P(x,t)\rangle = \frac{1}{A}\int [dx]\exp\left[-\int_0^t \frac{1}{4D}\left(\frac{\partial x}{\partial \tau}\right)^2 d\tau + \frac{\lambda^2}{2}\int_0^t\int_0^t d\tau_1 d\tau_2 \delta(x(\tau_1)-x(\tau_2))\right]. \tag{27}$$

If there is no diffusion, i.e., $D=0$, only one path $x(\tau)\equiv 0$ connects two ends, $x(0)=0$ and $x(t)=0$; then $\langle P(0,t)\rangle \to \exp[\lambda^2\delta(0)t^2/2]$, as $t\to\infty$. When $D\neq 0$, diffusion makes a big difference. First, there is an infinite number of possible paths now; $x\equiv 0$ is only one of them. Second, since the δ function has a nonzero value only as its argument is zero, $x(\tau)\equiv 0$ must be a singular path. Though it has the maximum value for the integrand, any deviation of $dx(\tau)$ from this path immediately gets zero from the δ function. Therefore, it is invalid to expand the integral in Eq. (27) around $x(\tau)\equiv 0$. The contribution to the integration from $x\equiv 0$ is negligible. Accordingly, $\langle P(0,t)\rangle$ must be $\ll \exp[\lambda^2 t^2\delta(0)/2]$, then $\ln\langle P(0,t)\rangle$ cannot increase faster than t^2. If we assume that as $t\to\infty$, $\langle P(0,t)\rangle \to \exp(\lambda^2 a_0 t^n)$, and constants a_0 and n can be determined by

$$a_0 t^n = \left.\frac{\partial \ln\langle P(0,t)\rangle}{\partial(\lambda^2)}\right|_{\lambda=0}. \tag{28}$$

Using the result

$$\frac{1}{A}\int [dx]\exp\left[-\int_{t_1}^{t_2}\frac{1}{4D}\left(\frac{\partial x}{\partial\tau}\right)^2 d\tau\right] = \frac{1}{2[\pi D(t_2-t_1)]^{1/2}}\exp\left\{-\frac{[x(t_2)-x(t_1)]^2}{4D(t_2-t_1)}\right\}, \tag{29}$$

we find that $a_0 t^n$ is given by

$$(D\pi t)^{1/2}\int_0^t d\tau_1\int_0^t d\tau_2 \int [dx]\exp\left[-\int_0^t\frac{1}{4D}\left(\frac{\partial x}{\partial\tau}\right)^2 d\tau\right]\delta(x(\tau_1)-x(\tau_2)) = \frac{1}{4}\left(\frac{\pi}{D}\right)^{1/2} t^{3/2}, \tag{30}$$

which is the same as Eq. (25).

A simple argument can further illustrate our result. From Eq. (1) $\langle P\rangle$ is effected by both diffusion and the environment $\lambda V(x)$. At time t, the diffusion spreads the population appreciably to the region $|x|\le 2\sqrt{Dt}$. The length scale thus is $\sqrt{Dt}$. Equation (27) reads

$$\langle P\rangle = M_x \exp\left[\tfrac{1}{2}\lambda^2\int_0^t\int_0^t \langle V(x(\tau_1))V(x(\tau_2))\rangle d\tau_1 d\tau_2\right],$$

where M_x denotes averaging over all paths. From a scaling argument, $\ln\langle P\rangle$ should have the form $\lambda^2 t^2/L$ where L has the dimensions of length. Then, L must have the order of $\sqrt{Dt}$, and hence $\ln\langle P\rangle \sim \lambda^2 t^{3/2}/\sqrt{D}$.

Extensive numerical simulations have also been performed. Averaging over the whole sample space is beyond the ability of our computer. To ensure a reliable result, we first perform a numerical simulation of Eq. (1) with $D=0$ and determine the number of samples necessary to produce a result which is consistent with the theoretical one, i.e., $\ln\langle P\rangle \sim t^2$. Then we use the same number of samples in the simulation of Eq. (1) with $D\neq 0$. It can be seen in Fig. 1 that the numerical result compares quite well with the theoretical solution. At $D\neq 0$, as t varies from 0 to 4000, for example, $\langle P(0,t)\rangle$ increases from 1 to the order of 10^{13}, but $\ln\langle P(0,t)\rangle/(\lambda^2 t^{3/2}/\sqrt{D})$ tends to a constant, $\sim\sqrt{\pi}/4$. The number of samples in a simulation increases with t from several hundred to more than one thousand. We have carried out simulations with different parameters. All of them give the same behavior as our analytical solution. Fluctuations do not cause any problem in the verification of our result. In Fig. 2, as t increases, the curve decreases instead of tending to a constant, which implies that $\ln\langle P(0,t)\rangle$ must grow slower than t^2 at $D\neq 0$.

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