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Multidimensional diffusion in random potentials

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It is shown that, in the long-time limit, d-dimensional diffusion in a Gaussian random potential has the logarithm of the average population $\ln\langle P\rangle$ growing as $t^{(2-d/2)}$. The dimension $d=4$ is critical. For $d\geq 4$, $\langle P\rangle$ only grows as a power of t. Numerical simulations have confirmed this result.

Diffusion in random media, where disorder involves presence of traps and sources, has recently received considerable attention.[1-4] In this Rapid Communication, we will discuss the following diffusion equation in d-dimensional space:

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

where D and λ are constants. $V(\mathbf{r})$ has a "white-noise" Gaussian distribution,

$$\langle V(r)\rangle=0,\ \ \langle V(\mathbf{r}_1)V(\mathbf{r}_2)\rangle=\delta(\mathbf{r}_1-\mathbf{r}_2)\,. \tag{2}$$

The initial condition is $P(\mathbf{r},0)=\delta(\mathbf{r})$. Equation (1) is related to many problems in physics, chemistry, and biology.[1-4] For example, we can consider that Eq. (1) describes a biological model. Then $P(\mathbf{r},t)d\mathbf{r}$ is the population of the bacteria at position $\mathbf{r}$ and time t. Previous studies[5,6] claimed that $\langle P(\mathbf{r},t)\rangle$, averaged over the Gaussian random potential, has the behavior

$$\lim_{t\to\infty}\frac{\ln\langle P(\mathbf{r},t)\rangle}{t^2}=\frac{\lambda^2}{2}\delta(0)\,. \tag{3}$$

The result in Eq. (3) was sufficient to trigger a debate.[7]

For the one-dimensional version of Eq. (1), an exact solution was recently derived.[4] In the long-time limit,

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

This result was confirmed by numerical simulations.[4] Equation (4) contradicts the former result in Eq. (3).

In this Rapid Communication, we will argue that in d-dimensional space ($d<4$),

$$\lim_{t\to\infty}\ln\langle P(\mathbf{r},t)\rangle/t^{2-d/2}=(\lambda^2/D^{2-d/2})\times\text{const}\,, \tag{5}$$

where const has a finite positive value. The magnitude of this constant has also been estimated. Dimension $d=4$ is critical. For $d\geq 4$, $\langle P(\mathbf{r},t)\rangle$ only grows as fast as a power of t. As shown in Figs. 1 and 2, extensive numerical simulations confirm Eq. (5) quite well for $d=1$ and 2.

Let us first consider a scaling transform. If we set $\mathbf{r}=\xi\mathbf{x}$ and $t=\eta\tau$ in Eq. (1), then

$$\frac{\partial P}{\partial \tau}=\frac{\eta D}{\xi^2}\frac{\partial^2 P}{\partial \mathbf{x}^2}+\eta\lambda V(\xi\mathbf{x})P\,. \tag{6}$$

Since $\langle V(\xi\mathbf{x}_1)V(\xi\mathbf{x}_2)\rangle=\delta(\mathbf{x}_1-\mathbf{x}_2)/\xi^d$, we have $V(\xi\mathbf{x})=V(\mathbf{x})/\xi^{d/2}$. The initial condition is now $P(\xi\mathbf{x},0)=\delta(\mathbf{x})/\xi^d$. In order to express the dependence of $P(\mathbf{r},t)$ on D and λ explicitly, we write it in the form

$$P(\mathbf{r},t)=g(\mathbf{r},t,D,\lambda)\,, \tag{7}$$

where g is some unknown function. Then, from Eq. (6), we have

$$g(\mathbf{r},t,D,\lambda)=g(\mathbf{r}/\xi,t/\eta,D\eta/\xi^2,\eta\lambda/\xi^{d/2})/\xi^d\,. \tag{8}$$

By selecting $\xi=(D/\lambda)^{2/(4-d)}$ and $\eta=(D/\lambda)^{4/(4-d)}/\lambda$, we have

$$P(\mathbf{r},t)=(\lambda/D)^{2d/(4-d)}g(\mathbf{r}(\lambda/\eta)^{2/(4-d)},\ t\lambda(\lambda/D)^{d/(4-d)},1,1)\,. \tag{9}$$

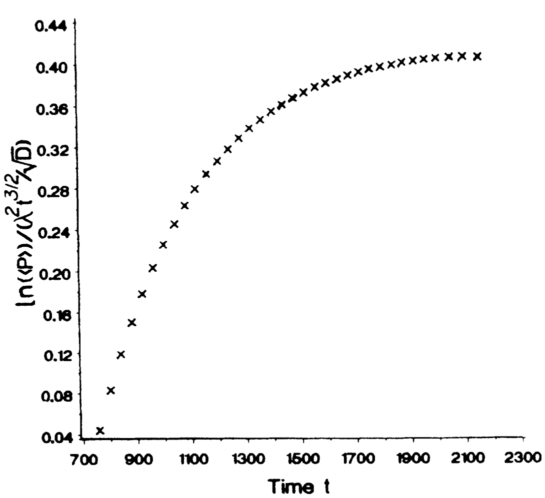

FIG. 1. One-dimensional numerical simulation. $\ln(\langle P\rangle)/(\lambda^2 t^{3/2}/\sqrt{D})$ vs time t. The lattice size is 2000, $\lambda=0.01$, and $D=0.1$. As t increases, the curve tends to a constant, $\sim\sqrt{\pi}/4$.

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At the center $\mathbf{r}=0$,

$$P(0,t)=(\lambda/D)^{2d/(4-d)}g_0(t\lambda(\lambda/D)^{d/(4-d)}), \quad (10)$$

where $g_0(y)=g(0,y,1,1)$. It is easy to understand that when $t\gg 1$, $\langle P(\mathbf{r},t)\rangle$ is of the same order as $\langle P(0,t)\rangle$, if $|\mathbf{r}|<\sqrt{Dt}$. Therefore, we shall explicitly consider $\langle P(0,t)\rangle$.

The scaling argument cannot further provide the form of function g or g_0. But Eq. (10) provides a criterion for any analytical result. For example, since the previous result in Eq. (3) cannot be expressed in the form of Eq. (10), it appears to be incorrect for the present problem. The form of Eq. (10) is also very useful in numerical calculations. We only need to perform numerical calculations for one set of λ and D. The results for other sets of λ and D can then be deduced from Eq. (10).

Let us now apply the path integral formulism[8,9] to study the behavior of g or g_0. From Eq. (1), the solution is given by

$$P(\mathbf{r},t)=\frac{1}{A}\int d\mathbf{r}\exp\left\{-\int_0^t d\tau\left[\frac{1}{4D}\left(\frac{\partial\mathbf{r}}{\partial\tau}\right)^2+\lambda V(\mathbf{r}(\tau))\right]\right\}, \quad (11)$$

where A is the normalization factor. The integration is over all paths between $\mathbf{r}(0)=0$ and $\mathbf{r}(t)=\mathbf{r}$. The Gaussian property of V in Eq. (2) enables us to find the average

$$\langle P(\mathbf{r},t)\rangle=\frac{1}{A}\int d\mathbf{r}\exp\left[-\int_0^t\frac{1}{4D}\left(\frac{\partial\mathbf{r}}{\partial t}\right)^2 d\tau+\frac{\lambda^2}{2}\int_0^t\int_0^t d\tau_1 d\tau_2\delta(\mathbf{r}(\tau_1)-\mathbf{r}(\tau_2))\right]. \quad (12)$$

Equation (11) can be written in the form

$$\langle P\rangle=M_{\mathbf{r}}\left[\exp\left(\frac{1}{2}\lambda^2\int_0^t\int_0^t d\tau_1 d\tau_2\delta(\mathbf{r}(\tau_1)-\mathbf{r}(\tau_2))\right)\right], \quad (13)$$

where $M_{\mathbf{r}}$ denotes averaging over all paths. In estimating Eqs. (12) and (13), we note that $\langle P\rangle$ is affected by both diffusion and the environment $\lambda V(\mathbf{r})$. As in the above biological model, the environment either enhances or reduces the growth of bacteria. Without diffusion, in long-time limit, the population in the areas with negative V would be eventually eliminated. In some sense, diffusion is an averaging process in which the densely populated areas (with big P) give their population to unpopulated areas. The diffusion rate is proportional to the population gradient. Therefore, in the presence of diffusion, the population in the area of negative V cannot be eliminated. During time interval t, the diffusion spreads the population appreciably to a sphere with radius of $\sqrt{Dt}$. The length scale thus is $\sqrt{Dt}$. From a scaling argument for Eq. (11), $\ln\langle P\rangle$ should have the form $\lambda^2 t^2/L^d$ where L has the dimension of length. Then, L must be of order $\sqrt{Dt}$, and hence $\ln\langle P\rangle\sim(\lambda^2/\sqrt{D^d})t^{2-d/2}$. We can further estimate

$$\ln\langle P(0,t)\rangle\sim\tfrac{1}{2}\lambda^2\int_0^t d\tau_1\int_0^t d\tau_2\int d\mathbf{r}(\tau_1)\int d\mathbf{r}(\tau_2)\delta(\mathbf{r}(\tau_1)-\mathbf{r}(\tau_2))/V_s^2, \quad (14)$$

where the integrals of $d\mathbf{r}(\tau_1)$ and $d\mathbf{r}(\tau_2)$ are taken in the sphere of radius $\sqrt{Dt}$ and V_s is the volume of that sphere, $V_s=\pi^{d/2}(\sqrt{Dt})^d/\Gamma(1+d/2)$. Then, we have, as $t\to\infty$,

$$\ln\langle P(0,t)\rangle/(t^{(2-d/2)}\lambda^2/D^{d/2})\sim\Gamma(1+d/2)/2\pi^{d/2}. \quad (15)$$

The constant at the right-hand side of Eq. (15) is only an estimate, i.e., not exact. For example, if we set $d=1$, it gives $\frac{1}{4}$ which is close to but not the same as the analytical result $\sqrt{\pi}/4$. The total population P_t can be estimated at $t\gg 1$,

$$\langle P_t\rangle\sim\langle P(0,t)\rangle\pi^{d/2}(\sqrt{Dt})^d/\Gamma(1+d/2). \quad (16)$$

Therefore, it is also true, $\ln\langle P_t\rangle\sim t^{(2-d/2)}\lambda^2/D^{d/2}$.

Extensive numerical simulations have also been performed. A detailed discussion about the method solving diffusion equation can be found in Ref. 10. In Figs. 1 and 2, the time step Δt and the space step a used in the numerical calculation are taken as the unit of time and length. From the von Neumann stability analysis,[10] we select $D\ll 1$ and $\lambda\ll D$. Numerical methods always convert the partial differential equations to difference equations. To simulate a continuum system, the size of the system must

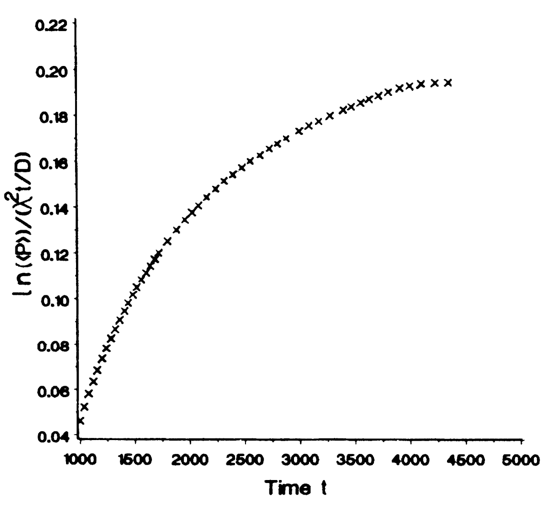

FIG. 2. Two-dimensional numerical simulation. $\ln(\langle P\rangle)/(\lambda^2 t/D)$ vs time t. The lattice size is 400×400, $\lambda=0.01$, and $D=0.1$. As t increases, the curve tends to a constant.

be much bigger than the space step a.[10] In addition, it is extremely important in this problem to make the system big enough to avoid the boundary effect. Typically, since systems in numerical simulations are finite, periodic boundary conditions are introduced to compensate some finite-size effect. But the present problem is so different that the periodic boundary conditions do not compensate any boundary effect. In order to illustrate our point, let us consider one-dimensional diffusion. Equation (1) is about diffusion in an infinite space, but in the numerical simulation one-dimensional diffusion on a finite system with the periodic boundary conditions is equivalent to diffusion on a finite ring. Then, if the size of the system L is small, there is strong "feed back" from the bounds through the periodic boundary conditions. It can be further shown that in the long-time limit, this boundary effect makes diffusion on a small ring fundamentally different from diffusion on an infinite system. As $\sqrt{Dt} \gtrsim L$, the population distribution on a small ring eventually becomes smooth. Then we can denote $\int P(x,t)dx = L\bar{P}(t)$ where $\bar{P}(t)$ is the space-average value of the population. From Eq. (1),

$$\int P(x,t)dx = \lambda \int V(x)P(x,t)dx \,, \tag{17}$$

which can be written as

$$L\bar{P}(t) = \lambda \bar{P}(t) \int V(x)dx \,. \tag{18}$$

The property of Gaussian random potential V in Eq. (2) enables us easily to evaluate the sample average on a small ring $\langle \bar{P}(t) \rangle$,

$$\ln(\langle \bar{P}(t) \rangle) \sim \tfrac{1}{2}\lambda^2 t^2 / L \,. \tag{19}$$

The above argument applies to diffusion in high dimensions, too. Therefore, in order to extend the results from a numerical simulation on a small system to diffusion on an infinite system, we must have the simulation free of any significant boundary effect. The required size of the system can be estimated as follows. As the time equals to $t\Delta t$, the front of the tails has moved to $x, y, \ldots = \pm ta$ in the numerical simulation. If ta is much bigger than the size of the system, the tail has already run around the system several times, accelerating the exponential growth. Even the population at the boundary then becomes sizable. To avoid this artificial "feedback" from the bounds, it is better to have the size of the system of the order of ta in calculating diffusion up to time $t\Delta t$. That the size of the system is made only bigger than $\sqrt{Dt}$ is found to be insufficient.

In this problem, 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 $D \neq 0$. Figure 1 presents a one-dimensional simulation. As shown from the figure, $\ln(\langle P \rangle)/(\lambda^2 t^{3/2}/\sqrt{D})$ tends to a constant $\sim \sqrt{\pi}/4$, which confirms the analytical result in Eqs. (4) and (5). At $D=0.1$, as t varies from 0 to 2000, for example, $\langle P(0,t) \rangle$ increases from 1 to the order of 10^5, but $\ln[\langle P(0,t) \rangle]/[(\lambda^2/\sqrt{D})t^{3/2}]$ 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.

Figure 2 is a simulation in two dimensions with the same numerical method as in one dimension. But now $\ln(\langle P \rangle)/(\lambda^2 t/D)$ tends to a constant in the limit $t \to \infty$, which confirms the result in Eq. (5).

[1] For example, see G. H. Weiss, J. Stat. Phys. **42**, 3 (1986), and references therein; K. Kang and S. Redner, Phys. Rev. A **32**, 435 (1985); **30**, 3362 (1984).

[2] F. C. Zhang, Phys. Rev. Lett. **56**, 2113 (1986); **59**, 1980 (1987).

[3] A. Engel and W. Ebeling, Phys. Rev. Lett. **59**, 1979 (1987); W. Ebeling, A. Engel, B. Esser, and Feistel, J. Stat. Phys. **37**, 369 (1984).

[4] R. Tao, Phys. Rev. Lett. **61**, 2405 (1988).

[5] Y. B. Zel'dovich, S. A. Molchanov, A. A. Ruzmaikin, and D. D. Sokolov, Zh. Eksp. Teor. Fiz. **89**, 2061 (1985) [Sov. Phys. JETP **62**, 1188 (1985)].

[6] J. Heinrichs and N. Kumar, J. Phys. C **17**, L741 (1984); **17**, 769; J. Heinrichs, Phys. Rev. Lett. **52**, 1261 (1984).

[7] For example, see S. Marianer and J. M. Deutsch, J. Phys. C **17**, L737 (1984), and references therein; R. B. Pandey, J. Phys. A **17**, L551 (1984).

[8] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[9] R. Tao and J. M. Luttinger, Phys. Rev. B **27**, 935 (1983).

[10] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge Univ. Press, Cambridge, 1986), pp. 615-667.