PHYSICAL REVIEW A VOLUME 42, NUMBER 2 15 JULY 1990

Brief Reports

Brief Reports are short papers which report on completed research which, while meeting the usual **Physical Review** *standards of scientific quality, does not warrant a regular article. (Addenda to papers previously published in the* **Physical Review** *by the same authors are included in Brief Reports.) A Brief Report may be no longer than $3\frac{1}{2}$ printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Critical volume in diffusion through random media

R. Tao
Department of Physics, Southern Illinois University, Carbondale, Illinois 62901
(Received 8 March 1990)

It has been found, very generally, that there is a critical volume of the diffusion space, Ω_c, for a class of diffusions in random media, characterized by $V(\mathbf{r})$ with a zero mean. If the size of the diffusion space is bigger than Ω_c, the total population increases with time. Otherwise, the total population decreases with time and will eventually vanish. An estimation of Ω_c is obtained by a variation method.

Diffusion in random media where disorder involves the presence of traps and sources, has recently received considerable attention, both for its intrinsic theoretical interest and for its many applications in physical and biological systems.[1-4] Examples of such systems would be chemical or physical reactions with random nucleation centers, the size of a polymer chain in random environment,[5,7] chain reaction with random fissile distribution, or biological multiplication with random nutrient concentration. In this work we will study diffusion through a d-dimensional random media which is enclosed by a trapping layer. Mathematically, the problem is described by the following equation:

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

where D is the diffusion constant and $n(\mathbf{r},t)$ vanishes on the boundary. We consider a class of random potential V that has a zero mean value and a nonzero but finite variance,

$$\langle V\rangle=0,\quad \langle V(\mathbf{r})V(\mathbf{r}')\rangle=g(|\mathbf{r}-\mathbf{r}'|)\ , \tag{2}$$

where the brackets denote statistical average, the function $g(r)$ is peaked at $r=0$. When r is small, $g(r)$ can be approximated as $g_0\exp[-(r/l)^2]$. The correlation length l is very short, much shorter than the typical length of the diffusion space, L. We have $\langle V^2\rangle=g_0>0$ and $\langle(\nabla V)^2\rangle=-\nabla^2 g(\mathbf{r})|_{\mathbf{r}=0}>0$. Initially, $n(\mathbf{r},0)=\delta(\mathbf{r})$. For such systems defined above, we pose the following question: In the long-time limit will $P(t)=\int n(\mathbf{r},t)d\mathbf{r}$ increase or decrease?

To illustrate our problem, we can consider the above equation describing a biological model. Initially, there is only a small population of bacteria at the center of a cell which is surrounded by an infinite absorbing layer. The random potential $V(\mathbf{r})$ characterizes the distribution of nutrient sources and traps. We are asking whether the total population of bacteria inside the cell will grow or diminish in the long-time limit.

The above equation can also describe a chain nuclear reaction. Then, our question is related to the condition for the chain reaction to be self-sustaining.

We have found that in such a class of problems there is a critical size of the diffusion space. If the volume enclosed by the boundary is bigger than this critical size, $P(t)$ increases with time. Otherwise, $P(t)$ decreases with time and eventually vanishes. This conclusion is general and related to the localization problem of random systems in quantum mechanics.[8] For nuclear chain reaction, our results are equivalent to the well-known problem of critical mass.[9]

Let us first examine the diffusion process in the above example. Though the potential seems to be "neutral" for its zero mean, in the diffusion process the bacteria can best fit the environment. They will concentrate in the region of positive V, and have only a small population in the region of negative V. Therefore, the net effect of the neutral potential increases the total population of bacteria. On the other hand, the traps on the boundary eliminate any approaching bacteria. This competition between the elimination on the boundary and growth through the diffusion determines the whole process. After integrating Eq. (1) over the whole space inside the boundary, we have

$$\frac{\partial}{\partial t}\int n(\mathbf{r},t)d\mathbf{r}=D\oint(\nabla n)d\sigma+\int V(\mathbf{r})n(\mathbf{r},t)d\mathbf{r}\ , \tag{3}$$

where $\oint$ denotes the integration on the boundary surface. The normal of the surface is chosen to point to the outside of the cell. Since $n(\mathbf{r},t)$ vanishes on the boundary, $(\nabla n)d\sigma$ is negative. We denote

$$P(t)=\int n(\mathbf{r},t)d\mathbf{r}=p(t)L^d\ , \tag{4}$$

where L^d is the volume of the cell. In d-dimensional space, roughly speaking, the absorption rate by the boundary $D\oint(\nabla n)d\sigma$, is proportional to the speed of bacteria reaching the boundary D/L and the surface area of the boundary $L^{(d-1)}$, i.e., $\sim L^{(d-1)}D/L = DL^{d-2}$. As stated earlier, the second term in Eq. (3) is related to the growth rate which is proportional to the volume of the cell L^d. Then Eq. (3) can be estimated as

$$\frac{\partial p(t)}{\partial t} \sim p(t)(-D/L^2+\eta) , \tag{5}$$

where η is the bulk growth rate per unit volume, a positive quantity which will be discussed in detail later. The critical length is then found to be $L_c \sim (D/\eta)^{1/2}$ and the critical volume is $\Omega_c \sim (D/\eta)^{d/2}$. If the size of the cell is smaller than Ω_c, the absorption by the boundary is dominated, the total population of bacteria decreases and vanishes in the long-time limit. If the size of the cell is bigger than Ω_c, the growth rate is stronger than the absorption by the boundary, and the total population of the bacteria in the cell increases with time.

A further consideration can relate this problem to the localization in quantum mechanics.[8] The following Schrödinger equation,

$$H\psi = -D\nabla^2\psi(\mathbf{r}) - V\psi(\mathbf{r}) = \lambda\psi(\mathbf{r}) , \tag{6}$$

describes a particle of mass $\hbar^2/2D$ moving in a potential $-V(\mathbf{r})$. Since the wave function stays in a finite region and vanishes on the boundary, the eigenvalues are discrete. Let the orthonormal eigenfunctions be ψ_n with eigenvalue λ_n. We can make all ψ_n real, then

$$\int \psi_l(\mathbf{r})\psi_j(\mathbf{r})d\mathbf{r} = \delta_{l,j} . \tag{7}$$

The ground state ψ_0 is nondegenerate and positive in the region, having no nodes. Then we can expand $n(\mathbf{r},t)$ as

$$n(\mathbf{r},t) = \sum_{n=0} \psi_n(0)\psi_n(\mathbf{r})e^{-\lambda_n t} , \tag{8}$$

satisfying $n(\mathbf{r},0)=\delta(\mathbf{r})$. Since $-\lambda_0 > -\lambda_1 > \cdots$, the term of the ground state will be dominant in the long-time limit,

$$n(\mathbf{r},t) \to \psi_0(0)\psi_0(\mathbf{r})e^{-\lambda_0 t} \quad \text{as } t\to\infty . \tag{9}$$

If λ_0 is negative, $n(\mathbf{r},t)$ will grow. If λ_0 is positive, $n(\mathbf{r},t)$ diminishes. For $\lambda_0=0$, $n(\mathbf{r},t)$ will be stabilized.

The ground-state eigenvalue is given by

$$\lambda_0 = D\int |\nabla\psi_0(\mathbf{r})|^2 d\mathbf{r} - \int V(\mathbf{r})|\psi_0(\mathbf{r})|^2 d\mathbf{r} . \tag{10}$$

The first term in Eq. (10) is the kinetic energy K which is always positive. K can be estimated as

$$K \sim D(\pi/L)^2 , \tag{11}$$

which decreases as the size of the cell decreases. Since $V(\mathbf{r})$ is random, the ground state is localized, concentrating in the regions of strong positive V and almost vanishing in the region of strong negative V. Then it is not difficult to see that $-\int V|\psi_0|^2 d\mathbf{r}$ is negative. An examination of Eqs. (9), (10), and (5) concludes that the kinetic energy is related to the absorption by the boundary, and the bulk growth rate per unit volume η is related to the potential energy,

$$\eta = \int V(\mathbf{r})|\psi_0(\mathbf{r})|^2 d\mathbf{r} . \tag{12}$$

We can estimate η and the critical volume by a variation method. Let the normalized nonperturbed ground state be ϕ_0, which is a positive and smooth function in the space. We set the trial wave function $\psi(\mathbf{r}) = \phi_0(\mathbf{r})\exp[\beta V(\mathbf{r})]$ where β is a positive variational parameter. This trial wave function shares many features with the true ground state. In the unperturbed case, $V=0$, the trial wave function becomes the true ground state. It is thus easy to understand that our trial wave function is a good approximation of the true ground state for a weak V. In the case of a strong V, the trial wave function is localized in the same way as the true ground state, concentrating in the region of strong positive V and almost vanishing in the region of strong negative V. Therefore, we expect that by varying the parameter β our trial wave function will provide a good approximation to the ground-state energy,

$$\lambda_0 \le \frac{D\int |\nabla\psi(\mathbf{r})|^2 d\mathbf{r} - \int V(\mathbf{r})|\psi(\mathbf{r})|^2 d\mathbf{r}}{\int |\psi(\mathbf{r})|^2 d\mathbf{r}} . \tag{13}$$

Let us first estimate the denominator. We write $e^{2\beta V} = \langle e^{2\beta V}\rangle + (e^{2\beta V} - \langle e^{2\beta V}\rangle)$, where $\langle e^{2\beta V}\rangle$ denotes its statistic average. Since V is random and has a very short correlation length, $e^{2\beta V} - \langle e^{2\beta V}\rangle$ must fluctuate around zero very fast. Then

$$\int d\mathbf{r}\phi_0^2(e^{2\beta V} - \langle e^{2\beta V}\rangle) = 0$$

and

$$\int |\psi(\mathbf{r})|^2 d\mathbf{r} = \int \phi_0^2 d\mathbf{r}\langle \exp(2\beta V)\rangle ,$$

since ϕ_0 is a smoothly varying real function. We denote

$$\langle \exp(2\beta V)\rangle = f(\beta) , \tag{14}$$

where the function $f(\beta)$ only depends on β, but its form is related to the distribution of the random potential. Similarly, in the numerator,

$$\int V(\mathbf{r})|\psi(\mathbf{r})|^2 d\mathbf{r} = \int \phi_0^2 \langle V\exp(2\beta V)\rangle .$$

Since $\langle V\exp(2\beta V)\rangle = \frac{1}{2}f'(\beta)$, we have

$$\int V(\mathbf{r})|\psi(\mathbf{r})|^2 d\mathbf{r} = \tfrac{1}{2}f'(\beta) . \tag{15}$$

The other term in the numerator is given by

$$D\int |\nabla\psi(\mathbf{r})|^2 d\mathbf{r} = D(\pi/L)^2 f(\beta) + D\beta^2 f(\beta)h(\beta) , \tag{16}$$

where $h(\beta)$ is defined as

$$h(\beta) = \langle (\nabla V)^2 \exp(2\beta V)\rangle / f(\beta) . \tag{17}$$

Substituting these results into Eq. (13), we obtain

$$\lambda_0 \le D(\pi/L)^2 + D\beta^2 h(\beta) - \tfrac{1}{2}f'(\beta)/f(\beta) . \tag{18}$$

The minimum of the right-hand side in Eq. (18) is obtained by varying the parameter β. We denote the minimum of $D\beta^2 h(\beta)-\frac{1}{2}f'(\beta)/f(\beta)$ as C, which is independent on L. Then

$$\lambda_0 \le D(\pi/L)^2 - C \ . \tag{19}$$

The critical length is $L_c \ge \pi\sqrt{D/C}$ and the critical volume is

$$\Omega_c \ge (\pi\sqrt{D/C}\,)^d \ . \tag{20}$$

The particular value of C depends on the distribution of the random potential V. For example, if V has a Gaussian distribution and ∇V and V can be treated as two independent random variables, we have

$$f(\beta)=\langle \exp(2\beta V)\rangle = \exp(2\beta\langle V^2\rangle), \quad h(\beta)=\langle(\nabla V)^2\rangle \ . \tag{21}$$

From Eq. (18) we have $C=\langle V^2\rangle)^2/(D\langle(\nabla V)^2\rangle$. Then for the Gaussian distribution,

$$\Omega_c \ge \{D\pi[\langle(\nabla V)^2\rangle]^{1/2}/\langle V^2\rangle\}^d \ . \tag{22}$$

For a one-dimensional random system in which $V(x)$ can be either $-\mu$ or μ on lattice sites with an equal probability, we have

$$f(\beta)=\cosh(2\beta\mu) \ . \tag{23}$$

If the lattice spacing is a, then

$$h(\beta)=2\mu^2/a^2 \ . \tag{24}$$

Then, if $\mu a^2/D \ll 1$, from Eq. (18), we have the critical length

$$L_c > D\pi\sqrt{2}/(\mu a) \ . \tag{25}$$

The situation near the critical volume needs some investigation. When L is close to L_c, λ_0 in Eq. (18) can be approximated as $\lambda_0 \sim -2D\pi^2(L-L_c)/L_c^2$. Since in a d-dimensional space $\Omega-\Omega_c \sim (\Omega_c)^{(d-1)/d}(L-L_c)d$, we can write the above expression in the form

$$\lambda_0 \sim -2D\pi^2(\Omega-\Omega_c)/(\Omega_c^{1+2/d}d) \ . \tag{26}$$

If $\Omega=\Omega_c-\epsilon$ where $\epsilon\sim 0^+$, the life time of the total population is

$$\tau \sim \Omega_c^{1+2/d}d/(2D\pi^2|\Omega-\Omega_c|) \ . \tag{27}$$

When $\Omega=\Omega_c+\epsilon$, τ in Eq. (27) gives the time necessary to have a significant increase in the total population. As $\Omega-\Omega_c \to \nu(\Omega-\Omega_c)$, $\tau\to\tau/\nu$.

This research was supported in part by Department of Energy and Natural Resources of Illinois State.

[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); A. Engel and W. Ebeling, *ibid.* **59**, 1979 (1987); W. Ebeling, A. Engel, B. Esser, and Feistel, J. Stat. Phys. **37**, 369 (1984).
[3]R. Tao, Phys. Rev. Lett. **61**, 2405 (1988); **63**, 2695 (1989).
[4]M. N. Rosenbluth, Phys. Rev. Lett. **63**, 467 (1989).
[5]M. E. Cates and R. C. Ball, J. Phys. (Paris) **49**, 2009 (1988).
[6]S. F. Edwards and M. Muthukumar, J. Chem. Phys. **89**, 2435 (1988).
[7]R. A. Guyer and J. Machta, Phys. Rev. Lett. **64**, 494 (1990).
[8]For example, see, P. W. Anderson, Phys. Rev. **109**, 1492 (1958); D. J. Thouless in *Ill-Condensed Matter,* edited by R. Balian, R. Maynard, and X. Toulouse (North-Holland, Amsterdam, 1979), p. 1; P. A. Lee and T. V. Ramarkrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[9]For example, see W. Finkelnburg, *Atomic Physics* (McGraw-Hill, New York, 1950), p. 305.