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Diffusion in a Random Potential: Hopping as a Dynamical Consequence of Localization

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A model of diffusion $\dot{\psi}(\mathbf{x},t)=\Delta\psi(\mathbf{x},t)+V(\mathbf{x})\psi(\mathbf{x},t)$ is studied, where $V(\mathbf{x})$ is the Gaussian random potential. It is found that the probability distribution function is concentrated (localized) at some metastable potential attractor, while the localization center hops discontinuously in search of a better metastable attractor. The sample-averaged localization-center displacement is found as $x_c \sim t/2\ln t$, i.e., it is sub-ballistic.

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Transport in random media and diffusion-controlled reaction and recombination have been classical topics. Recently there is much revived interest in these subjects because of wider connections recognized in physics, chemistry, and biology, and the deeper understanding gained in fractal and hierarchical nature related to these processes.[1] One particular model of this class is a random walk in a random-trapping environment. Previous analyses[2] show that the total survival probability is an exponentially decreasing function with a suitable exponent. The question of the relative spatio-temporal distribution rather than the total survival is addressed in this Letter.

A generalization of the random-trapping model is proposed which can be expressed as diffusion in a random medium:

$$\dot{\psi}(\mathbf{x},t)=\Delta\psi(\mathbf{x},t)+\lambda V(\mathbf{x})\psi(\mathbf{x},t), \tag{1}$$

where $\psi(\mathbf{x},t)$ is interpreted as the probability distribution function and note that $\int d^dx\,\psi(\mathbf{x},t)$ is not a conserved quantity as it is in random-random walk models.[3] $V(\mathbf{x})$ is a random variable with short-range correlation and λ measures the strength of random disorder. In analogy with a similar model[4] λ can be regarded as the inverse of the temperature (i.e., $\lambda=1/T$). All other constants have been absorbed in the units. In random-trapping models previously studied[2] it was shown that the total survival $\rho(t)=\int d^dx\,\psi(\mathbf{x},t)\sim\exp(-t^{\alpha})$, where α is the so-called survival exponent.

The focus in this Letter is to study the spatial fluctuations of $\psi(\mathbf{x},t)$, i.e., the relative probability distribution. Thus the first moment $\langle V(\mathbf{x})\rangle$ will remain unspecified since it does not contribute to the fluctuations.

Before going on to analyze Eq. (1), let us motivate it with an idealized biological problem: Suppose we study the evolution of a certain species which has an initial distribution $\psi(\mathbf{x},0)=\delta(\mathbf{x})$ and assume that the species can move in space via diffusion. Then introduce a "fitness" order parameter $V(\mathbf{x})$ taking both positive and negative values, which may represent a random distribution of nutrients and inhibitors. We want to know whether the species is relatively concentrated and if so how the population center moves in space, if it moves at all. [Another question, whether the total species is exponentially increasing or decreasing, which depends nontrivially on $\langle V(\mathbf{x})\rangle$, will be addressed elsewhere.] Similar processes probably can also be found in chemical-reaction systems.

We proceed to analyze the model by first giving qualitative understanding of Eq. (1). At least for strong disorder, we expect the distribution function $\psi(\mathbf{x},t)$ to be sharply localized. The question we ask is this: Given an initial distribution, say $\psi(\mathbf{x},0)=\delta(\mathbf{x})$, what is motion of the localization center? Clearly the origin (or places near the origin) may not be the best attractor (the place with finite spatial spread has highest combined V values); the population center would not be localized there *forever*. There is an ex-

ponential tail $\exp(-x/\xi)$ (where $x=|\mathbf{x}|$ and ξ is the assumed localization length) reaching out from origin; it covers many better attractors. Given enough time, $\psi(\mathbf{x},t)$ at some of these distant better attractors can outgrow (or outsurvive in random-trapping model) the $\psi(\mathbf{x},t)$ at the first attractor, thus resulting in a hop from one attractor to a better one. Since we assume an infinite sample size, any attractor is but a metastable potential trap. Better and better attractors can always be found over larger and larger spatial regions with longer and longer lifetimes spent at each attractor. There appears to be a natural hierarchy of potential barrier, distance, and time scales.[5] In the following the above statements are quantified.

We shall perform a variational analysis rather similar to that of Mott's variable-range hopping[6] for static Anderson localization. The ideas are best conveyed via Feynman path-integral language in space and time. $\psi(\mathbf{x},t)$ represents the sum of the contributions from all possible paths joining $(0,0)$ and $(\mathbf{x},t)$. In few dimensions, say one and two dimensions, we expect that the scaling behavior is governed by its zero-temperature fixed point.[4] We are looking for the most dominant $\psi(\mathbf{x},t)$ for a fixed time t, which receives contributions from a single dominant path, at least in the strong disorder limit. Using the above $\psi(\mathbf{x},t)$, the position of the localization center can be calculated; it is defined as $x_c(t)=\langle\langle\mathbf{x}\rangle\rangle_{\rm av}$, where $\langle\rangle_{\rm av}$ denotes a sample average.

We follow closely the strategy of Ref. 6. Suppose such a winning attractor at $\mathbf{x}$ for a given time t has the most dominant $\psi(\mathbf{x},t)$. The gain in the exponential of $\psi(\mathbf{x},t)$ is $t(E_x-E_0)$ and the cost of overcoming the potential barriers is $x\bar{E}$, where E_x is the largest value that can be found in a sample of size l_x, $E_0=V(0)$, and $\bar{E}$ is the average potential barrier height. We demand that for a given time t the total contribution to the dominant $\psi(\mathbf{x},t)$ be maximal, i.e.,

$$t(E_x-E_0)-x\bar{E}=\max. \tag{2}$$

To carry out the variation with respect to x we have to know E_x as a function of x. Assuming a Gaussian distribution,

$$P_x=\int_{E_x}^{\infty}\exp(-V^2)\,dV \tag{3}$$

is the probability of choosing a value equal to or larger than E_x in each trial. Since E_x is the largest value in a sample of size l_x ($l_x=|\mathbf{x}|$), then the chance that E_x is not chosen over x trials must be a finite number between 0 and 1, say $1/e$. We thus have

$$(1-P_x)^{l_x}=1/e. \tag{4}$$

For large x this implies $P_x\sim 1/l_x$; substituting the above P_x into (3) we obtain (using error-function expansions)

$$E_x=[\ln(|\mathbf{x}|)]^{1/2}, \tag{5}$$

to leading order when x is large. Substituting (5) into (2), we obtain to leading order

$$x_c(t)\simeq t/2\ln t, \tag{6}$$

which implies sub-ballistic motion of the localization center. We note in passing that in d dimensions the exponent in (4) should be replaced by x^d but $x_c(t)$ in (6) remains unchanged to leading order. If $V(\mathbf{x})$ is uniformly distributed instead of being Gaussian, a similar analysis can be carried out with the result

$$x_c\simeq t^{1/(d+1)}. \tag{7}$$

However, as soon as we raise the temperature from zero, the attractors consist of not just a single site but of several neighboring sites. It is well known (central limit theorem) that the sum of any kind of random numbers behaves approximately as Gaussian. Thus we expect (as evidenced by numerical simulations) that for flat randomness the result of x_c in (7) crosses over to that of (6) as the temperature rises from zero.

We performed simulations via the transfer matrix method[4,7] with various λ's to calculate $x_c=\langle\langle\mathbf{x}\rangle\rangle_{\rm av}$ as well as $x_s=(\langle\langle\mathbf{x}^2\rangle-\langle\mathbf{x}\rangle^2\rangle_{\rm av})^{1/2}$. The latter measures the spread of the localized distribution function. The results are displayed in Fig. 1.

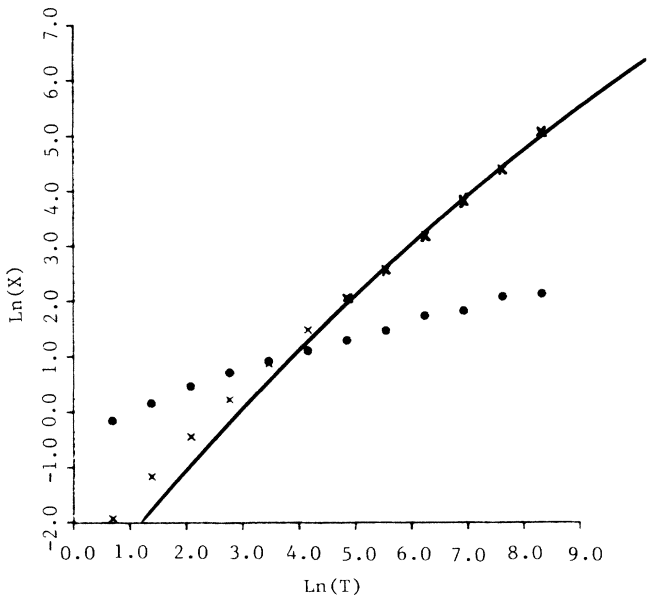

FIG. 1. In one dimension the simulations are done on a chain of 2500 sites, with 4086 time steps, and $\lambda=1.0$. The crosses indicate data for x_c and the circles for x_s; the curve $\ln x_c=\ln t-\ln(\ln t)+\text{const}$ is drawn for comparison. We see that x_c scales rather well, while x_s is slowly increasing with ever smaller slope. The data are averaged over 500 samples, and statistical errors are smaller than the symbol size.

The above variational analysis offers no hint as to how x_s should behave. Numerically we observed that the slow increase of x_s with t is probably due to the fact that the better attractors tend to occupy wider space. However, numerically we were not able to separate the information concerning how fast the localized $\psi(\mathbf{x},t)$ relaxes while x_c is hopping around.

Clearly the result $x_c \sim (t/2\ln t)$ cannot be true for all λ's and dimensions. Somewhere it must cross over to the diffusive behavior $x_c \sim \sqrt{t}$, but we are not yet at the stage to say where the transition may occur. We instead propose a conjecture for which we have some numerical evidence: Whenever $\psi(\mathbf{x},t)$ is localized, i.e., it has a localization center (time dependent) and is exponentially decreasing from this center, we always have (6) as a result, and the above variational analysis holds. Whenever $\psi(\mathbf{x},t)$ is extended we obtain the diffusive result $x_c \sim \sqrt{t}$.

In one dimension we performed simulations over an extensive temperature range, even for λ as low as 0.03, and we observed that x_c is always consistent with $t/(2\ln t)$. In two dimensions we observed different behaviors between $\lambda = 0.15$ and $\lambda = 0.05$, as shown in Fig. 2. However, we cannot rule out the possibility that the behavior $x_c \sim \sqrt{t}$ with $\lambda = 0.05$ is due to a long diffusive transient or that the localization length is comparable with the lattice size.

There is another important piece of information

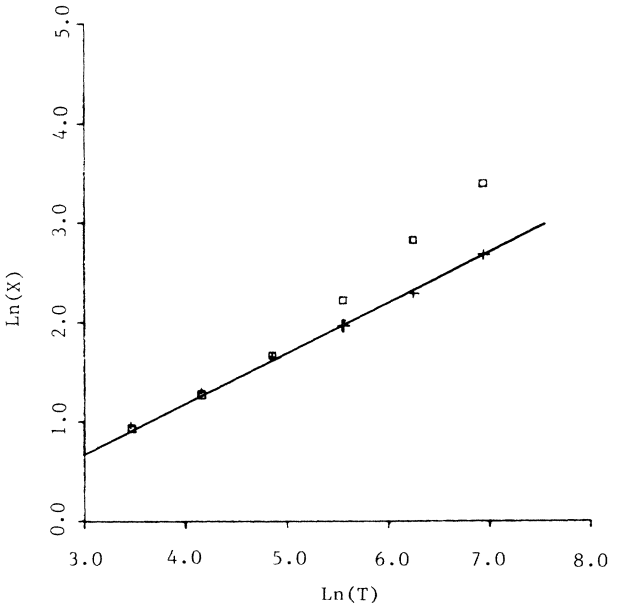

FIG. 2. While in one dimension it is observed that there is no qualitative change for x_c as λ varies, in two dimensions this figure shows distinctive behaviors between $\lambda = 0.15$ (squares) and $\lambda = 0.05$ (pluses). The line of $x_c = \sqrt{t}$ is drawn for comparison. The lattice size was 200×200, with 1024 time steps. Again 500 samples were averaged to obtain the data.

which is not contained in (6). Since the hopping is intermittent, we would like to know how long the localization center stays at each attractor, how far it will go next, and how much better the next attractor is with respect to the present one. These three quantities are closely related via (5) and (6); we need a third relation to reflect the discreteness of the hopping.

Suppose the localization center is now at $\mathbf{x}$, with its E_x and $t \sim 2x\ln|\mathbf{x}|$. Within a region of x around the origin there is no better attractor by definition. Over a region of size slightly larger than x there is a chance to find better attractors. Since $E_x \sim (\ln x)^{1/2}$ is a very slowly increasing function, the possible energy gain should be very small and thus a very long time to realize that hop is required. On the other hand, over very distant regions there are much better attractors available; however, long-distance hopping also requires a long time. The next immediate hop must be to one of the better attractors which requires the *least* time to realize. Attractors with E_x values in between would be skipped. Imagine that the next attractor is a distance x' away from the origin, has a value E_x' and that it requires a time t' to realize the hop. For this hop to be realized the total contribution has to be comparable to that of the present trap, i.e.,

$$t'E_x' - \bar{E}x' = t'E_x - \bar{E}x, \tag{8}$$

where $E_x' \simeq (\ln t')^{1/2}$. To first order this implies

$$t' \sim |\mathbf{x}' - \mathbf{x}|\bar{E}/(E_x' - E_x).$$

Moreover, we demand that t' be minimal. Carrying out the variation with respect to x' we obtain

$$E_x' \simeq E_x + 1/2E_x + O(1/E_x^2), \quad E_x > 1. \tag{9}$$

Thus, typically the localization center hops next to an attractor which is deeper by a finite amount while attractors with values in between will never be realized. The next probable location is

$$x' \sim \left[x + \frac{x}{2\ln(x)} \exp\left[1 + \frac{1}{4\ln(x)}\right]\right] \tag{10}$$

and the typical lifetime spent at the present attractor is $2x'\ln(x')$. We have not directly tested these results with systematic numerical simulations.

Incidentally, Eq. (1) arises in another physical situation as well: Consider an Ising-type model in which the coupling constants on the same layer are identical and uncorrelated between the layers. Then Eq. (1) would describe the interface configurations of the random-layered Ising system[4] in 2D. If we hold two ends of the interface at fixed positions then the results of this Letter tell us that the random pinning will distort the interface by as much as $L/4\ln L$, L being the linear dimension across the sample.

In summary we have analyzed a model of diffusion

in a random potential, which can be viewed as a generalization of the random-trapping model.[2] Our variational and numerical studies indicated that in low dimensionalities the distribution function hops from one localized attractor to another, obeying a scaling relation $x_c \sim t/(2\ln t)$. The reason that this x_c is larger than that of pure diffusion is that the randomness helps focus the distribution function so that it moves as a whole object. Such a displacement is clearly nonback-tracking because of energy nonconservation; thus the model results in a more efficient transport than that of pure diffusion.

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[1]For general issues on diffusion-controlled reaction and recombination processes see, e.g., a recent review article, G. H. Weiss, J. Stat. Phys. **42**, 3 (1986), and references therein.

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