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Classical Diffusion on a Random Chain

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A simple model of classical diffusion on a random chain is studied. The velocities to the right and to the left are calculated. When one changes continuously the probability distribution ρ of the hopping rates, a whole region is found where these two velocities vanish. In this region, the distance R covered by a particle during the time t behaves like $R \sim t^x$, where x depends continuously on ρ. The exponent x is calculated for a simple example.

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Recently, the problem of classical diffusion in a random medium has attracted a lot of interest.[1-4] In these works, the problem was studied on a lattice with random nearest-neighbor transfer rates which are symmetric: The probability of hopping from site i to site j was equal to the probability of hopping from site j to site i. Several interesting results were derived depending on the distribution of these random transfer rates.[2] A list of physical situations (the hopping conduction, magnetic models, etc.) leading to this problem can be found in Ref. 2.

Even more interesting seems to be the nonsymmetric case. In a discrete-time version, one can formulate the problem as follows. One considers a particle on a one-dimensional lattice. If the particle is on site i at time t, it will be at time $t+1$ either on site $i+1$ with probability p_i or on site $i-1$ with probability $q_i = 1 - p_i$. The problem is obvious if all the p_i are equal. However, if the p_i are randomly chosen with some probability distribution $\rho(p_i)$, one can observe very unexpected behaviors. One of the most striking results was obtained by Sinai[5] who has studied a case where the distribution $\rho(p_i)$ satisfies

$$\langle \ln[p_i/(1-p_i)] \rangle = \int \rho(p_i) dp_i \ln[p_i/(1-p_i)] = 0. \tag{1}$$

He finds that if a particle is on site 0 at time 0, then with probability 1 it will be at a distance $R \sim \ln^2 t$ at time t. This behavior differs completely from the usual diffusion (all the $p_i = \frac{1}{2}$) where $R \sim t^{1/2}$.

The purpose of this Letter is to show that other unexpected behaviors occur even when the constraint (1) is not present. We first show that there exists a finite velocity to the right (to the left) only if $\langle (1-p_i)/p_i \rangle < 1$ $[\langle p_i/(1-p_i) \rangle < 1]$. If these two inequalities are both unsatisfied, the distance R covered by the particle during the time t behaves like $R \sim t^x$, where x is an exponent depending continuously on the distribution ρ. For a simple distribution ρ, we give the expression of x as a function of the parameters which define ρ.

For this problem of diffusion, the first equation that one can write is an equation for $P_n(t)$ which is the probability for the particle to be on site n at time t. It is clear that $P_n(t)$ verifies

$$P_n(t+1) = q_{n+1} P_{n+1}(t) + p_{n-1} P_{n-1}(t). \tag{2}$$

To calculate the velocity V, it is easier to consider a lattice of N sites with periodic boundary conditions (site $N+n$ is identified with site n). After a very long time, the probability distribution $P_n(t)$ converges to an equilibrium probability distribution Q_n which satisfies

$$Q_n = q_{n+1} Q_{n+1} + p_{n-1} Q_{n-1}. \tag{3}$$

Then the velocity V is given by

$$V=[\sum_{n=1}^{N}(p_n-q_n)Q_n]/[\sum_{n=1}^{N}Q_n]. \tag{4}$$

It turns out that the Q_n can be determined explicitly as a function of all the p_i by using the recurrence (3), and by writing the periodic boundary condition $Q_{N+1}=Q_1$. The result can be written as

$$Q_n=(C/p_n)[1+\sum_{i=1}^{N-1}(\prod_{j=1}^{i}s_{n+j})], \tag{5}$$

where s_n is defined by

$$s_n=q_n/p_n=(1-p_n)/p_n \tag{6}$$

and C is just a normalization constant. Obviously, the boundary condition chosen here implies that $s_{N+n}=s_n$. From expressions (4) and (5) we can now calculate the velocity V for any choice of the p_i. In order to have a quantity which will be simpler to average and to study, we give the expression of the inverse velocity:

$$V^{-1}=\{\sum_{n=1}^{N}p_n^{-1}[1+\sum_{i=1}^{N-1}(\prod_{j=1}^{i}s_{n+j})]\}\times[N(1-\prod_{i=1}^{N}s_i)]^{-1}. \tag{7}$$

Now let us try to average V^{-1} over the possible choices of the p_i. Consider first the case where $\langle \ln s\rangle<0$ [i.e., $\langle \ln p\rangle>\langle\ln(1-p)\rangle$]. Then the product in the denominator of (7) can be neglected with probability 1 in the limit $N\to\infty$ and it becomes easy to average both sides of Eq. (7):

$$\langle V^{-1}\rangle=(1+\langle s\rangle)(1+\sum_{i=1}^{N-1}\langle s\rangle^i). \tag{8}$$

The series is convergent in the limit $N\to\infty$ only if $\langle s\rangle<1$. We conclude that there is a finite velocity for this problem only if $\langle s\rangle<1$ and in this case, the velocity is given by

$$\langle V^{-1}\rangle=(1+\langle s\rangle)/(1-\langle s\rangle). \tag{9}$$

If the distribution ρ was chosen such that $\langle \ln s\rangle<0$ but $\langle s\rangle>1$, the inverse velocity would be infinite. We shall see later that in this case, the distance R covered by the particle during the time t is no longer proportional to t but to t^x with $0<x<1$.

The calculation of $\langle V^{-1}\rangle$ can be done in the case $\langle \ln s\rangle>0$ in the same way as for $\langle \ln s\rangle<0$. One starts by neglecting 1 in the denominator of Eq. (7) and then one finds that $\langle V^{-1}\rangle$ is finite only if $\langle s^{-1}\rangle<1$. The result for V^{-1} is, in this case, $\langle V^{-1}\rangle=-(1+\langle s^{-1}\rangle)/(1-\langle s^{-1}\rangle)$. It may look arbitrary to average the inverse velocity V^{-1}. However, if $\langle s\rangle<1$ or $\langle s^{-1}\rangle<1$, one can show that the fluctuations of V^{-1} are small in the large-N limit [the simplest thing to show is that the fluctuations of V^{-1} are of order $N^{-1/2}$ if $\langle s^2\rangle<1$ or $\langle s^{-2}\rangle<1$]. This indicates that the velocity has small fluctuations, and therefore $\langle V^{-1}\rangle=\langle V\rangle^{-1}$.

At this stage, the main question is what happens if $\langle s\rangle>1$ and $\langle s^{-1}\rangle>1$. In order to simplify the calculations, we shall restrict ourselves to a simple distribution ρ which depends on two parameters α and p (for convenience we choose $p>\frac{1}{2}$):

$$\rho(p_i)=\alpha\delta(p_i-p)+(1-\alpha)\delta(p_i-(1-p)). \tag{10}$$

However, all the results presented here can be generalized to other distributions ρ. The main idea consists in showing that V^{-1} behaves like a power law N^y for almost all the samples in the limit $N\to\infty$. The choice of distribution (10) is motivated by the fact that the exponent y will have a simple expression as a function of the parameters α and p which define ρ.

For the distribution (10), a finite velocity exists if $\alpha>p$ (i.e., $\langle s\rangle<1$) or $\alpha<(1-p)$ (i.e., $\langle s^{-1}\rangle<1$) and the region we want to study is $1-p<\alpha<p$. Let us come back to formula (7). If $\langle \ln s\rangle<0$ (here it means that $\alpha<\frac{1}{2}$), we can again neglect the product in the denominator. Then by regrouping terms in (7), one can write V^{-1} as

$$V^{-1}=1+2\sum_{n=1}^{N-1}S_n+S_N, \tag{11}$$

where S_n is defined by

$$S_n=\frac{1}{N}\sum_{i=1}^{N}\prod_{j=1}^{n}s_{i+j}. \tag{12}$$

In the limit $N\to\infty$, if n remains finite, $S_n\to\langle s\rangle^n$ and so S_n increases with n. On the other hand, $S_N=\prod_{j=1}^{N}s_j$ vanishes with probability 1. Therefore, there are certainly in the sum (11) terms between $n=1$ and $n=N$ which are maximum and give the dominant contribution to V^{-1} in the limit $N\to\infty$. S_n is a sum of N terms and one could be tempted to use the central-limit theorem. This would be wrong because for most values of n, the number of terms in the sum (12) is too small to give the average $\langle s\rangle^n$. Therefore, with probability 1, S_n is not equal to $\langle S_n\rangle$.

We define $\Omega(m)$ as the number of terms in the sum S_n which are equal to $N^{-1}[(1-p)/p]^{n-2m}$. The average $\langle\Omega(m)\rangle$ is

$$\langle\Omega(m)\rangle=NC_n{}^m\alpha^{(n-m)}(1-\alpha)^m. \tag{13}$$

For large n, we see that, depending on m, $\langle\Omega(m)\rangle$ can be either much larger than 1 or much smaller than 1. The critical values $m_{\min}$ and $m_{\max}$ can be estimated by requiring that $\langle\Omega(m)\rangle \simeq 1$. If $m_{\min} < m < m_{\max}$, then $\langle\Omega(m)\rangle$ is large $[\langle\Omega(m)\rangle \gg 1]$; therefore with probability 1, $\Omega(m) = \langle\Omega(m)\rangle$. This is due to the fact that the fluctuations of $\Omega(m)$ are of order $\langle\Omega(m)\rangle^{1/2}$ only. On the other hand, if $m < m_{\min}$ or $m > m_{\max}$, $\langle\Omega(m)\rangle$ is small $[\langle\Omega(m)\rangle \ll 1]$ and then $\Omega(m) = 0$ with probability 1. For large n, the values $m_{\min}$ and $m_{\max}$ are the two solutions of

$$\ln N + m \ln\left(\frac{n(1-\alpha)}{m}\right) + (n-m)\ln\left(\frac{n\alpha}{n-m}\right) = 0. \quad (14)$$

It follows that S_n is given with probability 1 by

$$S_n = \sum_{m=m_{\min}}^{m_{\max}} C_n{}^m \alpha^{(n-m)}(1-\alpha)^m \left(\frac{1-p}{p}\right)^{n-2m}. \quad (15)$$

With this evaluation of S_n, we can come back to the calculation of V^{-1} by looking for the value $\tilde{n}$ which is dominant in sum (11). One finds that

$$\tilde{n} = \frac{\ln N}{(2\alpha-1)\ln[\alpha/(1-\alpha)]} \quad (16)$$

and

$$V^{-1} \sim S_{\tilde{n}} \sim N^{z-1} \quad (17)$$

with $z = \ln[p/(1-p)]/\ln[\alpha/(1-\alpha)]$.

To obtain the most probable value of S_n, we have completely ignored the correlations between the terms in the sums (11) and (12). A calculation taking these correlations into account would be more complicated, but the result would be the same apart from some factors $\ln N$ in Eq. (17). We have chosen $\Omega(m) \sim 1$ to determine $m_{\min}$ and $m_{\max}$. If we had replaced 1 by any other finite constant, the result would have been the same.

The fact that sum (11) was replaced by $S_{\tilde{n}}$ can be justified by looking at the behavior of S_n around $\tilde{n}$. One can estimate that there are $\sim \ln N$ terms in (11) which are comparable to $S_{\tilde{n}}$. Therefore (17) is again valid apart from factors of order $\ln N$.

We have shown that the inverse velocity $V^{-1} \sim N^{z-1}$ for a chain of N sites with periodic boundary conditions when $\frac{1}{2} < \alpha < p$. This means that to cover a distance $R \sim N$ the particle needs a time $t = V^{-1}N \sim N^z$. It is equivalent to say that the distance R covered by the particle during the time t behaves like $R \sim t^x$ with $x = 1/z$. It is interesting to notice that in (11), all the terms are positive and therefore the sign of V^{-1} is positive. This means that when $\alpha > \frac{1}{2}$, there is a systematic displacement to the right. If $\alpha < \frac{1}{2}$, V^{-1} becomes negative because the dominant term in the denominator of (7) is the product (Fig. 1).

In the limit of constraint (1) (here $\alpha \to \frac{1}{2}$), x vanishes and we find that R increases less rapidly than any power law. This is in good agreement with $R \sim \ln^2 t$ found by Sinai.[5] In the limit where $\langle s\rangle \to 1$ (here $\alpha \to p$) x tends to 1. We recover that in this limit, the distance starts to be proportional to the time.

In addition to the calculations presented in this Letter, we have done calculations on an infinite chain. In these other calculations, we took the time Fourier transform of Eq. (2) and we calculated the behavior of $P_n(\omega)$ for large n. We found results identical with those presented here.

We think that the power-law behavior found here is not of the same nature as the behavior found in Refs. 1 and 2. The two problems are actually different.[5] Here the distribution ρ is regular (i.e., all its moments are finite) but there is a jump at every unit time and the probability of jumping from site i to site j is not symmetric. On the contrary, in the case of symmetric hopping rates and continuous time, the average of the inverse transfer rate needs to be infinite to have a power-law behavior as shown in Refs. 1 and 2.

The main idea used here is that the most probable value of a quantity (here S_n) can be very different from its average. This idea was yet developed in the context of random magnets.[6] All the calculations presented here can be done in this other context. One has only to change the names of quantities: The inverse velocity becomes the magnetic susceptibility and S_n becomes the space-averaged correlation function. The power-law be-

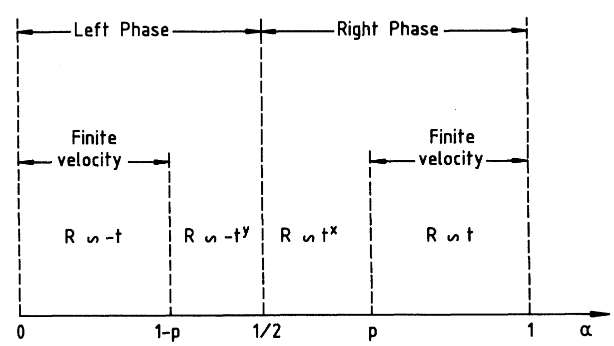

FIG. 1. Phase diagram for the distribution $\rho(p_i) = \alpha\delta(p_i - p) + (1-\alpha)\delta(p_i - (1-p))$. If $\alpha > \frac{1}{2}$, there is a systematic displacement to the right. The velocity is finite only if $\alpha > p$. For $\frac{1}{2} < \alpha < p$, the distance R covered during the time t is given by $R \sim t^x$ with $x = \ln[\alpha/(1-\alpha)]/\ln[p/(1-p)]$. The situation for $\alpha < \frac{1}{2}$ is symmetric.

haviors found here have also their analogs when one studies the effect of a magnetic field.[7]

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Note added.—After this work was submitted, Professor J. L. Lebowitz and Professor H. Spohn informed us that the same problem has been studied in a different way by mathematicians and similar results can be found in Refs. 8 and 9.

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Unbiased Estimation of Corrections to Scaling by Partial Differential Approximants

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High-temperature series for two bcc lattice models which interpolate between the Gaussian (or free-field) model and the $S=\frac{1}{2}$ Ising model are analyzed by partial differential approximants. Series to order 21 in both $x \propto 1/T$ and the interpolation parameter, y, yield unbiased estimates for the correction-to-scaling exponent, $\theta = 0.54 \pm 5$, and the susceptibility exponent, $\gamma = 1.2385 \pm 15$. The results are universal and agree tolerably with field-theoretic estimates and well with biased, one-variable analyses of general spin Ising models.

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An important qualitative prediction of the renormalization-group theory of critical phenomena is that the corrections to leading power-law behavior are determined in a universal way through a nontrivial correction-to-scaling exponent θ.[1] Thus a property $f(T, y)$, such as the susceptibility of a ferromagnetic system specified by an "irrelevant" parameter y, e.g., the ambient pressure, should vary as

$$f(T,y) \approx A(y)a_f \dot{t}^{-\psi}[1+C(y)c_f \dot{t}^{\,\theta}+\dots], \qquad (1)$$

when $\dot{t} \propto T - T_c(y) \to 0+$: The leading exponent ψ and the coefficients a_f and c_f depend on the property studied, but should otherwise be universal, i.e., independent of y; however, $\theta > 0$ ought to be independent of both y and f; only $A(y)$ and $C(y)$ should be nonuniversal.[1] Analyses by ratio and Padé-approximant techniques of high-temperature series expansions for lattice spin models have been strikingly successful in estimating leading exponents, such as γ for the susceptibility.[2] However, convincing, unbiased estimation, or even detection, of the confluent correction exponents and amplitudes has proved an elusive goal in single-variable series expansion studies. In this note we report an attack on the problem for two distinct $d=3$ (d = dimensionality) models which, as y varies from 0 to 1, interpolate smoothly between the exactly solvable Gaussian or free-field model and the standard, discrete spin-$\frac{1}{2}$ Ising model: See Fig. 1 where $x = J/k_B T$ with exchange parameter J. By applying *two-*

