DIFFUSIVE FLUCTUATIONS IN DIFFERENT REALIZATIONS OF A RANDOM MEDIUM

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Abstract

We study the fluctuations of the probability density $P(r,t)$ of diffusing particles to be at distance r at time t in the presence of random potentials, represented by random transition rates. We find an exact relation which expresses all the moments of $P(r,t)$ in terms of its first moment, for both quenched and annealed disorder and for any dimension. From this relation follows that anomalous diffusion implies non-trivial behavior of the moments of $P(r,t)$, such as an exponential divergence of the relative fluctuations for large r.

The random-walk (RW) model, has been widely used to describe transport properties in disordered systems[1-6]. In general, the randomness of the media can be characterized by two types of disorder: structural disorder and random potentials. Models for structural disorder include percolation clusters, random walks (RW), self-avoiding walks, or DLA. A common feature of all these models is that they are fractals on certain length scales[4,6]. Models for random potentials can be developed in terms of continuous time random walk (CTRW) and RW on regular lattices with a random distribution of transition rates, representing the random potentials[1,3,5].

In all these models, the crucial point is that transport can be anomalous, i.e., the mean square displacement of a random walk does not obey the common Fick's law $\langle r^2 \rangle = Dt$, but rather scales with time as $\langle r^2 \rangle = Dt^{\frac{2}{d_w}}$ where $d_w > 2$ is the anomalous diffusion exponent. This reflects the commonly seen feature of average slowing down the motion of a particle in a disordered medium, which is of interest for many applications[1,5].

When transport properties of such models are discussed, a central role is played by the propogator $P(r,t)$, which is the probability of finding a RW at time t at a distance r from its starting point $r = 0$. In disordered systems, $P(r,t)$ itself can be regarded as a random variable provided that we index it with a variable relating to different realizations of disorder. This variable corresponds to the density of independent particles diffusing in this medium. Moments of $P(r,t)$ with respect to the configurational disorder contain information on the relation between the static disorder and the dynamical process.

In this paper, we discuss disordered systems which are described by random distribution of transition rates on regular lattices. We show rigorously that anomalous diffusion leads to a non conventional scaling behavior of the probability density, which is reflected in the divergence of its relative fluctuations for large r. We find a general relation, applicable to all the varieties of this model, i.e., quenched or annealed disorder, in any dimension, which connects all of the moments of $P(r,t)$ with respect to different realizations to its first moment.

Consider N different realizations of the disordered system, in which a random walker starts at the origin at time $t = 0$ and moves until time t. Then

$$\langle P^q(r,t) \rangle = \frac{1}{N} \sum_{i=1}^{N} P_i^q(r,t) \, , \tag{1}$$

where $P_i(r,t)$ is the probability that in the i'th realization the RW has reached r at time t, and $\langle . \rangle$ represents averaging over the N realizations. For simplicity, we will consider in what follows the moments of the propogator relative to its value at the the origin, i.e., we deal with the variables $u_i(r,t) = P_i(r,t)/P_i(0,t)$.

Within the framework of this definition, an indication of non-conventional scaling is that $\langle u^q(r,t) \rangle$ is not asymptotically (in time) proportional to $\langle u(r,t) \rangle^q$. Our calculation of the q'th moment will be based on an expression for $\langle u^q(r,t) \rangle$ in terms of the first moment evaluated at a shifted value of r.

For this purpose we first define the parameters of the underlying RW and specify the parameters to be used in the subsequent analysis. Let $p(\mathbf{j})$ be the probability density that the displacement of the RW in a single step is equal $\mathbf{j}$. We will assume this function to be symmetric in the sense that $\langle p(\mathbf{j}) \rangle = 0$ and to have finite second moments, i.e.,

$$\sum_r j_k j_l p(\mathbf{j}) < \infty \, , \qquad k, l = 1, 2, ..., d \, , \tag{2}$$

where d is the dimensionality of the space. For simplicity we will assume that all of the second moments are equal a constant σ, and that the second order correlations all vanish. More general cases can be analyzed but provide no essentially new information. We return to the problem of evaluating $\langle u^q(r,t) \rangle$ as defined in Eq. (1) under these assumptions.

At a fixed t, we can decompose the sum over $P_i^q(r,t)$ into contributions from RWs which have taken exactly n steps at time t. The variable n can take on all non-negative integer values. Let the number of realizations out of the total N having this property be $N_n(t)$ so that

$$\sum_{n=0}^{\infty} N_n(t) = N \, . \tag{3}$$

We can appeal to the law of large numbers to assert that

$$\lim_{N \to \infty} \frac{N_n(t)}{N} = \Phi_n(t) \, , \tag{4}$$

where $\Phi_n(t)$ is the probability density that exactly n steps have been taken until time t. Let $u_i(r,t|n)$ be the normalized distribution of the displacement at time t of a RW in the i'th realization, conditional on there having been exactly n steps at that time. It follows that

$$\langle u^q(r,t)\rangle = \frac{1}{N}\sum_{n=0}^{\infty}\sum_{i=1}^{N_n} u_i^q(r,t|n)\,. \tag{5}$$

However, the definition of the model used in this analysis implies that the propogator for being at a given displacement is known once the number of steps is known, i.e., one may write $P_i^q(r,t|n) \equiv P(r,n)$ which depends neither on i nor on t. It therefore follows that (for large t)

$$\langle u^q(r,t)\rangle = \frac{1}{N}\sum_{n=0}^{\infty} N_n(t) u^q(r,n) \sim \sum_{n=0}^{\infty} \Phi_n(t) u^q(r,n)\,. \tag{6}$$

Equation (6) can be simplified by noting that the restriction indicated in Eq. (2) is equivalent to the statement that the limit $t \to \infty$ also implies $n \to \infty$. An appeal to the central limit theorem allows us to conclude that $u(r,n)$ can be approximated in this limit as a Gaussian, hence in the large t limit we have

$$u(r,n) \sim \exp\left(-\frac{r^2}{2\sigma^2 n}\right)\,. \tag{7}$$

The long time form of the q'th power of this function, in turn, can be expressed as the rather simple expression

$$u^q(r,n) \sim u(r\sqrt{q},n)\,. \tag{8}$$

This asymptotic relation allows us to express $\langle u^q(r,t)\rangle$ as

$$\langle u^q(r,t)\rangle \sim \sum_{n=0}^{\infty} u(r\sqrt{q},n)\Phi_n(t) = \langle u(r\sqrt{q},t)\rangle\,. \tag{9}$$

Thus the q'th moment of $u(r,t)$ is related to the first moment of this function with a shifted argument. This result is independent of dimension and valid for quenched or annealed disorder.

We now find an expression for the histogram $N(\log 1/u)$, i.e., the distribution of u over the different realizations, for given r and t. For this purpose, we use the alternative expression for the moments

$$\langle u^q(r,t)\rangle = \int_0^{\infty} N(\log 1/u) u^q d(\log 1/u)\,. \tag{10}$$

Identifying Eq. (10) with Eq. (9) we find

$$N(\log 1/u) \;=\; \Phi_{\frac{r^2}{\log 1/u}}(t)\frac{r^2}{(\log 1/u)^2}\,. \tag{11}$$

Let us now discuss the implications of these results. For systems in which the diffusion is regular, i.e., $\langle r^2\rangle = Dt$ for large t and the averaged probability density is a Gaussian $\langle u(r,t)\rangle = \exp(-\frac{r^2}{Dt})$, it follows from (9) that

$$\langle u^q(r,t)\rangle = \langle u(r\sqrt{q},t)\rangle \;=\; \langle u(r,t)\rangle^q\,. \tag{12}$$

This is what we will term a regular scaling of the moments. An example for this situation is a CTRW model in which the pausing time probability density $\psi(t)$ has a finite first moment $\langle t\rangle$. In the large t limit, n is also large, allowing us by a renewal-theoretic argument[11] to replace it by $t/\langle t\rangle$. With this substitution we derive the expected Gaussian approximation $\langle u(r,t)\rangle$

$$\langle u(r,t)\rangle \sim \exp\left(-\frac{\langle t\rangle r^2}{2\sigma^2 t}\right) = \exp\left(-\frac{\rho^2}{2\tau}\right)\,, \tag{13}$$

in which we have set $\rho = r/\sigma$ and $\tau = t/\langle t\rangle$. Moreover, in this case $\Phi_n(t)$ may be calculated exactly, and has the form $\Phi_n(t) = t^n e^{-t}/n!$, and it therefore follows from (11) that the distribution of u takes the form

$$N(\log 1/u) \;=\; \frac{t^{r^2/(\log 1/u)}e^{-t}}{\Gamma(r^2/(\log 1/u)+1)}\frac{r^2}{(\log 1/u)^2}\,. \tag{14}$$

On the other hand, when the diffusion is anomalous, i.e., $\langle r^2\rangle = Dt^{2/d_w}$ and

$$\langle u(r,t)\rangle \sim \exp\left[-\left(\frac{r}{t^{1/d_w}}\right)^\delta\right]\,, \tag{15}$$

where d_w and $\delta = \frac{d_w}{d_w-1}$, it follows from (9) that

$$\langle u^q(r,t)\rangle = \langle u(r\sqrt{q},t)\rangle \;=\; \langle u(r,t)\rangle^{q\delta/2}\,. \tag{16}$$

i.e., there is non-trivial scaling of the moments. This behavior is called multifractality[6–9]. An example for this situation is furnished by a CTRW model with $\psi(t) \sim T^\alpha/t^{\alpha+1}$, where $0<\alpha<1$. For this case the probability density is known[10] to have the form (15) with $\delta = \frac{2}{2-\alpha}$.

Let us now derive an expression for $\Phi_n(t)$ in this case, and thus find the histogram $N(\log 1/u)$ and also confirm the result (16) explicitly.

We define a dimensionless time $\tau = t/T$. The Laplace transform of $\psi(\tau)$ can be shown to have the small-s expansion

$$\mathcal{L}\{\psi(\tau)\} = \hat{\psi}(s) \sim 1 - s^\alpha \sim e^{-s^\alpha} . \tag{17}$$

The Laplace transform of $\Phi_n(\tau)$ is known to be

$$\mathcal{L}\{\Phi_n(\tau)\} = \hat{\Phi}_n(s) = \frac{1-\hat{\psi}(s)}{s}\hat{\psi}^n(s) , \tag{18}$$

which, in the limit $s \to 0$, is approximated by

$$\hat{\Phi}_n(s) \sim s^{\alpha-1} e^{-ns^\alpha} . \tag{19}$$

Thus the long time behavior of $\Phi_n(t)$ can be found by inverting this transform. We can write the inversion integral as

$$\begin{aligned} \Phi_n(\tau) &\sim \frac{1}{2\pi i}\int_\Gamma \frac{1}{s^{1-\alpha}} e^{-ns^\alpha + s\tau} ds \\ &= \frac{1}{2\pi i}\left(\frac{n}{\tau}\right)^{\frac{\alpha}{\alpha-1}} \int_\Gamma \frac{1}{\xi^{1-\alpha}} \exp\left[-\Omega(\xi^\alpha - \xi)\right] ds , \end{aligned} \tag{20}$$

in which Γ indicates the Bromwich contour, and Ω is the parameter

$$\Omega = \left(\frac{n}{\tau^\alpha}\right)^{\frac{1}{1-\alpha}} . \tag{21}$$

In the regime $\Omega >> 1$ we can evaluate the integral approximately by using the steepest descent method. In this way we find

$$\Phi_n(\tau) \sim \left(\frac{n^{2\alpha+1}}{\tau^{3\alpha}}\right)^{\frac{1}{2(\alpha-1)}} \exp\left[-C\left(\frac{n}{\tau^\alpha}\right)\right] . \tag{22}$$

It therefore follows from (11) that the histogram for this case takes the form

$$N(\log 1/u) \sim \tau^{\frac{3\alpha}{2(1-\alpha)}} r^{\frac{1-4\alpha}{1-\alpha}} (\log 1/u)^{\frac{6\alpha-3}{2(1-\alpha)}} \exp\left[-C\left(\frac{r^2}{(\log 1/u)\tau^\alpha}\right)\right] . \tag{23}$$

Note that since (22) is valid only for $n >> \tau^\alpha$ (23) is valid only for $\log 1/u << \frac{r^2}{\tau^\alpha}$, and cannot be valid for large $\log 1/u$.

Let us now return to Eq. (11) which we approximate in the long time limit as

$$\langle u^q(r,\tau)\rangle \sim \int_0^\infty u(r\sqrt{q},n)\Phi_n(\tau)dn\,, \tag{24}$$

where Eq. (22) is used to furnish an expression for $\Phi_n(\tau)$. While the resulting integral cannot be evaluated exactly, we can again appeal to the steepest descent method to find the exponential term in the resulting approximation. The exponential term in the integrand of (24) is

$$\langle u^q(r,\tau)\rangle \sim \exp\left[-C\left(\frac{n}{\tau^\alpha}\right) - \frac{q\rho^2}{2n}\right]\,, \tag{25}$$

and the value of n that maximizes this exponent is proportional to $q^{\frac{1-\alpha}{2-\alpha}}$ from which follows that

$$\ln\langle u^q(r,\tau)\rangle \sim q^{\frac{1}{2-\alpha}} \ln\langle u(r,\tau)\rangle\,, \tag{26}$$

which agrees with our general result in Eq. (16) (applicable for all systems with anomalous diffusion) for the CTRW case with $\psi(t) \sim T^\alpha/t^{\alpha+1}$.

Multifractal behavior of moments as indicated by Eqs. (16) and (26) have been discovered for various simulated systems[7,8], but has been established analytically only for some specific models[9]. This behavior indicates that there is no single scaling exponent in terms of which all the moments scale and is reflected, for example, in divergence of the relative fluctuations of $u(r,t)$ as follows.

Using Eq. (16), the relative fluctuations of $u(r,t)$ can be expressed in terms of the first moment

$$\left(\frac{\Delta u}{u}\right)^2 \equiv \frac{\langle u^2(r,t)\rangle - \langle u(r,t)\rangle^2}{\langle u(r,t)\rangle^2} = \frac{\langle u(r,t)\rangle^\delta - \langle u(r,t)\rangle^2}{\langle u(r,t)\rangle^2}\,. \tag{28}$$

Since $\delta < 2$, for large r, where $\langle u(r,t)\rangle << 1$, the second term in the nominator can be neglected, and one obtains

$$\left(\frac{\Delta u}{u}\right)^2 = \frac{1}{\langle u(r,t)\rangle^{2-\delta}}\,, \tag{29}$$

i.e., the relative fluctuations diverge as $\langle u(r,t)\rangle$ goes to zero, or r goes to infinity. For the CTRW model discussed above, the form of $\langle u(r,t)\rangle$ is known explicitly[10], and one finds

$$\left(\frac{\Delta u}{u}\right)^2 = \frac{1}{\langle u(r,t)\rangle^{2-\delta}} = \exp\left[(2-\delta)\left(\frac{br}{t^{1/d_w}}\right)^\delta\right]\,, \tag{30}$$

i.e., the relative fluctuations diverge stronger then exponentially as the distance from the origin increases.

This expression corresponds to a measurable quantity. Consider N independent diffusing particles in the presence of random potentials. Then, $P(r,t)$ is just the (normalized) density for particles to be found at distance r at time t. Equation (29) then implies that the relative fluctuations of this quantity would diverge as r increases.

It has recently been suggested[7,8,9], that such multifractal behavior is related to the existence of an algebraic long-tail in the histogram $N(\log 1/u)$. On the contrary, we find that both Eq. (14) and (23) have an algebraic long tail behavior, but while the histogram of Eq. (14) does not correspond to a multifractal behavior, that of Eq. (23) does correspond to such behavior. This can be understood by looking at Eq. (10) which can be rewritten as

$$\langle u^q(r,t)\rangle = \int_0^\infty N(\log 1/u)e^{-q(\log 1/u)}d(\log 1/u)\,. \tag{31}$$

In other words, $\langle u^q(r,t)\rangle$ is just the Laplace transform of $N(\log 1/u)$, and therefore, the asymptotic behavior of the latter, is related only to the behavior of $\langle u^q(r,t)\rangle$ for small q. In particular, according to a Tauberian theorem, if $N(\log 1/u) \sim (\log 1/u)^{-2}$ for large $(\log 1/u)$ (as in (14)), then $\langle u^q(r,t)\rangle \sim 1 - Aq\ln q \sim e^{-Aq}$ for small q (excluding a logarithmic correction), i.e., only the small q behavior is non-multifractal. However, in such cases, this small q behavior may indicate the existence of a q_{min}, in which a crossover between multifractal and non-multifractal regimes occurs, such that for $q < q_{min}$ the behavior of the moments is non-multifractal. Such features have been found in other systems[12]. Note that Eq.(16) is valid only for large value of the argument in the exponent, and says nothing about the behavior for small q. Therefore does not rule out the possibility of such a crossover.

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