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Analysis of self-averaging properties in the transport of particles through random media

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We investigate self-averaging properties in the transport of particles through random media. We show rigorously that in the subdiffusive anomalous regime, transport coefficients are not self-averaging quantities. These quantities are exactly calculated in the case of directed random walks. In the case of general symmetric random walks a perturbative analysis around the effective medium approximation is performed.

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The analysis of transport of particles in random media has interest for physical systems since the transport mechanism is the basis of many physical phenomena [1–4]. The effect of disorder in the behavior of such systems can be normal, if only a quantitative change of the transport parameters occurs, or anomalous when a qualitative change is induced by the disorder. This anomalous behavior is of great interest in the physics of disordered media and has been observed in almost all kind of physical phenomena, from electrical conductivity to thermal properties [2–4]. There is no general theory for anomalous transport because in general the involved phenomena are not unique. An important class of anomalous behaviors are those due to restrictions in the motion of particles imposed by the disorder. If this restriction is strong the motion of the particle is subdiffusive and, as a consequence, anomalies in the observed phenomena occur.

An important characteristic associated with the anomalous behavior is the sample to sample dependence of the measured quantities. Strong sample to sample fluctuations are observed in most cases of anomalous behavior [4]. In a normal situation the transport coefficients are usually sample independent, while for strong disorder transport coefficients are supposed not to be self-averaging quantities. The existence of sample to sample fluctuations is problematic either from experimental or theoretical points of view. On the one hand, experiments are usually performed over a few samples. On the other hand, systematic analysis of disorder effects have been usually based on the probability density of diffusing particles averaged over random media configurations. The study of systems without self-averaging properties implies the calculation of averaged products of probabilities or some equivalent function, which is a rather difficult task. Only a few works have been devoted to the analysis of self-averaging properties in special cases. In [5] a case of weak disorder was investigated, while [6] and [7] deal with cases of directed random walks. In recent works sample to sample fluctuations of first passage times in asymmetric random walks [8] have been investigated. Also, and related to sample to sample fluctuations, there are some works dealing with sample averaging of powers of the probability [9].

In this Rapid Communication we perform a systematic analysis of the self-averaging properties of systems described by random walks (RW's) on regular lattices with a random distribution of transition rates. We introduce a method based on the renormalization of some coefficients of the evolution equations to obtain averaged products of probabilities. This method generalizes the one previously used in [10] for the calculation of single averaged probabilities. We apply the method, which we believe to be of rather wide applicability, to the general symmetric RW and to the directed RW in one dimension. It is shown rigorously that for strong quenched disorder the transport coefficients are not self-averaging.

We consider a general transport problem in which a particle moves in a lattice with random transition rates. The position of the particle at a time t is denoted by $r(t)$ and the quantities of interest are mean functions of the position $F(r)$. Defining $P(r,t)$ as the probability of finding the particle in r at time t, the observed quantities are given by

$$F(t)=\sum_{r} F(r)P(r,t). \tag{1}$$

In principle, these quantities are dependent on the particular configuration of the medium. A complete description of these quantities can be achieved by using averaged moments of the form

$$\langle F^n(t)\rangle = \sum_{r_1,r_2,\ldots,r_n} F(r_1)\cdots F(r_n)\langle P(r_1,t)\cdots P(r_n,t)\rangle, \tag{2}$$

where $\langle\cdots\rangle$ indicates the average over all possible configurations of the medium. The self-averaging character of $F(t)$ can be derived from its variance. We analyze this character in the asymptotic time regime of systems with infinite size. In this case the self-averaging property is defined by means of the magnitude of the fluctuations of the transport coefficients in different realizations of disorder. A zero dispersion means self-averaging of the corresponding coefficient. The same definition has already been used in transport problems [6,7]. Other kinds of methods used in transport problems [5,4] and spin glass theory [11] consider samples of finite size. Then self-averaging properties are studied by taking the limit of infinite size for different configurations.

The study of sample to sample fluctuations of the transport coefficients can be achieved from the calculation of the averaged products of probabilities. In the following we focus on this problem in a transport model with a probability governed by a master equation with random coefficients w_r as

$$\partial_t P(r,t) = L_0 P + L_L w_r L_R P, \tag{3}$$

where L_0, L_L, and L_R are linear operators. In a standard transport model these operators are linear combinations of shift operators, $L(r)=\Sigma_i a_i E_i(r)$, such that $E_i(r)P(r,t)=P(r+i,t)$ and w_r are random transition rates.

The starting point of our method is the introduction of an effective medium with memory [10]. In this way (3) can be written in terms of Laplace transforms as

$$sP(r,s)-P_0(r)=[L_0+L_L\phi(s,r)L_R]P(r,s) + L_L[w_r-\phi(s,r)]L_RP(r,s), \tag{4}$$

where $P_0(r)$ is the probability at $t=0$ and $\phi(r,s)$ is the transition probability of the effective medium that will be determined below. Taking the integral form of (4) and iterating, a development in powers of the random transition rate $\theta_s(r)=w_r-\phi(s,r)$ is obtained [10]. Now we renormalize $\theta_s(r)$ by performing a summation of all terms in which contiguous indices take the same value [10], obtaining

$$P(r,s)=G_s(r,r')P_0(r') + \sum_{n=1}^{\infty} \Phi_s(r_1)\cdots\Phi_s(r_n)G_s^L(r,r_1) \times J_s(r_1,r_2)\cdots J_s(r_{n-1},r_n)G_s^R(r_n,r')P_0(r'), \tag{5}$$

where summation over repeated indices is understood and the sum is restricted to terms with different contiguous indices. This renormalization corresponds to the one loop resummation in diagrammatic representations, also known as single site approximation in condensed matter. The renormalized random transition rate is given by

$$\Phi_s(r)=\frac{\theta_s(r)}{1-J_s(r,r)\theta_s(r)} \tag{6}$$

and the functions $G_s^{L,R}$ and J_s are defined by

$$G_s^R(r,r')=L_R(r)G_s(r,r'), G_s^L(r,r')=L_L^\dagger(r')G_s(r,r'), \tag{7}$$

$$J_s(r,r')=L_R(r)L_L^\dagger(r')G_s(r,r'), \tag{8}$$

$G_s(r,r')$ being the propagator of the deterministic part of (4), $L_0+L_L\phi L_R$. Finally, the transition probability $\phi(r,s)$ is defined by the effective medium approximation (EMA) condition [10]: $\langle\Phi_s(r)\rangle=0$. When the model is translationally invariant the propagator is only dependent on the difference of site positions and the effective medium is homogeneous, that is, ϕ is not dependent on the position.

The averaged products of probabilities can be directly calculated from (5). These products are more conveniently expressed in terms of $\delta P(r,s)$, defined as the difference between the exact probability and that obtained with the effective medium: $\delta P(r,s)=P(r,s)-G_s(r,r')P_0(r')$. In this way the averaged products of $\delta P(r,t)$ are obtained from (5) as series in moments of $\Phi_s(r)$. Since self-averaging is equivalent to a null dispersion, to analyze the self-averaging character of the transport coefficients only $\langle P(r,s)\rangle$ and $\langle P(r,s)P(r',s)\rangle$ must be considered. The method outlined above can be used to obtain these quantities in a large variety of problems. Here we consider the directed RW and the general symmetric RW in one-dimensional (1D) media with quenched disorder.

(*a*) *Directed random walk (DRW) in 1D.* In the DRW only steps in one direction are allowed. Despite its simplicity several phases or anomalous behaviors appear depending on the intensity of disorder [6]. In one dimension the master equation modeling the DRW can be written as:

$$\partial_t P(n,t) = -[1-E_{-1}(n)]w_nP(n,t). \tag{9}$$

The anomalous phases can be classified according to the intensity of disorder, which is related to the existence of inverse moments of the random term w_n. If we restrict our analysis to the long time behavior of the velocity, only the existence of the first inverse moment is relevant. Taking a probability distribution $\rho(w_n)=(1-\alpha)w_n^{-\alpha}$ the weak disordered phase corresponds to the existence of the first inverse moment ($\alpha<0$), and the strong disordered phase to $\langle w_n^{-1}\rangle\to\infty$ $(1>\alpha>0)$. Other cases concerning transients can be found in [6].

The application of the method to this case is straightforward. The propagator $G_s(n,m)$ is zero when $n<m$ and for $n\geqslant m$ we have

$$G_s(n,m)=\frac{\phi(s)^{n-m}}{[s+\phi(s)]^{n-m+1}}. \tag{10}$$

Using the EMA condition we obtain the transition probability of the effective medium $\phi(s)=R^{-1}(s)-s$ where the function $R(s)=\langle(s+w)^{-1}\rangle$ has been calculated in Ref. [6]. Since in the DRW only steps in one direction are possible, only terms in (5) with ordered indices $r_1>r_2>\cdots>r_n$ are different from zero. Then $\langle\delta P(r,s)\rangle=0$ and $\langle P(r,s)\rangle$ is exactly given by the EMA. It is also possible to obtain exact expressions for the averaged products of the moment generating function defined as $F(x,s)=\Sigma_{i=0}^{\infty}x^iP(i,s)$. The factorial moments $f_n(s)$ can be obtained by taking the derivative of $F(x,s)$ at $x=1$. All these quantities are sample dependent. The averaged products of factorial moments can be calculated by means of averaged products of generating functions as

$$\langle f_n(s)\cdots f_m(s)\rangle=\left.\frac{\partial^{n,\ldots,m}\langle F(x,s)\cdots F(y,s)\rangle}{\partial x^n\cdots\partial y^m}\right|_{x=\cdots=y=1}. \tag{11}$$

In general, any self-averaging property can be analyzed with the knowledge of the averaged products of generating functions. Let us consider as an example the analysis of the behavior of the factorial moments and assume the asymptotic form $f_n(s)\sim a_n s^{\alpha_n}$, where a_n is in principle a sample dependent quantity. The averaged value of a_n and its dispersion can be obtained from $\langle F(x,s)\rangle$ and from $D(x,y,s)$

$=\langle[F(x,s)-\langle F(x,s)\rangle][F(y,s)-\langle F(y,s)\rangle]\rangle$. From (5) we obtain the exact expression of the averaged products of generating functions:

$$\langle F(x,s)\rangle=\frac{1}{s+\phi(s)(1-x)}, \qquad (12)$$

$$D(x,y,s)=\frac{\langle\Phi_s^2\rangle}{[s+\phi(s)]^2}\frac{(1-x)(1-y)}{[s+(1-x)\phi(s)][s+(1-y)\phi(s)]}\times\frac{1}{[1-A(s)xy]}, \qquad (13)$$

where $A(s)=\{\phi(s)^2[s+\phi(s)]^2s^2\langle\Phi_s^2\rangle\}[s+\phi(s)]^{-4}$ and the renormalized random transition is $\Phi_s=[s+\phi(s)]\{[w-\phi(s)]/(w+s)\}$. From these expressions we immediately have the calculation of moments and their sample to sample dispersions. In the weak disordered phase, after calculation of $R(s)$ and $\langle\Phi_s^2\rangle$, one obtains a ballistic behavior, $\langle\bar{r}(t)\rangle\sim vt$, with a velocity $v=\langle w^{-1}\rangle^{-1}$, that is a self-averaging quantity. In the strong disordered phase one obtains, in agreement with [6,7], a subballistic behavior, $\langle\bar{r}(t)\rangle\sim b\,t^{(1-\alpha)}$ with a coefficient with mean value $\langle b\rangle=\sin[\pi(1-\alpha)]/[\pi(1-\alpha)\Gamma(2-\alpha)]$, that is not self-averaging. The relative variance of b is $\sigma_r^2(b)=\langle(b-\langle b\rangle)^2\rangle/\langle b\rangle^2=\alpha/(2-\alpha)$. The dispersion increases $[\sigma_r(b)\to 1]$ for stronger disorder $(\alpha\to 1)$.

(*b*) *Symmetric random walk (SRW) in 1D.* There are two models of symmetric RW, the random trap (RT) and random barrier (RB) models. The master equations corresponding to both models are written in our formulation as

$$\partial_t P(n,t)=[1-E_{-1}(n)]w_n[E_{+1}(n)-1]P(n,t) \qquad (14)$$

for the random barrier and

$$\partial_t P(n,t)=[E_{-1}(n)+E_{+1}(n)-2]w_nP(n,t) \qquad (15)$$

for the random trap. The anomalous behavior induced by the disorder is, in both cases, well known [1]. The different phases can be classified following the definitions of [1]. We recall that for model A (weak disorder) the inverse moments of w_n, $\beta_M=\langle(w_n)^{-M}\rangle$ $(M=1,2,\ldots)$ are finite, while models B (marginal case, $\alpha=0$) and C (strong disorder, $0<\alpha<1$) are based on a probability distribution $\rho(w_n)=(1-\alpha)\,w_n^{-\alpha}$ $[w_n\in(0,1)]$, such that inverse moments diverge. In all cases the long time behavior of the sample averaged diffusion coefficient has been exactly calculated. However, sample to sample fluctuations have not been investigated until now. The sample averaged quantities are the same for RT and RB in one dimension [10]. The same results are also obtained from (5) for the self-averaging properties.

The application of the method to RB and RT models is also straightforward, but it is not possible to obtain exact expressions as in the DRW case. The propagator $G_s(n,m)$ and the functions $J_s(n,m)$ are given in [10] for all kinds of disorder. The transition probability of the effective medium $\phi(s)$ has also been calculated in [10] from the EMA condition. In this reference we obtained the exact asymptotic behavior of the averaged mean square displacement $\langle\overline{x^2}(s)\rangle$ in the frequency domain, which is directly related to the diffusivity. The results derived from the EMA for each type of disorder (A, B, and C) are given by

$$\overline{x^2}(s)_{EMA}=\frac{2}{s^2\beta_1}\left(1+\frac{\beta_2-\beta_1^2}{2\beta_1^2}(\beta_1 s)^{\frac{1}{2}}+O(s)\right), \qquad (16)$$

$$\overline{x^2}(s)_{EMA}=\frac{4}{s^2|\ln(s)|}\left(1-\frac{\ln|\ln(s)|}{|\ln s|}+O(|\ln s|^{-1})\right), \qquad (17)$$

$$\overline{x^2}(s)_{EMA}=2\left[\frac{\sin(\pi\alpha)}{(1-\alpha)\pi 2^{\alpha}}\right]^{2/(2-\alpha)}s^{(3\alpha-4)/(2-\alpha)}+O(s^{(5\alpha-6)/(4-2\alpha)}). \qquad (18)$$

The exact results can be expressed as corrections to the results given by the EMA as

$$\langle\overline{x^2}(s)\rangle\sim\overline{x^2}(s)_{EMA}[1+\alpha(s)], \qquad (19)$$

where the first corrections are

$$\alpha_A(s)=\frac{1}{12\beta_1^3}(\beta_2-\beta_1^2)^2s, \qquad (20)$$

$$\alpha_B(s)=\frac{(\pi^2+16\ln 2-20)}{|\ln s|^2}, \qquad (21)$$

$$\alpha_C(s)=(4\ln 2-5+\pi^2/4)\alpha^2+O(\alpha^3\ln\alpha). \qquad (22)$$

In the weak disordered case the behavior is normal and the EMA reproduces exactly the first and second terms of $\langle\overline{x^2}\rangle$. In the marginal case B the EMA is exact up to terms of order smaller than $|\ln s|^{-3}$ [10]. In the strong disordered case the behavior is subdiffusive and the EMA does not reproduce exactly the coefficient of the leading term [10]. Expressions (19)–(22) have been diagrammatically calculated in [10] by using cumulants and projection operators. We can obtain the same result from (5) in a much more simple way in terms of moments and single functions. This simplicity allows us to calculate more involved quantities and to analyze self-averaging properties. For instance, to analyze the sample to sample fluctuations of the generalized diffusion coefficient we have calculated $\langle\overline{x^2}^{\,2}\rangle$ which depends on the averaged product of probabilities. As in the above case the exact result can be expressed as corrections to the EMA result as

$$\langle\overline{x^2}(s)^2\rangle\sim\overline{x^2}(s)_{EMA}^2[1+\gamma(s)], \qquad (23)$$

where the correction terms are

$$\gamma_a=\frac{\beta_1^{-3/2}(\beta_2-\beta_1^2)}{4}s^{1/2}, \qquad (24)$$

$$\gamma_b=\frac{1}{|\ln s|}, \qquad (25)$$

$$\gamma_c=\alpha/2+O(\alpha^2). \qquad (26)$$

These terms have been calculated from a diagrammatic representation of the averaged products of (5). A detailed description of this method will be presented elsewhere. Finally, from (19) and (23) we can extract several conclusions. For weak and strong disorder the dispersion of the particle can be taken, in the long time limit, as $\overline{x^2} \sim a_1 s^{\alpha_1} + a_2 s^{\alpha_2}$, where the coefficients are in principle sample dependent quantities. In the weak disordered case the behavior is diffusive and we have $\overline{x^2} \sim a_1 s^{-2} + a_2 s^{-7/4}$, where the first coefficient is self-averaging but the second is sample dependent with a zero mean value and a variance $\sigma^2(a_2) = \beta_1^{-7/2}(\beta_2 - \beta_1^2)$. In the strong disordered case the behavior is subdiffusive, $\overline{x^2} \sim c_1 s^{-(4-3\alpha)/(2-\alpha)}$ and c_1 is not self-averaging. The mean value of the coefficient c_1 can easily be calculated for small α from (19) and (22) ($\langle c_1 \rangle = 4\alpha + O(\alpha^3)$). As we will show elsewhere its dispersion can be also obtained in the same way, $\sigma^2(c_1) = 2\alpha^3 + O(\alpha^4 \ln \alpha)$. Finally, the marginal case B is similar to the weak case with logarithmic corrections and we have $\overline{x^2} \sim b_1 s^{-2} |\ln s|^{-1} + b_2 s^{-2} |\ln s|^{-3/2}$. The first coefficient is self-averaging but b_2 is sample dependent with a zero mean value and a variance $\sigma^2(b_2) = 16$.

In summary, we have presented here a general method to study self-averaging properties in the transport of particles through random media. Our analysis of both DRW and SRW shows rigorously that when the behavior of a quantity is normal its long time behavior is sample independent. On the contrary, in anomalous diffusion phases the self-averaging property is not satisfied. The method introduced in this Rapid Communication can easily be applied to other one-dimensional problems and it can also be extended to more dimensions. Some of these applications will be presented elsewhere.

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