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 (EMA) is performed.

The analysis of transport of particles in random media has interest in physical systems since the transport mechanism is on the basis of many physical phenomena. The effect of disorder in the behavior of such systems can be normal, if only a quantitative change of the transport parameters occur, 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. 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 to 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. 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 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 a case of weak disorder was investigated, while and deal with cases of directed random walks. In recent works sample to sample fluctuations of first passage times in asymmetric random walks have been investigated. Also, and related with sample to sample fluctuations, there are some works dealing with sample averaging of powers of the probability.

In this Letter we perform a systematic analysis of the self-averaging properties of systems described by random walks (RW) 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 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 magnitudes 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:

\[
F(t) = \sum_r F(r)P(r, t).
\]

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

\[
\langle F^n(t) \rangle = \sum_{r_1 r_2 \cdots r_n} F(r_1) \cdots F(r_n)P(r_1, t) \cdots P(r_n, t),
\]

where \( \langle \cdots \rangle \) indicate average over all possible configurations of the medium. The self-averaging character of \( F(t) \) can be derived from its variance. A zero dispersion is equivalent to self-averaging. This dispersion can be obtained 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:
\[ \partial_t P(R,t) = L_0 P + L_L w_r L_R P, \]  
where \( L_0, L_L \), and \( L_R \) are linear operators. In a standard transport model these operators are linear combinations of shift operators, \( L(r) = \sum_i a_i E_i(r) \), 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 \( [11] \). In this way \( [14] \) can be written in terms of Laplace Transforms as

\[ sP(r,s) - P_0(r) = [L_0 + L_L \phi(s,r)L_R]P(r,s) + L_L[w_r - \phi(s,r)L_R]P(r,s), \]  
where \( P_0(r) \) is the probability at \( t = 0 \) and \( \phi(s,r) \) is the transition probability of the effective medium that will be determined below. Taking the integral form of \( [11] \) and iterating, a development in powers of the random transition rate \( \theta(r) = w_r - \phi(s,r) \) is obtained \( [11] \). Now we renormalize \( \theta(r) \) by performing a summation of all terms in which contiguous indexes take the same value \( [10] \), obtaining

\[ P(r,s) = G_s(r,rt)P_0(rt) + \sum_{n=1}^{\infty} \Phi_s(r_1) ... \Phi_s(r_n)G_s^L(r,rt)J_s(r_2,rt) ... J_s(r_n,rt), \]  
where summation over repeated indexes is understood and the sum is restricted to terms with different contiguous indexes. This renormalization corresponds to the one loop resummation in diagrammatic representations, also known as single site approximation in condensed matter. The renormalized random transition is given by

\[ \Phi_s(r) = \frac{\theta_s(r)}{1 - J_s(r,r)\theta_s(r)} \]  
and the functions \( G_s^{L,R} \) and \( J_s \) are defined by

\[ G_s^R(r,rt) = L_R(r)G_s(r,rt), \quad G_s^L(r,rt) = L_L^\dagger(rt)G_s(r,rt), \]  
being \( G_s(r,rt) \) the propagator of the deterministic part of \( [4] \), \( L_0 + L_L \phi L_R \). Finally, the transition probability \( \phi(s,r) \) is defined by the Effective Medium Approximation (EMA) condition \( [12] \): \( \langle \Phi_s(r) \rangle = 0 \). 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, \( \phi \) is not dependent on the position.

The averaged products of probabilities can be directly calculated from \( [3] \). 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: \( \delta P(r,s) = P(r,s) - G_s(r,rt)P_0(rt) \). In this way the averaged products of \( \delta P(r,t) \) are obtained from \( [3] \) 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 \( \langle P(r,s)P(rt,s) \rangle \) must be considered. The method outlined above can be used to obtain these magnitudes in a large variety of problems. Here we consider the directed RW and the general symmetric RW in one-dimensional 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:

\[ \partial_t P(n,t) = -(1 - E_{-1}(n))w_n P(n,t). \]  

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 \( p(w_n) = (1 - \alpha)\delta^{n-\alpha} \) the weak disordered phase correspond 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 \( [8] \).

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

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

Using the EMA condition we obtain the transition probability of the effective medium \( \phi(s) = R^{-1}(s) - s \) where the function \( R(s) = (s + w)^{-1} \) has been calculated in Ref. \( [8] \). Since in the DRW only steps in one direction are possible, only terms in \( [4] \) with ordered indexes \( r_1 > r_2 > ... > r_n \) 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 \( F(x,s) = \sum_{i=1}^{\infty} x^i \rho(i,s) \). 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

\[ \langle f_n(s) ... f_m(s) \rangle = \left. \frac{\partial^{n+...+m} F(x,s) ... F(y,s)}{\partial x^n ... \partial y^m} \right|_{x=...=y=1}. \]
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 \( f_n(s) \approx a_n s^{\alpha_n} \), where \( a_n \) is in principle a sample dependent quantity. The averaged value of \( a_n \) and its dispersion can be obtained from (5) and from \( D(x,y,s) = \langle (F(x,s) - (F(x,s)) (F(y,s) - (F(y,s))) \rangle. \)

From (3) we obtain the exact expression of the averaged products of generating functions:

\[
(F(x,s)) = \frac{1}{s + \phi(s)(1-x)} \tag{12}
\]

\[
D(x,y,s) = \frac{(\Phi^2_s)}{(s + \phi(s))^2} \left[ \frac{(1-x)(1-y)}{s + \phi(s)} \right] \tag{13}
\]

where \( A(s) = [\phi(s)^2(s + \phi(s))^2 s^2(\Phi^2_s)(s + \phi(s))^{-4} \) and the renormalized random transition is \( \Phi_s = (s + \phi(s)) \left[ (w - \phi(s))/(w + s) \right]. \)

From these expressions it is immediate the calculation of moments and their sample to sample dispersions. In the weak disordered phase, after calculation of \( R(s) \) and \( (\Phi^2_s) \), one obtains a ballistic behavior, \( (\tau(t)) \sim vt \), with a velocity \( v = (w^{-1})^{-1} \), that is a self–averaging quantity. In the strong disordered phase one obtains, in agreement with [6], [7], a subballistic behavior, \( (\tau(t)) \sim b t^{(1-\alpha)} \) with a coefficient with mean value \( (b) = \sin(\pi(1-\alpha))/((\pi(1-\alpha)\Gamma(2-\alpha)) \), that is not self–averaging. The relative variance of \( b \) is \( \sigma^2_r(b) = (b - (b))^2)/(b)^2 = \alpha/(2-\alpha). \) 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:

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

for the random barrier and

\[
\partial_t P(n,t) = (E_{-1}(n) + E_{+1}(n) - 2) w_n P(n,t) \tag{15}
\]

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 \( w_n \), \( \xi_M^A = \langle w_n \rangle^{-M} \) \( (M = 1, 2, ...) \) 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 magnitudes 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 like in the DRW case. The propagator \( G_n(n,m) \) and the functions \( J_k(n,m) \) are given in \([10]\) for all kinds of disorder. The transition probability of the effective medium \( \phi(s) \) has been also calculated in \([10]\) from the EMA condition. In this reference we obtained the exact asymptotic behavior of the averaged mean square displacement \( \langle x^2(s) \rangle \) in the frequency domain, which is directly related with the diffusivity. The results derived from the EMA for each type of disorder (A, B and C) are given by:

\[
\langle x^2(s)_{EMA} \rangle = \frac{2}{s^2 \beta_4} \left( 1 + \frac{\beta_2 - \beta_1^2}{2 \beta_1^2} (\beta_1 s)^2 + O(s) \right) \tag{16}
\]

\[
\langle x^2(s)_{EMA} \rangle = \frac{4}{s^2 \ln|s|} \left( 1 - \frac{\ln|\ln(s)|}{\ln|s|} + O(|\ln|s||^{-1}) \right) \tag{17}
\]

\[
\langle x^2(s)_{EMA} \rangle = 2 \left[ \frac{\sin(\pi \alpha)}{((1-\alpha)\pi 2^n)} \right]^{2/(2-\alpha)} \left( s^{-\alpha} \right) + O(s^{n-\alpha}). \tag{18}
\]

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

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

where the first corrections are

\[
\alpha_A(s) = \frac{1}{12 \beta_1^2} (\beta_2 - \beta_1^2)^2 s \tag{20}
\]

\[
\alpha_B(s) = \frac{(\pi^2 + 16 \ln 2 - 20)}{|\ln|s||^2} \tag{21}
\]

\[
\alpha_C(s) = (4 \ln 2 - 5 + \pi^2/4) s + O(\alpha^3 \ln \alpha). \tag{22}
\]

In the weak disordered case the behavior is normal and the EMA reproduces exactly the first and second terms of \( \langle x^2 \rangle \). In the marginal case B the EMA is exact up to terms of order smaller than \( |\ln|s||^{-3} \). In the strong disordered case the behavior is subdiffusive and the EMA does not reproduce exactly the coefficient of the leading term \([13]\). Expressions (19)–(22) have been diagrammatically calculated in \([10]\) by using cumulants and projection operators. We can obtain the same result from \([3]\) 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 \( \overline{x^2(s)} \) 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

\[
\overline{x^2(s)} \sim \overline{x^2(s)}_{EMA}(1 + \gamma(s)),
\]

where the correction terms are

\[
\gamma_a = \frac{\beta_1^2 (\beta_2 - \beta_1^2)}{4} s^{\frac{1}{2}}.
\]

\[
\gamma_b = \frac{1}{\ln s}.
\]

\[
\gamma_c = a/2 + O(\alpha^2).
\]

These terms have been calculated from a diagrammatic representation of the averaged products of \( \overline{x} \). 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 sample dependent with a zero mean value and a variance \( \sigma^2 \). In the weak disordered case the behavior is subdiffusive, \( \overline{x^2} \sim c_1 s^{-(4-3\alpha)/(2-\alpha)} \) and \( \gamma_1 \) is not self-averaging. The mean value of the coefficient \( c_1 \) can be easily calculated for small \( \alpha \) from (19) and (23) \( (c_1) = 4\alpha + O(\alpha^3) \). 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 \( \overline{x^2} \sim c_1 s^{-(4-3\alpha)/(2-\alpha)} \ln s \). 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 on random media. Our analysis of both DRW and SRW shows rigorously that when the behavior of a magnitude is normal its long time behavior is sample independent. By the contrary in anomalous diffusion phases the self-averaging property is not satisfied. The method introduced in this letter can be easily applied to other one dimensional problems and it can be also extended to more dimensions. Some of these applications will be presented elsewhere.

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