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An alternative approach to the Terwiel cumulants expansion in disordered media

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Abstract. In the context of the study of diffusion in disordered media we present an alternative way to obtain the Terwiel cumulants expansion. Our approach starts from a formal solution of the master equation (ME) associated with the model of the nearest-neighbour random walk in a one-dimensional disordered chain. We apply our formalism to the analysis of a finite-effective-medium-like approximation.

1. Introduction

Diffusion is a determinant process in many phenomena occurring in disordered media. Of particular interest are the diffusion-controlled reactions which often occur in physical, chemical or biological systems. As examples of these processes we can mention the chemical reaction of two components in which one of them is fixed and the other one wanders around until they meet and react [1]; or, in the field of biology, the absorption of ligand molecules by acceptor centres located on a cell's surface [2]. In many systems it is necessary to consider the effect of disorder on the behaviour of quantities of physical interest [3, 4]. These effects may be only quantitative modifications that preserve the diffusion or involve a more profound change. Disorder imposes restrictions on the movement of the particles. When the disorder becomes strong enough, these restrictions lead to an anomalous behaviour.

In this paper we consider a finite one-dimensional lattice bounded by perfect traps. A particle is allowed to diffuse on the lattice until it is captured by one of the traps. Disorder is introduced by assigning to each site of the lattice a transition rate that is a stochastic variable (site disorder). The transition rate ω_i gives the jumping probability per unit time from site i to any of its nearest neighbours: $i \pm 1$ (symmetric random walk). The random variables $\{\omega_i\}$ are supposed to be mutually independent and with identical density of probability $\rho(\omega)$. The time that the particle spends on each lattice site before it jumps to any of its neighbouring sites is a random variable whose average moments are given by

$$\bar{t^n} = (2\omega_i)^{-n} \qquad n = 1, 2, \ldots .$$

If the density of probability $\rho(\omega_i)$ gives finite values for the average

$$\left\langle \frac{1}{\omega_i^2} \right\rangle \equiv \int \rho(\omega_i) \frac{\mathrm{d}\omega_i}{\omega_i^2}$$

we say that the system has a weak disorder; otherwise the disorder is strong. Some authors prefer to call 'strong disorder' the case where both $\langle \frac{1}{\omega_i} \rangle$ and $\langle \frac{1}{\omega_i^2} \rangle$ diverge. A convenient family of probabilities distributions $\rho(\omega_i)$ for the random variables ω_i is given by

$$\rho_\alpha(\omega) = \begin{cases} (1-\alpha)\omega^{-\alpha} & \omega \in [0, 1] \\ 0 & \text{otherwise} \end{cases}$$

where the parameter $\alpha < 1$ characterizes the disorder. For $\alpha < -1$ the inverse second moment

$$\left\langle \frac{1}{\omega^2} \right\rangle \equiv \int_0^1 \frac{\rho_\alpha(\omega)\,\mathrm{d}\omega}{\omega^2}$$

is finite and we have *weak disorder*. For $-1 < \alpha < 1$ the second inverse moment diverges and we have the so-called *strong disorder*.

Among the properties of the system that we are interested in are the asymptotic behaviour ($t \to \infty$) of the averaged survival probability and the statistics of the first-passage time (FPT). Such average is taken over realizations of the disorder. For weak disorder the system behaves, for long times, as an homogeneous one with an effective transition rate ω_{eff} given by

$$\omega_{eff} = \left\langle \frac{1}{\omega} \right\rangle^{-1}$$

while for short times this effective transition rate is

$$\omega_{eff} = \langle \omega \rangle.$$

The study of particles diffusion in one-dimensional disordered media has attracted the attention of many authors in the last two decades [5–12]. Since it is not possible, in general, to exactly solve the associated ME for a given realization of the disorder, several approximated procedures have been developed to solve an *averaged ME* [11]. These techniques have yielded the long-time behaviour for physically relevant quantities for any kind of disorder. Instead, our approach starts by writing a formal solution of the ME in Laplace space, for a given realization of the disorder. Using straightforward algebra we will be able to express the averaged solution as a series in terms of the known Terwiel cumulants [13]. This scheme allows us to reobtain several results in a much simpler way.

The outline of the paper is as follows. In section 2 we describe the model and define the survival probability and the FPT for a homogeneous system; in section 3 we analyse a disordered system and obtain a formal solution in terms of Terwiel cumulants. The asymptotic behaviour for systems with weak disorder is also given; in section 4 a finite-effective medium approximation is obtained from the Terwiel expansion.

2. The FPT statistics

Assuming that the process can be modelled by a particle that makes a random walk on a regular one-dimensional disordered lattice, to each site of the lattice is assigned a random variable ω_n that gives the jump probability per unit time to any of the two nearest neighbours (sites $n + 1$ and $n - 1$). Since the jump probability per unit time is constant the resulting diffusion will be Markovian. Let us stress that once the random variable ω_n is chosen, its value is kept fixed, i.e. we have *quenched* disorder in the lattice. The density of the probability distribution for ω is given by the function $\rho(\omega)$.

The position of the particle in the chain is governed by the ME

$$\frac{\mathrm{d}G_{ij}(t)}{\mathrm{d}t} = \sum_{k=1}^{N} H_{ik} G_{kj}(t) \qquad i, j = 1, \ldots, N \tag{2.1}$$

where $G_{ij}(t) \equiv G(i, t|j, t_0 = 0)$ is the conditional probability that the walker is at site i at time t given that it started from site j at time $t_0 = 0$. N is the number of sites in the lattice and the matrix H is defined below. In matrix notation the equation (2.1) can be rewritten in the form

$$\frac{\mathrm{d}G}{\mathrm{d}t} = HG \tag{2.2}$$

where the matrix H has the general form

$$H \equiv M\Omega. \tag{2.3}$$

The matrix M depends on the boundary condition and Ω is the diagonal matrix

$$\Omega = \begin{pmatrix} \omega_1 & 0 & . & . & 0 \\ 0 & \omega_2 & 0 & . & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & . & . & \omega_N \end{pmatrix}.$$

If we assume that the sites $i = 0$ and $i = N + 1$ are absorbing, the matrix M adopts the form

$$M = \begin{pmatrix} -2 & 1 & . & . & 0 \\ 1 & -2 & 1 & . & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & . & 1 & -2 \end{pmatrix}.$$

By Laplace transforming equation (2.2) we obtain

$$-G(0) + z\tilde{G}(z) = H\tilde{G}(z)$$

which leads to

$$\begin{aligned} \tilde{G}(z) = (z - H)^{-1}G(0) &= (z - M\Omega)^{-1}G(0) \\ &= (z - M\Omega)^{-1} \end{aligned} \tag{2.4}$$

with $\tilde{G}(z)$ the Laplace transform of the matrix $G(t)$. $G(0)$ is the identity matrix.

The sum

$$F_j(t) \equiv \sum_i G_{ij}(t) \tag{2.5}$$

represents the survival probability of the walker at time t, that is, the probability that a walker that started from site j at time $t_0 = 0$ is still somewhere on the lattice at time t. The probability density $g_j(t)$ for FPT is given by

$$g_j(t) = -\frac{\mathrm{d}F_j}{\mathrm{d}t}.$$

Thus, the mean value of the FPT for the particle, starting at site j, is given by

$${}^{(1)}T_j = \int_0^\infty g_j(t)t\,\mathrm{d}t = -\int_0^\infty t\frac{\mathrm{d}F_j}{\mathrm{d}t}\mathrm{d}t = \int_0^\infty F_j(t)\,\mathrm{d}t \tag{2.6}$$

where we have assumed that $tF_j(t) \sim 0$ for $t \to \infty$. In terms of the Laplace transform of $F_j(t)$,

$$\tilde{F}_j(z) = \int_0^\infty \mathrm{e}^{-zt}F_j(t)\,\mathrm{d}t = \sum_i \tilde{G}_{ij}(z)$$

the mean value ${}^{(1)}T_j$ is given by

$${}^{(1)}T_j = \tilde{F}_j(z = 0).$$

Similarly, higher moments ${}^{(k)}T_j$ of the FPT can be obtained from

$${}^{(k)}T_j = \int_0^\infty g_j(t)t^k \, \mathrm{d}t = (-1)^{k+1}k \frac{\mathrm{d}^{k-1}\,\tilde{F}_j(z)}{\mathrm{d}z^{k-1}}|_{z=0}.$$

Therefore, the FPT statistics can be obtained from the knowledge of the matrix $\tilde{G}_{ij}(z)$ at z near to zero.

3. The Terwiel cumulants expansion

The values of ${}^{(k)}T_j$ will depend on the particular set of values taken by the random variable $\{\omega_i\}$ for a given realization of the disorder. Usually we will be interested in an average of these quantities over realizations of the disorder. This average can be formally carried out by introducing a projection operator $\mathcal{P}$ which averages over disorder:

$$\mathcal{P}Q \equiv \langle Q \rangle \equiv \int \mathrm{d}\omega_1\,\rho(\omega_1) \int \mathrm{d}\omega_2\,\rho(\omega_2) \ldots \int \mathrm{d}\omega_n\,\rho(\omega_n) Q$$

for any quantity Q. Obviously we have the identity

$$Q = \mathcal{P}Q + (1 - \mathcal{P})Q. \tag{3.1}$$

For the moments ${}^{(k)}T_j$ we have

$$\begin{aligned}\langle {}^{(k)}T_j \rangle = \mathcal{P}({}^{(k)}T_j) &= (-1)^{k+1}k\mathcal{P}\frac{\mathrm{d}^{k-1}}{\mathrm{d}z^{k-1}}\tilde{F}_j(0)|_{z=0} \\ &= (-1)^{k+1}k\frac{\mathrm{d}^{k-1}}{\mathrm{d}z^{k-1}}\sum_i \langle \tilde{G} \rangle_{ij}(z)|_{z=0}.\end{aligned} \tag{3.2}$$

Let us now evaluate the average $\langle \tilde{G}_{ij}(z) \rangle$. We start by splitting the transition probabilities ω_n in their average, γ, and random parts, η_n, such that $\langle \omega_n \rangle = \gamma$ (and $\langle \eta_n \rangle = 0$) and $\omega_n = \gamma + \eta_n$. Thus the matrix Ω can be written as

$$\Omega = \Gamma + \eta \tag{3.3}$$

where $\Gamma = \gamma I$ and $\eta = \mathrm{diag}(\eta_1, \ldots, \eta_N)$. By replacing the decomposition (3.3) in (2.4), and using the Dyson expansion, it is straightforward to verify the identity

$$\tilde{G}(z) = \tilde{G}^0(z) + \tilde{G}^0(z)M\eta\tilde{G}(z) \tag{3.4}$$

with $\tilde{G}^0(z) \equiv (z - M\Gamma)^{-1}$. Because the matrix $\tilde{G}^0$ does not depend on the disorder, the average of the matrix $\tilde{G}$ can be written as follows:

$$\mathcal{P}\tilde{G} = \tilde{G}^0 + \tilde{G}^0\mathcal{P}M\eta\tilde{G} = \tilde{G}^0 + \tilde{G}^0\mathcal{P}M\eta[\mathcal{P}\tilde{G} + (1 - \mathcal{P})\tilde{G}] \tag{3.5}$$

where we have used the identity (3.1). Furthermore

$$(1 - \mathcal{P})\tilde{G} = \tilde{G}^0(1 - \mathcal{P})M\eta\tilde{G} = \tilde{G}^0(1 - \mathcal{P})M\eta[\mathcal{P}\tilde{G} + (1 - \mathcal{P})\tilde{G}]. \tag{3.6}$$

By iterating (3.6) and using this result in (3.5) we get

$$\mathcal{P}\tilde{G} = \tilde{G}^0 + J\mathcal{P}\{1 + \eta J(1 - \mathcal{P}) + \eta J(1 - \mathcal{P})\eta J(1 - \mathcal{P}) + \ldots\}\eta\mathcal{P}\tilde{G} \tag{3.7}$$

with $J \equiv \tilde{G}^0 M$. In this way we arrive at a formal equation for $\langle \tilde{G} \rangle$

$$\langle \tilde{G} \rangle = \tilde{G}^0 + J\left\langle \frac{1}{1 - \eta J(1 - \mathcal{P})}\eta \right\rangle \langle \tilde{G} \rangle. \tag{3.8}$$

The terms involved in this expansion of $\langle[1-\eta J(1-\mathcal{P})]^{-1}\eta\rangle$ are known as the Terwiel cumulants [13]. An expansion in terms of the Terwiel cumulants has been used to write an approximated ME [11], instead of making the expansion directly from the formal solution as is done here. The expressions obtained in that form are rather complex.

The expression (3.8) allows us to write $\langle\tilde{G}\rangle$ down in terms of $\tilde{G}^0$:

$$\langle\tilde{G}\rangle = \left\{1 - J\left\langle\frac{1}{1-\eta J(1-\mathcal{P})}\eta\right\rangle\right\}^{-1}\tilde{G}^0. \tag{3.9}$$

Expanding $\langle\tilde{G}_{ij}(z)\rangle$ around $z=0$,

$$\langle\tilde{G}_{ij}(z)\rangle = \sum_{k=0}^{\infty} A_{ij}^{(k)} z^k$$

it is easy to verify the identity:

$$\langle{}^{(k)}T_j\rangle = (-1)^{k+1}k!\sum_{i=1}^{N} A_{ij}^{(k-1)}. \tag{3.10}$$

Thus, in order to evaluate the average of the moments ${}^{(k)}T_j$ we need the coefficients $A_{ij}^{(k)}$. By replacing the expansions of $\tilde{G}^0$ and J near $z=0$

$$\tilde{G}^0 = -\frac{M^{-1}}{\Gamma} + \frac{M^{-2}}{\Gamma^2}z + \cdots$$
$$J \equiv \tilde{G}^0 M = -\frac{1}{\Gamma} + \frac{M^{-1}}{\Gamma^2}z + \cdots$$

in the equation (3.9) for $\langle\tilde{G}\rangle$, we obtain for the coefficients $A_{ij}^{(0)}$ and $A_{ij}^{(1)}$ the values:

$$\begin{aligned} A_{ij}^{(0)} &= -\left\langle\frac{1}{\omega_i}\right\rangle M_{ij}^{-1} \\ A_{ij}^{(1)} &= \sum_l \left\langle\frac{1}{\omega_i}M_{il}^{-1}\frac{1}{\omega_l}\right\rangle M_{lj}^{-1} \\ &= \left\langle\frac{1}{\omega}\right\rangle^2 M_{ij}^{-2} + \left(\left\langle\frac{1}{\omega^2}\right\rangle - \left\langle\frac{1}{\omega}\right\rangle^2\right) M_{ii}^{-1}M_{ij}^{-1} \end{aligned} \tag{3.11}$$

where we have used the fact that $\langle\frac{1}{\omega_i}\frac{1}{\omega_j}\rangle = \langle\frac{1}{\omega}\rangle^2$ if $i \neq j$ due to the independence of the variables ω_i and ω_j.

The expression for $A_{ij}^{(0)}$ shows that, at long times, the system behaves as a homogeneous one with an effective transition rate ω_{eff} given by

$$\omega_{eff} \equiv \left\langle\frac{1}{\omega}\right\rangle^{-1}.$$

The coefficient of the linear term in z is related to the fluctuation of the random variable $\frac{1}{\omega_i}$.

In the case of strong disorder the results just obtained are no longer valid. In particular, as follows from equation (3.11), the moments of the FPT diverge. It is of interest to study the form that these divergencies take place. A way to perform that study is to evaluate the magnitudes involved in the frame of a finite effective approximation scheme. Therefore, in the next section we present, from the Terwiel expansion obtained previously, an effective-medium-like approximation.

4. Finite-effective-medium-like approximation from the Terwiel expansion

In general it is not easy to evaluate $\langle \tilde{G}_{ij}(z)\rangle$ for disordered systems with an arbitrary value of N. However, there are various approximation methods. Among these methods is the finite-effective-medium approximation which gives the correct result for small and large values of the parameter z [6–11]. This approximation can be obtained in the following way: consider a finite one-dimensional lattice with jumping probability between nearest neighbour equal to Γ in every site except in the site l where the jumping probability is ω (single impurity problem at site l). In this approximation one requires that the average over the values of ω of the propagator $\tilde{G}^{(i)}(z,\Gamma,\omega,l)$ associated with this single impurity problem be equal to the propagator $\tilde{G}^0(z,\Gamma)$ corresponding to an homogeneous chain with jumping probability equal to Γ in every position in the chain. Because the value of Γ resulting from this requirement depends on the position l and on the Laplace parameter z, it will be denoted by $\Gamma_l(z)$. Hence

$$\int \tilde{G}^{(i)}_{jk}(z,\Gamma_l,\omega)\rho(\omega)\,\mathrm{d}\omega = \tilde{G}^0_{jk}(z,\Gamma_l). \tag{4.1}$$

The probability density $\rho(\omega)$ used in the last equation is the same as the one defined for the disordered system. It can be shown that the value Γ_l must be independent of the indices jk of the matrix element used to write equation (4.1). The propagator $\tilde{G}^{(i)}$ is given by

$$\tilde{G}^{(i)}(z,\Gamma_l,\omega) = (z - M\Omega)^{-1} \equiv (z - M\Gamma_l - M\Delta)^{-1}$$

where Δ is a matrix with zero entries except for the element ll, which is equal to $\Delta_l = \omega - \Gamma_l(z)$. It is straightforward to verify the identity

$$\tilde{G}^{(i)} = \tilde{G}^0 + \left(\frac{\tilde{G}^0 M}{1 - J_{ll}\Delta_l}\right)\tilde{G}^0.$$

Replacing this expression in equation (4.1) we obtain

$$\int \frac{\Delta_l\rho(\omega)\,\mathrm{d}\omega}{1 - \Delta_l(\tilde{G}^0 M)_{ll}} = 0 \tag{4.2}$$

or equivalently

$$\int \frac{\rho(\omega)\mathrm{d}\omega}{1 - \Delta_l J_{ll}} = 1. \tag{4.3}$$

This equation gives us the values of $\Gamma_l(z)$. In figure 1 we show the values of Γ_l as a function of z, for l at the beginning and at the middle of the chain, for weak disorder and for a particular case of strong disorder.

Equation (4.3) can be obtained as an approximated solution of our exact formal expression given in equation (3.8). In fact this equation can be rewritten in

$$\langle\tilde{G}\rangle = \tilde{G}^0 + (\langle J\eta\rangle + \langle J\eta(1-\mathcal{P})J\eta\rangle + \langle J\eta(1-\mathcal{P})J\eta(1-\mathcal{P})J\eta\rangle + \cdots)\langle\tilde{G}\rangle. \tag{4.4}$$

Since η is already diagonal, if we neglect off-diagonal of the matrix J, i.e. if we take $J_{lj} \sim \delta_{lj}J_{ll}$, equation (4.4) leads us to

$$\begin{aligned}\langle\tilde{G}_{lj}\rangle \sim \tilde{G}^0_{lj} &+ (\langle J_{ll}\eta_l\rangle + \langle J_{ll}\eta_l(1-\mathcal{P})J_{ll}\eta_l\rangle \\ &+ \langle J_{ll}\eta_l(1-\mathcal{P})J_{ll}\eta_l(1-\mathcal{P})J_{ll}\eta_l\rangle + \cdots)\langle\tilde{G}_{lj}\rangle.\end{aligned} \tag{4.5}$$

For a fixed value of the index l the expression inside the bracket can be arranged in the form

$$\left\langle\frac{J_{ll}\eta_l}{1 - J_{ll}\eta_l}\right\rangle \frac{1}{1 + \langle\frac{J_{ll}\eta_l}{1 - J_{ll}\eta_l}\rangle}. \tag{4.6}$$

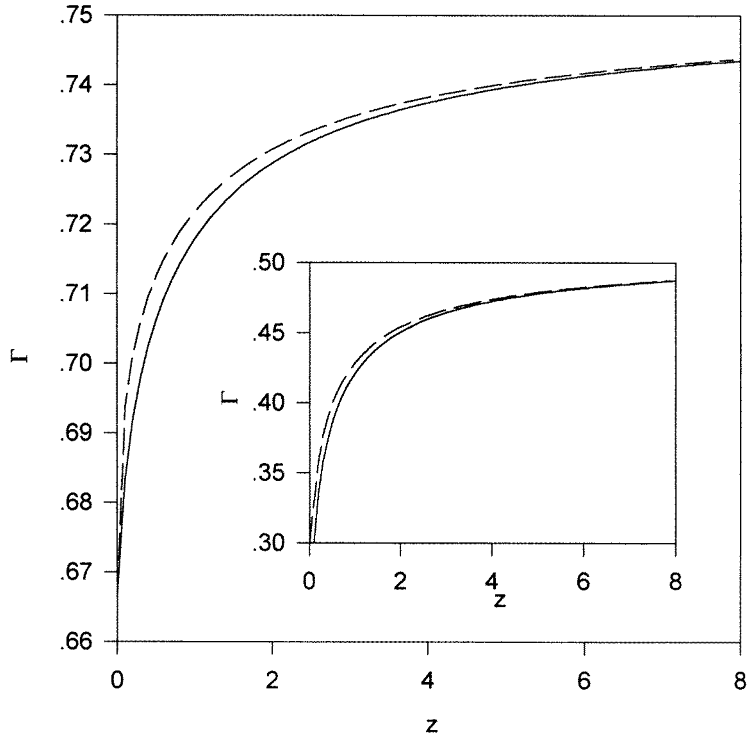

Figure 1. Graphs of the effective hopping transition $\Gamma(z, l)$ for $l = 1$ and $l = 15$ for a lattice with $N = 30$ and for weak disorder. The inset shows the same function for strong disorder with the parameter that characterizes the disorder $\alpha = 0$.

Hence the requirement $\langle\tilde{G}_{lj}\rangle = \tilde{G}^0_{lj}$ leads to the condition

$$\left\langle \frac{J_{ll}\eta_l}{1 - J_{ll}\eta_l} \right\rangle = 0 \tag{4.7}$$

or equivalently

$$\left\langle \frac{1}{1 - J_{ll}\eta_l} \right\rangle = 1. \tag{4.8}$$

This equation coincides with equation (4.3) that gives the value of the jumping probability Γ_l in finite-effective-media-like approximation when the impurity is at site l. Note that with this value of Γ_l we will have that, in general, $\langle\tilde{G}_{rk}\rangle \neq \tilde{G}^0_{rk}$ for $r \neq l$.

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