

Microscopic Approach to Random Walks

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Abstract In the present paper the microscopic approach to random walk models is introduced. For any particular model it provides a rigorous way to derive the transport equations for the macroscopic density of walking particles. Although it is not more complicated than the standard random walk framework it has virtually no limitations with respect to the initial distribution of particles. As a consequence, the transport equations derived with this method almost automatically give answers to such important problems as aging and two point probability distribution.

Keywords Continuous time random walk model · Aging · Two-point probability function · Coupled random walks

1 Introduction

Random walk models are known almost to any scientist independent of his field of research. The random walk of drunk sailors is the microscopic model of the classical diffusion. The continuous time random walks (CTRW) [1–4] extended our knowledge into the field of anomalous diffusion, connected to the fractional diffusion equations (FDE) and generalized the central limit theorem [5–7]. The fractional diffusion equations are now applied for description of a wide variety of phenomena in physics, biology and finance [8–12]. Usually one uses them as the classical diffusion equation without getting into the details of their derivation. However, when more delicate and particular questions require an answer, the whole derivation of corresponding transport equations has to be done from the very beginning. There are several types of such problems. The first one is the aging in anomalously slow evolving subdiffusive systems. Its physical examples are glasses, granular and colloidal systems, transport in random environments [13–18]. Several papers were devoted to the detailed study of this process [19–23]. Another nontrivial and very recent work is related to the analysis of the two-point probability distribution of random walks important for the analysis

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of the real experimental data. Multi-point correlation functions can be measured experimentally and provide indispensable information on the underlying stochastic process which could not be recovered from a single point data. Two independent methods were suggested to address this problem [24, 25].

In this article we demonstrate that after the exact and general transport equation for a random walk model is derived, the solution of the above mentioned problems of aging and two-point distributions follows automatically. That gives a clear and complete understanding of their nature.

The structure of the paper is as follows. We first introduce the standard continuous time random walk model. On its basis we show how the macroscopic transport equations are derived by using microscopic distributions. Then, these general transport equations are applied to the problem of aging and the two-point probability distribution. We discuss the results in the concluding section.

2 Standard CTRW Model

First we describe the standard CTRW [1–4] setup. Although the analysis below is one-dimensional, its generalization to higher dimensions is quite straightforward. Consider a particle or an ensemble of independent particles performing jumps which are alternated by some waiting periods. The distribution of jump lengths is governed by the probability density function $g(x)$ and the distribution of waiting times by $\psi(\tau)$. We assume that the waiting times are independent of the jump lengths (decoupled) and both are independent of the particle's position and current time. PDFs g and ψ characterize the random walk system and determine its asymptotic properties. Our goal now is to derive the transport equation for the macroscopic density of particles $n(x, t)$. The time evolution is of course determined by the initial distribution of particles. However, before defining the initial condition in the most general form a short comment is necessary. Consider some point on a line where the particles perform their random walk. At any given moment of time there are particles which arrived at this point some time before. Note that for each particle this time can be different. As a consequence, the time, when a particle leaves this point, is also different. Therefore, the outgoing flow of particles from a given point in general can not be described just by the total number of particles in this point. This observation motivates us to introduce the microscopic distribution of particles with respect to the times they spent in a given point until the observation time: $N(x, t, \tau)$. The quantity N defines how many particles in the point x at the moment of time t have arrived there time τ ago (i.e. at the time $t - \tau$). We will also call the time τ the "life time" of the particle in a given point. The total number of particles in the given point is obviously given by the integral of N over all possible life times [26]:

$$n(x, t) = \int_0^{\infty} N(x, t, \tau) d\tau. \quad (1)$$

Note the infinite limit of integration. If the system of particles was created at $t = 0$, the upper limit should be set to the current observation time t . We, however, will keep the infinity for the sake of generality. Now we are in a shape to define the most general initial condition for the system of walking particles. Assume that when the observation is started ($t = 0$) the particles have some distribution of life times $N_0(x, \tau)$. The corresponding macroscopic initial condition is given by:

$$n_0(x) = \int_0^\infty N_0(x, \tau) d\tau. \tag{2}$$

This initial distribution could be artificially created or could be a result of the previous evolution, for example. The simplest initial condition for the system created at $t = 0$ would be $N_0(x, \tau) = n_0(x)\delta_+(\tau)$. We continue, however, with a general form.

For the following computations we will need an expression for the survival probability, i.e. the probability not to make a jump before the time t , $\Psi(t)$. It is easily expressed as: $\Psi(t) = 1 - \int_0^t \psi(\tau) d\tau$. We have already mentioned the flow of particles from a given point, $Q(x, t)$, which shows how many particles leave a certain point per unit of time. It was first introduced in [26], and is given by the following conditional probability formula (probability for a particle to jump away after a waiting time τ provided that it has survived this time in the given point) [26, 27]:

$$Q(x, t) = \int_0^\infty \frac{N(x, t, \tau)\psi(\tau)}{\Psi(\tau)} d\tau. \tag{3}$$

The crucial point here is that the outgoing flow of particles is not simply proportional to the total number of particles in a given point. It depends on the microscopic distribution N . The only exception is the exponential waiting time: $\psi(\tau) = (1/\tau_0)\exp(-\tau/\tau_0)$. In this case $\psi \propto \Psi$. They just cancel out each other in the above integral and flow becomes proportional to the number of particles.

By using the expression for the outgoing flow of particles, we can write down the balance equations. Before doing so, it is convenient to separate the microscopic density into two parts. The first one, N_1 , represents particles which survived from the initial distribution $N_0(x, \tau)$ (for such particles $\tau \geq t$). The second one, N_2 , is formed by the evolution of random walks (for them $\tau < t$). By using again the conditional probability formula we can write [28]

$$N_1(x, t, \tau) = \frac{N_0(x, \tau - t)\Psi(\tau)}{\Psi(\tau - t)}, \quad \tau \geq t. \tag{4}$$

For N_2 we use the balance equation. All such particles were created as a result of outgoing flow of particles from all other points in the past. This flow is weighted by the probability to make a jump of a current length and by the probability to stay in a point after the arrival.

$$N_2(x, t, \tau) = \int_{-\infty}^{+\infty} g(x')\Psi(\tau)Q(x - x', t - \tau)dx', \quad \tau < t. \tag{5}$$

Now we can have a look on the expression for the outgoing flow. Substituting $N = N_1 + N_2$ in (3) and using (4,5) we have:

$$\begin{aligned} Q(x, t) &= \int_t^\infty \frac{N_1(x, t, \tau_1)\psi(\tau_1)}{\Psi(\tau_1)} d\tau_1 + \int_0^t \frac{N_2(x, t, \tau_1)\psi(\tau_1)}{\Psi(\tau_1)} d\tau_1 \\ &= \int_t^\infty \frac{N_0(x, \tau_1 - t)\psi(\tau_1)}{\Psi(\tau_1 - t)} d\tau_1 \\ &\quad + \int_{-\infty}^{+\infty} g(x') \int_0^t \psi(\tau_1)Q(x - x', t - \tau_1)dx' d\tau_1. \end{aligned} \tag{6}$$

The second term has a convolution form and represents the random walks evolution of particles. The first one is a source term. It depends explicitly on the history of particles at $t = 0$ which is included into the initial distribution over the lifetimes, $N_0(x, \tau)$.

Now we can solve (6) with a help of Fourier-Laplace transform. Indexes k and p denote Fourier and Laplace components respectively.

$$Q_{k,p} = \frac{\left(\int_t^\infty \frac{N_{0,k}(\tau_1-t)\psi(\tau_1)}{\Psi(\tau_1-t)} d\tau_1\right)_p}{1 - \psi_p g_k}.$$

Expression for N_2 immediately follows from (5): $N_{2,k,p} = g_k e^{-p\tau} \Psi(\tau) Q_{k,p}$.

Macroscopic density of particles is given by the integral of N with respect to τ and is composed of two components $n = n_1 + n_2$

$$n_1(x, t) = \int_t^\infty N_1(x, t, \tau) d\tau, \quad n_2(x, t) = \int_0^t N_2(x, t, \tau) d\tau.$$

After combining all these results and simple arithmetics, we obtain the Fourier-Laplace transform of the macroscopic density of particles with arbitrary initial distribution over the lifetimes:

$$n_{k,p} = \frac{\Psi_p n_{0,k}}{1 - \psi_p g_k} + \frac{1 - g_k}{1 - \psi_p g_k} \int_0^\infty N_{0,k}(\tau) \left(\frac{\Psi(\tau + t)}{\Psi(\tau)} - \Psi(t) \right)_p d\tau. \tag{7}$$

Here $n_0(x)$ is the macroscopic initial condition, $n_0(x) = \int_0^\infty N_0(x, \tau) d\tau$. There are now two terms. The first one gives the standard answer for the CTRW model. The second one is responsible for the influence of the initial distribution over the lifetimes. If all particles were created at $t = 0$, then $N_0(\tau) = n_0(x)\delta_+(\tau)$ and this term vanishes. It also vanishes, if ψ is exponential, as we mentioned before. Then we have the common expression for the Green's function of the CTRW model [4, 26]:

$$n_{k,p} = \frac{\Psi_p n_{0,k}}{1 - \psi_p g_k}. \tag{8}$$

The general form of (7) does not contain any assumptions about initial conditions or any other simplifying steps. It is exact. It is well known that the asymptotic form of the (8) for the subdiffusion regime can be written in terms of the fractional diffusion equation with fractional derivative with respect to time. It is also known that the solutions of this asymptotic equation do not possess the semi-group property. Since (7) contains the whole pre-history in its source term, it preserves the semi-group property of its solutions. With this general transport equation (7) we are able to address the problems of aging and two-point correlation functions.

3 Aging

In a broad sense the aging can be understood as the dependence of the measurement results on the age of the system. Assume that the system was prepared a time t_1 (aging time) ago. The first measurement was performed after this time elapsed, at $t = 0$. We would like to

know how the evolution of the system for times $t > 0$ depends on the aging time t_1 . It is quite clear that for exponential waiting time distribution there is no memory at all. However, for subdiffusive systems (when the mean waiting time is infinite) the effect of the previous evolution is dramatic. The reason of the aging effect is a nontrivial distribution of lifetimes at the moment of the first measurement. It is determined by the previous evolution during the aging time (source term of (7)). The longer is the aging time, the slower is the dynamic of N_1 —particles of the initial distribution which remain sitting. Only in the course of time the dynamics becomes dominated by walking particles described by N_2 and leads to the expected scaling of diffusion.

In order to solve the aging problem, we need to find the distribution of life times resulted from the previous evolution during the aging time t_1 . The following steps are technical and describe how to reconstruct $N(x, t = t_1, \tau)$ by knowing $n(x, t_1)$ and t_1 . We will reuse these calculations for the next section of the two-point probability distribution.

First we need to reconstruct the initial distribution of particles at $t = -t_1$, when the system was created. It is possible due to the following property of the Green’s function. The solution at any moment of time is given by the convolution of the initial distribution and the Green’s function. Therefore, after Fourier transform we obtain:

$$n_k(t_1) = G_k(t_1)\tilde{n}_{0,k}.$$

Here $G(x, t)$ is the Green’s function given by (8) and $\tilde{n}_{0,k}$ is the distribution of particles at preparation. From the above expression we easily find $\tilde{n}_0(x)$. Since we can reconstruct $\tilde{n}_0(x)$ anyway, let us for simplicity of the following calculations assume $\tilde{n}_0(x) = \delta(x)$.

When the system was created, we had $N_0(x, \tau) = \delta(x)\delta_+(\tau)$. Therefore the microscopic density $N(x, t, \tau)$ can be written as (see (4,5)):

$$\begin{aligned} N(x, t, \tau) &= \Psi(\tau)\delta(t - \tau)\delta(x) \\ &\quad + \int_{-\infty}^{+\infty} g(x')\Psi(\tau)Q(x - x', t - \tau)dx' \\ &\equiv \Psi(\tau)B(x, t - \tau), \end{aligned} \tag{9}$$

where $B(x, t)$ is some unknown function. We now set $t = t_1$. By using the fact that $n(x, t_1) = \int_0^{t_1} N(x, t_1, \tau)d\tau$ and (9) we find:

$$n(x)_s = \left(\int_0^{t_1} \Psi(\tau)B(x, t_1 - \tau)d\tau \right)_s,$$

where index s denotes the Laplace transform with respect to t_1 . By using the property of the Laplace transform of the convolution integrals we are able to find $B_s(x)$:

$$B_s = n_s/\Psi_s.$$

By applying the Laplace transform to (9) we find the expression for the Laplace transform of $N(x, t = t_1, \tau)$:

$$N_s(\tau) = \Psi(\tau)e^{-s\tau}B_s = \Psi(\tau)e^{-s\tau}(n_s/\Psi_s).$$

For the $n_s(x)$ we can use the Green’s function answer (8) with $n_{0,k} \equiv 1$, so in the final form:

$$N_{s,k}(\tau) = \frac{\Psi(\tau)e^{-s\tau}}{1 - \psi_s g_k}, \tag{10}$$

where k is the Fourier transform with respect to x . Now we are ready to write down the final answer for the aging diffusion:

$$n_{k,s,p} = \frac{\Psi_p \Psi_s}{(1 - \psi_p g_k)(1 - \psi_s g_k)} + \frac{1 - g_k}{1 - \psi_p g_k} \frac{1}{1 - \psi_s g_k} ([\Psi(t_1 + t)]_{p,s} - \Psi_p \Psi_s). \tag{11}$$

It is easy to check that the above equation gives the right expression for the density of particles at the moment of time $t + t_1$. If we start from a delta function at the preparation of the system, obviously its density at $t + t_1$ will be given by the Green's function $G(x, t + t_1)$ (8). One has to apply the double Laplace transform and compare it with (11). The following formula for the double Laplace transform can be used:

$$[f(t + t_1)]_{s,p} = \frac{f_s - f_p}{p - s}.$$

It can be shown that both expressions coincide. Note that in [21] a different solution of aging (sub)diffusion equation was obtained. The details of this difference are discussed in [29]. In our setup the whole distribution at the first measurement is assumed to be known. It allows to reconstruct the microscopic distribution over the life times and therefore the source term in (7) completely. It means also that the probability distribution of times, when a first jump after the beginning of the observation occurs, is different from $\psi(\tau)$ and explicitly depends on the position of a particle. In [21] the probability of the first jump after the aging time is uniform with respect to the coordinate and depends only on the aging time.

Let us briefly discuss the properties of the (11). It is evident that if the aging time, t_1 , is zero, (11) turns to the standard transport equation of the CTRW model [4]. This is also the case for the exponential waiting time distribution function $\psi(\tau)$. For any other $\psi(\tau)$ the source term is not zero. The most pronounced effect of aging can be seen for the subdiffusive regime, i.e. for those $\psi(\tau)$ which have infinite mean waiting time $\langle \tau \rangle$. A usual form for the waiting time PDF with an infinite mean is a power law:

$$\psi(\tau) = \frac{\gamma}{(1 + t)^{1+\gamma}}, \tag{12}$$

with $0 < \gamma < 1$. For this example we show how to work with the general answer (11). We will be interested in the asymptotic properties of the solution. It means that large temporal and spatial scales, $x, t \gg 1$, are considered. In Fourier-Laplace space that corresponds to the small values of k and p . We will also assume that the aging time is large $t_1 \gg 1$ ($s \ll 1$). For the distribution of jump lengths we chose such a function, that the mean square of the jump length is finite. For small k, p , and s instead of the full Fourier and Laplace transforms we can take their expansions. For the waiting time distribution (12) it has the form: $\psi_p = 1 - \Gamma(1 - \gamma)p^\gamma + O(p)$. For the symmetric jump lengths distribution with mean square $\langle x^2 \rangle$ the expansion is: $g_k = 1 - \langle x^2 \rangle k^2 / 2 + O(k^4)$. By substituting these expansions into the general formula (11) we get the asymptotic answer in Fourier Laplace space for the density of particles. Its back transform in real time/space can be represented in the integral form and is quite involved. It allows however to see that the density is non-negative and normalized, as it should be. Here we just give the answer for the temporal behavior of the mean square

displacement. It can be computed without explicit knowledge of the density by the formula

$$\langle x^2(t) \rangle = \int_{-\infty}^{+\infty} x^2 n(x, t) dx = -(d^2/dk^2)n_k(t)|_{k=0}.$$

In real time for large t and t_1 we get the following asymptotic behavior (cf. [21]):

$$\langle x^2(t, t_1) \rangle = \frac{\langle x^2 \rangle}{\Gamma(1 + \gamma)\Gamma(1 - \gamma)} [(t + t_1)^\gamma - t_1^\gamma]. \tag{13}$$

Here the aging effect is clearly seen. Only for $t_1 = 0$ mean square displacement follows the expected subdiffusive scaling t^γ . For any other $t_1 > 0$ the dynamics is slower and only asymptotically tends to the scaling regime. This effect can be qualitatively explained as follows. In the subdiffusive regime the frequency of jumps decays with time. It is easy to check that the flow of particles from all points $\int_{-\infty}^{+\infty} Q(x, t) dx$ decays as $t^{-1+\gamma}$. It means that for a longer aging time, longer time is required before a particle will make the first jump after the observation has started. It corresponds to the slower dynamics of the mean square displacement. Only for $t \gg t_1$ the self-similar profile of subdiffusion starts to dominate.

To conclude this section, we have shown that the general equation taking into account the microscopic details of random walks is applicable to the problem of aging. It shows that the microscopic distribution of particles other their life times is responsible for the aging effect. Now we turn to the closely related problem of the two point probability distribution in random walks.

4 Two-Point Probability Distribution

There are two recent papers considering the two-point probability distributions in CTRW models. In the first one, by Baule and Friedrich [24], the fractional diffusion equation for the two-point PDF was derived from the basic Langevin equation for the Brownian particle. In the second paper of Barkai and Sokolov [25], probabilistic approach was used for the CTRW model. Both papers reproduce the same result for the two-point PDF. It should be stressed that in our case this answer immediately follows from the general transport equation.

Let us specify the problem we are aiming to solve. Assume that a particle has started at the moment of time $t = 0$ from the point $x = 0$. We let the particle perform its random walk during the time t_1 and then measure its coordinate $x = x_1$. After letting it to evolve for another $t' > 0$, at the time $t_2 = t_1 + t'$ we measure its second position: $x = x_2$. The goal now is to obtain the joint probability distribution function of finding a walker at x_1 at time t_1 and at x_2 at time t_2 , *provided it has started at zero*:

$$p(x_1, t_1; x_2, t_2|0, 0). \tag{14}$$

The same quantity was calculated in [24, 25].

In this section we are going to apply (7) to this particular setup and find the above two-point PDF (14).

In order to obtain the PDF for the two-point distribution it is now sufficient to choose the initial data properly. We have two times: t_1 and t_2 . The point t_1 will serve as the initial condition for (7). Namely, after starting at zero (without any history) we are able to calculate the probability of finding the particle in $x = x_1$ at $t = t_1$, $n(x_1, t_1)$ by using the simple answer with the Green's function (8). This we will take as $n_0(x)$. In order to predict the following

evolution during the time t' , we need to know the distribution over the life times in the point $x = x_1$ at $t = t_1$, $N(x = x_1, t = t_1, \tau)$, which we will use instead of $N_0(x, \tau)$. The time t_1 we also take as the upper limit of the integration in (7). Now we find $N(x = x_1, t = t_1, \tau)$. Actually, the answer was already calculated for the aging problem, so we just reuse it:

$$N_{s,k_1}(\tau) = \frac{\Psi(\tau)e^{-s\tau}}{1 - \psi_s g_{k_1}}, \tag{15}$$

where k_1 denotes the Fourier transform with respect to x_1 . We note that $p(x_1, t_1, x_2, t_2) = p(x_1, t_1, x_2, t_1 + t')$ depends on two space and time variables. By taking double Fourier and Laplace transforms of this expression we will obtain $p_{k_1, k_2, s, p}$, with the following correspondence of variables: $t_1 \leftrightarrow s, t' \leftrightarrow p, x_1 \leftrightarrow k_1, x_2 \leftrightarrow k_2$. By substituting the above (15) into (7) and taking the double Laplace and Fourier transform we obtain:

$$p_{k_1, k_2, s, p} = \frac{\Psi_p \Psi_s}{(1 - \psi_p g_{k_2})(1 - \psi_s g_{k_1})} + \frac{1 - g_{k_2}}{1 - \psi_p g_{k_2}} \frac{1}{1 - \psi_s g_{k_1}} ([\Psi(t_1 + t')]_{p,s} - \Psi_p \Psi_s). \tag{16}$$

The answer (16) represents the Fourier-Laplace transform of the two-point probability density. It can be checked that it coincides with (23) in [25] (the following relation in the Laplace space might be helpful for these calculations: $\Psi_p = (1 - \psi_p)/p$) and (20) in [24]. The calculations of corresponding moments and quantities of interest are of course the same as in [24, 25].

5 Discussion and Conclusions

In the present paper, an additional step in the microscopic description of random walks was made. It has allowed us to derive more general transport equations which involve the distributions of particles over their lifetimes. Such a description provides exact and complete picture of the random walk dynamics. It was shown that the general transport equation successfully described aging phenomena and two-point probability distribution. We argue that the microscopic approach should be used for the derivation of macroscopic transport equations each time when a new model or setup is considered. One of the additional examples is the random walk model with a coupled transition kernel, when the jump lengths and waiting times are correlated with each other [30]. It should be noted that the above approach was applied to the standard CTRW model with instantaneous jumps between the trapping points. There exist however a generalized model taking into account the finite velocity of particles during their motion from one resting point to another [31–33]. Even more general model of multistage random walks assumes that a particle can undergo a complicated stochastic process for a random time until it is trapped again [34]. In these models particles could be divided into two groups: trapped in a given point and passing through this point. Therefore, not only the microscopic distribution of sitting particles but also the pre-history of flying particles determines the following evolution. A possible influence of the initial distribution of flying particles was only mentioned in [27] and definitely should be studied in greater detail in the future.

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