Diffusion in Presence of External Anomalous Noise

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(Received 7 January 1988)

We present a theory to study external non-Markovian noise in diffusion processes by using the multistate continuous-time random walk. We show that if the external noise is anomalous the effective Green's function of the walker has no long-time tails. We study the internal fluctuations in presence of non-Markovian noise.

PACS numbers: 05.40.+j, 02.50.+s

Recently there has been considerable interest in various aspects of dynamic disorder such as diffusive transport on a spatially and dynamically disordered lattice,[1] diffusion-influenced reactions where the reactivity of the species fluctuates in time,[2] and external fluctuations in master equations.[3,4] The starting point of the above references is a master equation (ME) with dynamically disordered transition rates. In Refs. 1 and 2 the Liouville master-equation approach has been used[5,6]; in the work of Sancho and co-workers,[3,4] on the other hand, the functional calculus was employed.[7,8]

The continuous-time random-walk (CTRW) theory is found to be an attractive approach to tackle these problems.[9,10] In this Letter we study a CTRW in presence of dynamical disorder, generalizing the external noise to a non-Markovian stochastic process. This situation cannot be straightforwardly analyzed neither starting from the Liouville master equation nor by use of functional calculus techniques.

Assuming the noise to be a two-level non-Markovian process we can represent the situation as a CTRW with two internal states.[11] The transition matrix characterizing the diffusion process in presence of an external non-Markovian dichotomic noise in the multistate CTRW theory must be written as

$$\psi(s,s';t)=\begin{vmatrix} M_{11}(s,s';t)\phi_{11}(t) & M_{12}(s;t)f_{12}(t) \\ M_{21}(s;t)f_{21}(t) & M_{22}(s,s';t)\phi_{22}(t)\end{vmatrix}, \tag{1a}$$

$$M_{11}(s,s';t)=B_1(s,s')\exp[-\textstyle\sum_{s''}B_1(s'',s')t],$$

$$M_{22}(s,s';t)=B_2(s,s')\exp[-\textstyle\sum_{s''}B_2(s'',s')t],$$

$$M_{21}(s;t)=\exp[-\textstyle\sum_{s'}B_1(s',s)t], \tag{1b}$$

$$M_{12}(s;t)=\exp[-\textstyle\sum_{s'}B_2(s',s)t].$$

Here

$$M_{ii}(s,s',t)dt=B_i(s,s')\exp[-\textstyle\sum_{s''}B_i(s'',s')t]dt$$

is the probability that the walker ends its sojourn in s', after a time between t and $t+dt$ since it arrived in s', by means of a jump to s when the noise is in the state i $(i=1,2)$. $M_{ij}(s;t)$ $\langle i\neq j\rangle$ is the probability that the walker is still in the site s after a time t since it arrived at s, with the noise in the level j. $f_{ij}(t)\,dt$ is the probability that the noise being at the level j at $t=0$, it makes a transition to i at time between t and $t+dt$, and $\phi_{ii}(t)$ is the probability that the noise is still in the level i after a time t since it arrived at this level.

The structure of the transition matrix is due to the *external character of the noise:* Its elements are a product of a probability density and a probability; for example $f_{12}(t)$ is associated with the noise and $M_{12}(s;t)$ with the walker for a fixed noise value. Then the elements $\psi_{ij}(s,s';t)$ acquire the form of a probability density as is usual in the multistate CTRW theory.[11]

In this Letter we assume equal transition probabilities for the noise: $f_{21}(t)=f_{12}(t)=f(t)$. Then the probability that the noise remains fixed in the level i is $\phi_{ii}(t)=1-\int_0^t f(t')dt'=\phi(t)$.

In Eq. (1b) we have assumed that *for each fixed value of the noise* the walker is governed by a ME; this is the consequence of the exponential time dependence $\{B_i(s,s')\exp[-\sum_{s''}B_i(s'',s')t]\}$ for the walker's waiting time.

General framework.— The formal solution of the multistate CTRW problem [for translational-invariant transition matrix $\psi(s-s';t)$] is[11,12]

$$\tilde{\mathbf{P}}(k,u)=\tilde{\boldsymbol{\phi}}(u)[\mathbf{I}-\boldsymbol{\psi}(k,u)]^{-1}\mathbf{P}(k,t=0), \tag{2}$$

where Laplace $(t\to u)$ and Fourier $(s\to k)$ transforms have been used [we use the tilde to specify the Laplace transform of a function; the Fourier transform is characterized by the argument (k) of the function]; for example,

$$\tilde{\mathbf{P}}(k,u)=\sum_s l^{iks}\int_0^\infty l^{-ut}\mathbf{P}(s,t)dt. \quad (3)$$

Here $P_i(s,t)$ is the joint probability for the walker to be at site s *and* the noise in the state i at time t. The diagonal matrix $\tilde{\boldsymbol{\phi}}(u)$ is

$$\tilde{\phi}_{ij}(u)=\left[1-\sum_{l=1}^{2}\tilde{\psi}_{lj}(k=0,u)\right]u^{-1}\delta_{ij}. \quad (4)$$

The effective Green's function of the walker, averaged over the external noise, is

$$P(s,t)\equiv\sum_{i=1}^{2}P_i(s,t)=\mathcal{L}_u^{-1}\mathcal{F}_k^{-1}\left\{\sum_{ijl=1}^{2}\tilde{\phi}_{ij}(u)[\mathbf{I}-\tilde{\boldsymbol{\psi}}(k,u)]_{jl}^{-1}P_l(k,t=0)\right\}. \quad (5)$$

The Laplace and Fourier transform of the matrix Eq. (1a) is

$$\tilde{\boldsymbol{\psi}}(k,u)=\begin{vmatrix}B_1(k)\tilde{\phi}(u+B_1(k=0)) & \tilde{f}(u+B_2(k=0))\\ \tilde{f}(u+B_1(k=0)) & B_2(k)\tilde{\phi}(u+B_2(k=0))\end{vmatrix}, \quad (6a)$$

where

$$\tilde{\phi}(u+B_i(k=0))=\frac{1-\tilde{f}(u+B_i(k=0))}{u+B_i(k=0)}. \quad (6b)$$

The effective Green's function for the walker, in Fourier-Laplace representation, can be obtained from Eqs. (5) and (6). Its long-time behavior can be studied by analysis of the $u\to 0$ limit. We consider two different cases for the waiting-time density of the noise $f(t)$.

(I) $f(t)$ has finite first moment $\langle t_{\text{noise}}\rangle$. Then

$$\tilde{f}(u)\underset{u\to 0}{\sim}1-\langle t_{\text{noise}}\rangle u, \quad (7a)$$

which implies that

$$\tilde{f}(u+B_i(k=0))\underset{u\to 0}{\sim}a_{i0}+a_{i1}u, \quad (7b)$$

where

$$a_{i0}=1-B_i(k=0)\langle t_{\text{noise}}\rangle,\qquad a_{i1}=-\langle t_{\text{noise}}\rangle. \quad (7c)$$

(II) $f(t)$ has an infinite first moment (non-Markovian limit). Then

$$\tilde{f}(u)\underset{u\to 0}{\sim}1-\beta u^{\gamma};\ \ 0<\gamma<1, \quad (8a)$$

implying that

$$\tilde{f}(u+B_i(k=0))\underset{u\to 0}{\sim}b_{i0}+b_{i1}u, \quad (8b)$$

where

$$b_{i0}=1-\beta[B_i(k=0)]^{\gamma},\qquad b_{i1}=-\beta\gamma[B_i(k=0)]^{\gamma-1}. \quad (8c)$$

Note that $B_i(k=0)\neq 0$ as can be seen from Eq. (1b). This means that even if the noise is anomalous the effective random walk has no long-time tails.

The behavior of $\tilde{f}(u+B_i(k=0))$ in the limit $u\to 0$ is linear in u because of the shift of its argument in both (I) and (II). Then we write, in general,

$$\tilde{f}(u+B_i(k=0))\underset{u\to 0}{\sim}f_{i0}+f_{i1}u, \quad (9)$$

where $f_{i0}=a_{i0}$ (b_{i0}) and $f_{i1}=a_{i1}$ (b_{i1}) in cases (I) and (II), respectively.

The effective Green's function.—The effective Green's function of the walker (in the limit $u\to 0$) is obtained with Eq. (9) in expressions (6a) and (6b):

$$\tilde{P}(k,u)\underset{u\to 0}{\sim}\frac{D(k)}{E(k)u+F(k)}. \quad (10)$$

Here

$$D(k)=[B_1(k)+B_2(k)](f_{20}-1)(1-f_{10})+B_1(k)(1+f_{10})(1-f_{20})+B_2(k=0)(1+f_{20})(1-f_{10}), \quad (11a)$$

$$E(k)=2\{B_1(k)[B_2(k=0)f_{11}+f_{10}-1]+B_2(k)[B_1(k=0)f_{21}+f_{20}-1]+B_1(k)B_2(k)[f_{11}(f_{20}-1)+f_{21}(f_{10}-1)]$$
$$+[B_1(k=0)+B_2(k=0)](1-f_{10}f_{20})-B_1(k=0)B_2(k=0)(f_{10}f_{21}+f_{11}f_{20})\}, \quad (11b)$$

$$F(k)=2\{B_1(k)B_2(k=0)(f_{10}-1)+B_2(k)B_1(k=0)(f_{20}-1)+B_1(k)B_2(k)(f_{10}-1)(f_{20}-1)$$
$$+B_1(k=0)B_2(k=0)(1-f_{10}f_{20})\}. \quad (11c)$$

As initial conditions we have assumed that the walker's position is known precisely, and that the noise state is in equilibrium:

$$\mathbf{P}(s,t=0)=\delta_{s,0}\begin{pmatrix}1/2\\1/2\end{pmatrix}. \quad (12)$$

When the waiting time of the noise $[f(t)]$ and the statistics of the transition of the walker $[B_i(k)]$ are known, all terms in Eq. (10) can be found and the calculation of $P(s,t)$ is reduced to quadratures.

Remark.— We have presented a theory to take into account external non-Markovian noise in diffusion processes by means of the multistate CTRW. This approach allows us to conclude that even if the external noise has long-time tails the effective Green's function for the walker will not conduce to anomalous diffusion.

Particular example.— As an example we assume that the transition probability of a one-step ME becomes a random function of time because of the presence of an external noise. We represent the influence of the noise by adding a random function to the transition probability.

For each realization the noise-functional Markovian ME is

$$\partial R(s;t,[\xi(t)])/\partial t = \{[\exp(-\partial/\partial s)-1][q_0+q_1\xi(t)]+[\exp(\partial/\partial s)-1]p_0\}R(s;t;[\xi(t)]), \quad (13a)$$

where $R(s;t;[\xi(t)])$ is a functional of the noise realization $[\xi(t)]$. Here $\xi(t)$ is a two-state Markovian process which takes values $\pm\Delta$ and has correlation time λ^{-1}:

$$\langle\xi(t)\rangle_{\xi(t)}=0;\ \langle\xi(t)\xi(t')\rangle_{\xi(t)}=\Delta^2\exp[-\lambda\,|t-t'|\,] \quad (13b)$$

(the requirement of positivity of the transition probability implies that $q_0-q_1\Delta\geq 0$).

By setting $\xi(t)=\Delta$ and $\xi(t)=-\Delta$ in Eq. (13a) we can obtain the ME which governs the walker's evolution for each fixed value of the noise. The expressions for $B_1(s,s')\equiv B_\Delta(s,s')$ and $B_2(s,s')\equiv B_{-\Delta}(s,s')$ of Eq. (1b) (in Fourier representation) are

$$B_\Delta(k)=(q_0+q_1\Delta)l^{ik}+p_0l^{-ik},$$
$$B_{-\Delta}(k)=(q_0-q_1\Delta)l^{ik}+p_0l^{-ik}. \quad (14)$$

Using the fact that $\xi(t)$ is a two-level Markovian noise characterized by Eq. (13b) we can deduce the functions $f_{ij}(t)$ and $\phi_{ij}(t)$ of Eq. (1a):

$$f_{12}(t)=f_{21}(t)=(\lambda/2)\exp[-(\lambda/2)t],$$
$$\phi_{11}(t)=\phi_{22}(t)=\exp[-(\lambda/2)t]. \quad (15)$$

The transition matrix is obtained from Eqs. (14) and (15). If we restore the expression of $\tilde{\psi}_{ij}(k,u)$ in Eq. (5) the exact effective Green's function of the walker can be written as

$$\mathbf{P}(s,t)=\mathcal{L}_u^{-1}\mathcal{F}_k^{-1}\{\tilde{\mathbf{P}}_\Delta(k,u)+\tilde{\mathbf{P}}_{-\Delta}(k,u)\}. \quad (16)$$

This is in agreement with the results of Ref. 3 where the effective Green's function is found by averaging over the realization of the noise:

$$\mathbf{P}(s,t)=\langle\mathbf{R}(s;t;[\xi(t)])\rangle_{\xi(t)}. \quad (17)$$

The scheme presented in this Letter offers the possibility to study the influence of external non-Markovian noise in the internal fluctuations of the system, with use of a nonexponential (anomalous) waiting-time noise [case II Eq. (8a)]. The study of the thermodynamic limit will be published elsewhere.[13]

Discussion.—This approach can be straightforwardly generalized to the case of an n-level external noise. The evolution equation for the effective Green's function can be studied by generalization of the resolvent-matrix method[14]; the application of this technique to external noise is in progress.[15] Also the analysis of local dynamical disorder and simultaneous static and dynamical disorder will be subject of further work.

One of the authors (C.E.B.) deeply acknowledges the hospitality of Centro Atómico Bariloche where this work was done. This work has been partially supported by Grant NO. PID3012000/85 from Consejo National de Investigaciones Científicas y Técnicas, Argentina, and Grant No. PID746/86 from Consejo Provincial de Investigaciones Científicas y Technológicas, Córdoba, Argentina.

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