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Generalized Master Equation for Space-Time Coupled Continuous Time Random Walk *

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The generalized master equation for the space-time coupled continuous time random walk is derived analytically, in which the space-time coupling is considered through the correlated function $g(t) \sim t^{\gamma}$, $0 \le \gamma < 2$, and the probability density function $\omega(t)$ of a particle's waiting time t follows a power law form for large t: $\omega(t) \sim t^{-(1+\alpha)}$, $0 < \alpha < 1$. The results indicate that the expressions of the generalized master equation are determined by the correlation exponent γ and the long-tailed index α of the waiting time. Moreover, the diffusion results obtained from the generalized master equation are in accordance with the previous known results and the numerical simulation results.

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The continuous time random walk theory (CTRW) as one of the various methods to describe anomalous diffusion is now widely used to explain the anomalous transport phenomena in physical, biological, geological and economic systems, since it was introduced by Montroll *et al.*[1] and Weiss *et al.*,[2] see Refs. [3–6] and references therein. The CTRW model is based on the idea that the jump length and the waiting time of a walker between two successive jumps are drawn from a joint probability density function (PDF) $\psi(x,t)$.[4] The jump length PDF can be deduced from $\lambda(x) = \int_0^{\infty} dt\psi(x,t)$ and the waiting time PDF can be deduced from $\omega(t) = \int_{-\infty}^{\infty} dx\psi(x,t)$, respectively. Note that the PDF for a particle to be at x at t, denoted by $W(x,t)$, in the Fourier–Laplace space, is given by

$$W(k,s) = \frac{1-\omega(s)}{s}\frac{1}{1-\psi(k,s)}, \qquad (1)$$

where $\omega(s)$ is the Laplace form of $\omega(t)$, $\psi(k,s)$ and $W(k,s)$ are the Fourier–Laplace transforms of $\psi(x,t)$ and $W(x,t)$, respectively. If the jump length and waiting time are coupled, it is the coupled CTRW, the joint PDF is $\psi(x,t) = \lambda(x|t)\omega(t)$, where $\omega(t)$ is referred to as the PDF of waiting time, and $\lambda(x|t)$ denotes the conditional PDF relating jump length and waiting time. There have been several coupled CTRW approaches proposed including CTRW with correlated jump length,[7,8] CTRW with correlated waiting time,[7,9] and space-time coupled CTRW processes, such as the Lévy walk.[6,10,14–17]

Different from the Lévy walk, we proposed a space-time coupled CTRW model,[10–12] in which the jump length is correlated with waiting time through a correlated function $g(t) = C_{\gamma}t^{\gamma}$, $0 \le \gamma < 2$ is the correlation exponent, and C_{γ} is a constant with units $\mathrm{m}^2/\mathrm{s}^{\gamma}$. In this coupled model, the PDF of the waiting time follows a power law form: $\omega(t) \simeq C_0 t^{-(1+\alpha)}, 0 < \alpha < 1$, for long time limit $t \to \infty$. Here, a constant C_0 is defined by $C_0 = C/|\Gamma(-\alpha)|$ with a scale factor C, and the Laplace transform of $\omega(t)$ is $\omega(s) = 1 - Cs^{\alpha}$, $s \to 0$. The PDF of the conditional jump length is a Gaussian-like function:[13] $\lambda(x|t) = \frac{1}{\sqrt{2\pi g(t)}}\exp[-\frac{x^2}{2g(t)}]$, where $g(t)$ as the variance is a function of time instead of a given constant, and the joint PDF of a random particle is

$$\psi(x,t) = \lambda(x|t)\omega(t) = \frac{1}{\sqrt{2\pi g(t)}}\exp\Big[-\frac{x^2}{2g(t)}\Big]\omega(t). \qquad (2)$$

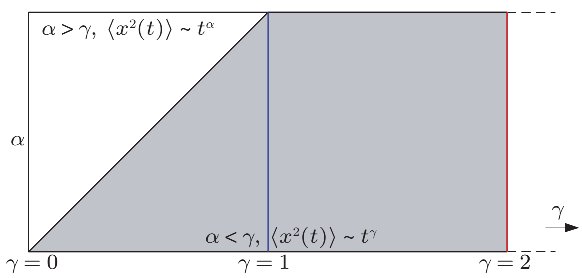

Fig. 1. (Color online) The white area shows the case $\alpha > \gamma$ and $\langle x^2(t)\rangle \sim t^{\alpha}$, the grey area shows the case $\alpha < \gamma$ and $\langle x^2(t)\rangle \sim t^{\gamma}$, the blue line denotes the case of $\gamma = 1$, which is normal diffusion, and the red line denotes the case of $\gamma = 2$, which is ballistic diffusion.

The diffusion result mean square displacement (MSD) for this coupled model can be deduced analytically,[10] the diffusive type and behavior are determined by the correlation exponent γ, the long-tailed index α of waiting time, and the competition between α and γ. The diffusion results are displayed in Fig. 1.

However, the generalized master equation (GME) for this coupled model is still unresolved; apparently, to understand the coupled CTRW model, it is meaningful to acquire the expression of the GME. Considering this, in this study, we are dedicated to deducing

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the GME for the coupled CTRW model; the results obtained in this study show that the diffusion results MSD $\langle x^2(t)\rangle$ can be directly deduced from the GME, which are in accordance with the previous known results.

The joint PDF Eq. (2) in the Fourier–Laplace space is

$$\begin{aligned}\psi(k,s) =& \mathscr{L}\{\exp[-\frac{1}{2}k^2 g(t)]\omega(t)\}\\ =& 1 - Cs^{\alpha} - \frac{1}{2}C_0 C_{\gamma} k^2 \mathscr{L}\{t^{-(1+\alpha-\gamma)}\}, \quad (3)\end{aligned}$$

Substituting Eq. (3) into Eq. (1), we have

$$W(k,s) = \frac{1}{s}\frac{1}{1+\frac{1}{2}C_{\gamma}\frac{1}{|\Gamma(-\alpha)|}k^2 s^{-\alpha}\mathscr{L}\{t^{-(1+\alpha-\gamma)}\}}. \quad (4)$$

From Eq. (4) we can see that the following calculation around Eq. (4) is determined by the calculation of the term $\mathscr{L}\{t^{-(1+\alpha-\gamma)}\}$. Considering $0 \le \gamma < 2$ and $0 < \alpha < 1$, the following calculation can be divided into two cases: the $\gamma \ge \alpha$ case and the $\gamma < \alpha$ case.

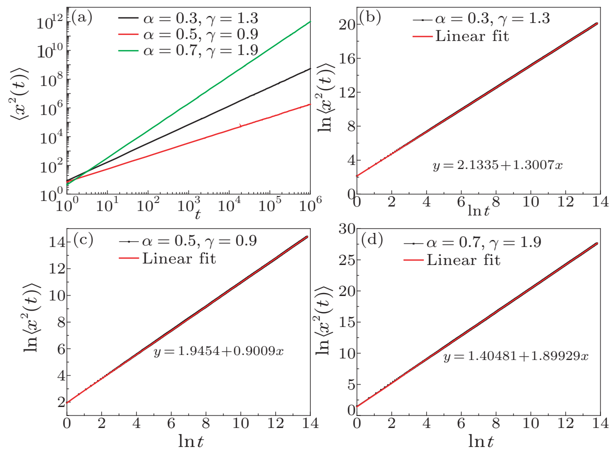

Fig. 2. (Color online) The MSD $\langle x^2(t)\rangle$ varying with time t for $\gamma > \alpha$ with three different cases: $\alpha = 0.5$, $\gamma = 1.3$; $\alpha = 0.5$, $\gamma = 0.9$; and $\alpha = 0.7$, $\gamma = 1.9$. The log-log plot of $\langle x^2(t)\rangle$ versus t corresponding to the three cases are displayed in (b)–(d), respectively.

For the case of $\gamma \ge \alpha$, the joint PDF in the Fourier–Laplace space Eq. (3) is

$$\begin{aligned}\psi(k,s) =& 1 - Cs^{\alpha} - \frac{1}{2}C_0 C_{\gamma} k^2 \mathscr{L}\{t^{-(1+\alpha-\gamma)}\}\\ =& 1 - Cs^{\alpha} - \frac{1}{2}C_0 C_{\gamma}\Gamma(\gamma-\alpha)k^2 s^{\alpha-\gamma}. \quad (5)\end{aligned}$$

Correspondingly, Eq. (4) turns into

$$W(k,s) = \frac{1}{s}\frac{1}{1+\frac{C_{\gamma}\Gamma(\gamma-\alpha)}{2|\Gamma(-\alpha)|}k^2 s^{-\gamma}}. \quad (6)$$

After the inverse Fourier–Laplace transform, then we obtain

$$\frac{\partial W(x,t)}{\partial t} = {}_0D_t^{1-\gamma}K_1\frac{\partial^2}{\partial x^2}W(x,t), \quad (7)$$

which is just the GME for the coupled CTRW model to describe the diffusive process for the $\gamma \ge \alpha$ case, ${}_0D_t^{1-\gamma}$ is the Riemann–Liouville operator, and $K_1 = \frac{C_{\gamma}\Gamma(\gamma-\alpha)}{2|\Gamma(-\alpha)|}$ is the diffusion coefficient. Apparently, from Eq. (7),

$$\langle x^2(t)\rangle = \frac{2K_1}{\Gamma(1+\gamma)}t^{\gamma} \quad (8)$$

can be directly deduced.[4] The numerical results of MSD varying with time for the $\gamma > \alpha$ case are displayed in Fig. 2, in which these three cases $\alpha = 0.5$, $\gamma = 1.3$; $\alpha = 0.5$, $\gamma = 0.9$; and $\alpha = 0.7$, $\gamma = 1.9$ chosen as the representation are considered, and the linear fitting slopes of the numerical results are 1.3007, 0.9009 and 1.89929, which are all in very good agreement with the expected values. The numerical results for the $\gamma = \alpha$ case is displayed in Fig. 3, in which $\gamma = \alpha = 0.5$ chosen as the representation is considered, the linear fitting slope of the numerical results is 0.52248, which is in very good agreement with the expected value. In this work, the numerical calculation is to simulate the continuous time random-walk trajectories directly, along with $N = 10^5$ test particles for the ensemble. We set the PDF of the waiting time as $\omega(t) = (10^{-3})^{\alpha}\alpha t^{-(1+\alpha)}(t \ge 10^{-3})$ in all the numerical simulations.

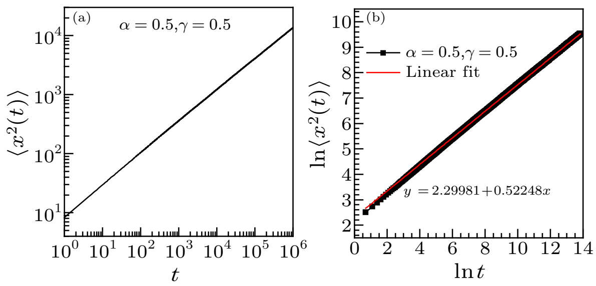

Fig. 3. (Color online) The MSD $\langle x^2(t)\rangle$ varying with time t for $\gamma = \alpha$ with $\alpha = 0.5$ and $\gamma = 0.5$. The log-log plot of $\langle x^2(t)\rangle$ versus t is displayed in the right.

A closed-form solution for Eq. (7) can be found in terms of the Fox functions,[4] and the results are

$$W(x,t) = \frac{1}{\sqrt{4\pi K_1 t^{\gamma}}}H_{1,2}^{2,0}\left[\frac{x^2}{4K_1 t^{\gamma}}\,\middle|\,\begin{matrix}(1-\gamma/2,\gamma)\\ ((0,1),(\frac{1}{2},1))\end{matrix}\right]. \quad (9)$$

For the case of $\gamma < \alpha$, $0 < \gamma < 1$ and $0 < \alpha < 1$ at the same time, thus $\alpha - \gamma + 1 > 1$, considering

$$\mathscr{L}\{C_0 t^{-(1+\alpha-\gamma)}\} = 1 - Cs^{\alpha-\gamma}, \quad (10)$$

where $C_0 = \frac{C}{|\Gamma(\gamma-\alpha)|}$. Thus we obtain

$$\mathscr{L}\{t^{-(1+\alpha-\gamma)}\} = \frac{|\Gamma(\gamma-\alpha)|}{C}(1 - Cs^{\alpha-\gamma}). \quad (11)$$

Then for the case of $\gamma < \alpha$, the joint PDF in Fourier–Laplace space Eq. (3) is

$$\psi(k,s) = 1 - Cs^{\alpha} - \frac{C_{\gamma}|\Gamma(\gamma-\alpha)|}{2|\Gamma(-\alpha)|}k^2(1 - Cs^{\alpha-\gamma}), \quad (12)$$

and

$$W(k,s) = \frac{1}{s}\frac{1}{1+\frac{C_\gamma|\Gamma(\gamma-\alpha)|}{2C|\Gamma(-\alpha)|}k^2(s^{-\alpha}-Cs^{-\gamma})}. \quad (13)$$

Now we introduce an intermediate variable $a=\alpha-\gamma$ and $0<a<1$ apparently, then we have

$$W(k,s) = \frac{1}{s}\frac{1}{1+\frac{C_\gamma|\Gamma(\gamma-\alpha)|}{2C|\Gamma(-\alpha)|}k^2 s^{-\gamma}(s^{-a}-C)}. \quad (14)$$

For $t\to\infty$, which is $s\to 0$ correspondingly, the term $s^{-a}-C\to s^{-a}$, therefore

$$W(k,s) = \frac{1}{s}\frac{1}{1+\frac{C_\gamma|\Gamma(\gamma-\alpha)|}{2C|\Gamma(-\alpha)|}k^2 s^{-\alpha}}. \quad (15)$$

After the inverse Fourier–Laplace transform, we obtain

$$\frac{\partial W(x,t)}{\partial t} = {}_0D_t{}^{1-\alpha}K_2\frac{\partial^2}{\partial x^2}W(x,t), \quad (16)$$

which is just the GME for the coupled CTRW model to describe the diffusive process for the $\gamma<\alpha$ case. Here $K_2=\frac{C_\gamma|\Gamma(\gamma-\alpha)|}{2C|\Gamma(-\alpha)|}$ is the diffusion coefficient. Apparently, from Eq. (16),

$$\langle x^2(t)\rangle = \frac{2K_2}{\Gamma(1+\alpha)}t^\alpha \quad (17)$$

can be directly deduced.[4] The numerical results of MSD varying with time for the $\gamma<\alpha$ case are displayed in Fig. 4, in which these three cases $\alpha=0.3$, $\gamma=0.1$; $\alpha=0.5$, $\gamma=0.3$; and $\alpha=0.7$, $\gamma=0.1$ chosen as the representation are considered, and the linear fitting slopes of the numerical results are 0.29971, 0.49958 and 0.6995, which are all in very good agreement with the expected values.

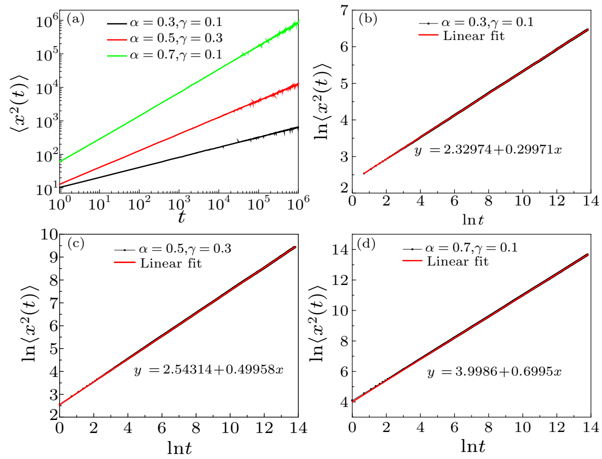

Fig. 4. (Color online) The MSD $\langle x^2(t)\rangle$ varying with time t for $\gamma<\alpha$ with three different cases: $\alpha=0.3$, $\gamma=0.1$; $\alpha=0.5$, $\gamma=0.3$; and $\alpha=0.7$, $\gamma=0.1$. The log-log plots of $\langle x^2(t)\rangle$ versus t corresponding to the three cases are displayed in (b)–(d), respectively.

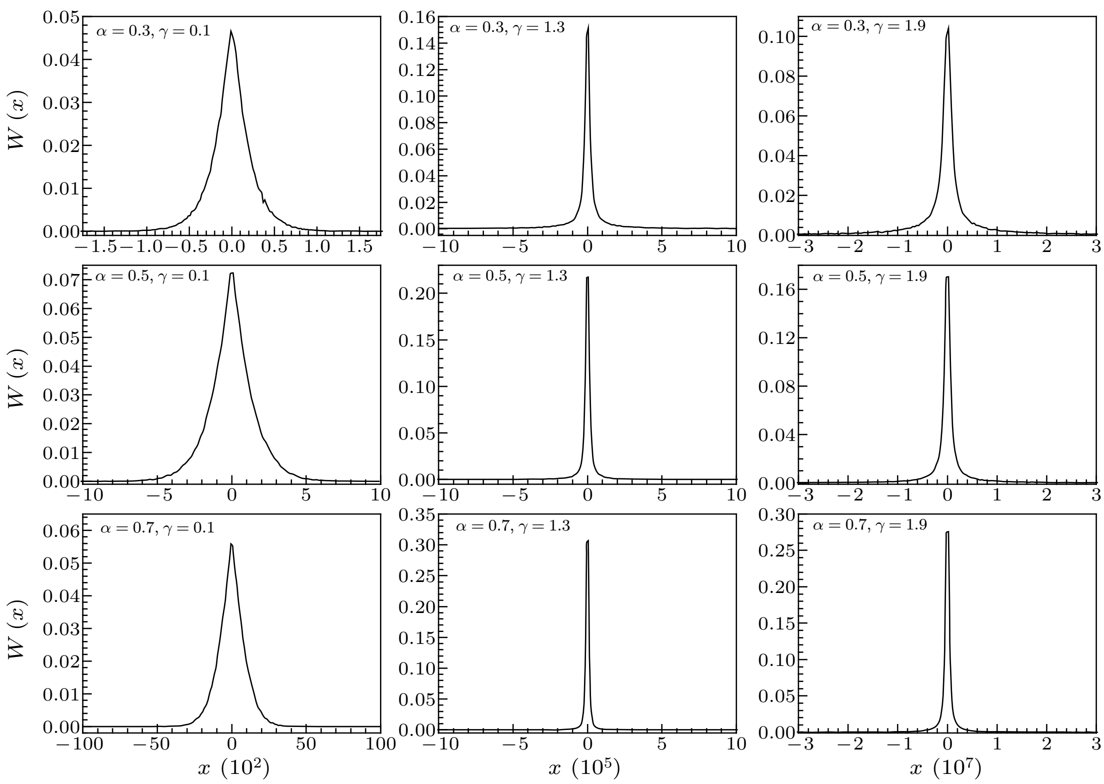

Fig. 5. (Color online) The value of $W(x,t)$ for the $\gamma\geq\alpha$ and $\gamma<\alpha$ cases with nine pairs of different α and γ at time $t=10^6$. The cusp shape of the $W(x,t)$ is distinct.

Again, a closed-form solution for Eq. (16) can be found in terms of Fox functions,[4] and the results are

$$W(x,t)=\frac{1}{\sqrt{4\pi K_2 t^{\alpha}}}H^{2,0}_{1,2}\left[\frac{x^2}{4K_2t^{\alpha}}\,\middle|\,\begin{matrix}(1-\alpha/2,\alpha)\\((0,1),(\frac{1}{2},1))\end{matrix}\right]. \tag{18}$$

Apparently, the diffusion results (8) and (17) deduced from the GME Eqs. (7) and (16) are in accordance with the known results by calculating the second partial derivation of the characteristic function.[10] Moreover, the solutions (9) and (18) to Eqs. (7) and (16) are expressed in terms of the Fox functions, which means that compared with the much smoother shape for the Brownian diffusion, the propagator $W(x,t)$ should display a pronounced cusp shape.[4] The numerical results of $W(x,t)$ for both the $\gamma \geq \alpha$ case and the $\gamma < \alpha$ case are displayed in Fig. 5, from which we can see that the distributions of $W(x,t)$ for different cases display cusp shapes as expected.

In summary, the GMEs for the space-time coupled CTRW have been derived analytically, and the concrete expressions of the GME have also been determined by the correlation exponent γ and the long-tailed index α of the waiting time. The diffusion results MSD can be directly acquired from the GME (Eqs. (8) and (17)), which are in accordance with the previous known results.[10] Furthermore, from the GME we can obtain that the propagator $W(x,t)$ will display a pronounced cusp shape instead of the smooth Gaussian shape.

References

[1] Montroll E W and Weiss G H 1965 *J. Math. Phys.* **6** 167
[2] Scher H and Montroll E W 1975 *Phys. Rev.* B **12** 2455
[3] Bouchaud J P and Georges A 1990 *Phys. Rep.* **195** 127
[4] Metzler R and Klafter J 2000 *Phys. Rep.* **339** 1
[5] Metzler R, Jeon J H, Cherstvy A G and Barkai E 2014 *Phys. Chem. Chem. Phys.* **16** 24128
[6] Zaburdaev V, Denisov S and Klafter J 2015 *Rev. Mod. Phys.* **87** 483
[7] Iyengar N et al 1996 *Am. J. Physiol.* **271** R1078
[8] Blumen A, Zumofen G and Klafter J 1989 *Phys. Rev.* A **40** 3964
[9] Meerschaert M M, Nane E and Xiao Y 2009 *Stat. Probab. Lett.* **79** 1194
[10] Liu J and Bao J D 2013 *Physica* A **392** 612
[11] Liu J and Bao J D 2013 *Chin. Phys. Lett.* **30** 020202
[12] Liu J et al 2016 *Acta Phys. Sin.* **65** 160502 (in Chinese)
[13] Klafter J and Sokolov I M 2011 *First Steps in Random Walks: From Tools to Applications* (Oxford: Oxford University Press)
[14] Shlesinger M F, Klafter J and Wong Y M 1982 *J. Stat. Phys.* **27** 499
[15] Shlesinger M F, West B J and Klafter J 1987 *Phys. Rev. Lett.* **58** 1100
[16] Klafter J, Blumen A and Shlesinger M F 1987 *Phys. Rev.* A **35** 3081
[17] Barkai E, Aghion E and Kessler D A 2014 *Phys. Rev.* X **4** 021036