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Continuous-time random walk: exact solutions for the probability density function and first two moments

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Abstract. We consider decoupled continuous time random walk model with finite characteristic waiting time and approximate jump length variance. We take the waiting time probability distribution given by a combination of exponential and Mittag-Leffler function. Using this waiting time probability distribution we investigate diffusion behaviors for all the time. We obtain exact solutions for the first two moments and probability distribution for force-free and linear force cases. Due to the finite characteristic waiting time and jump length variance the model presents, for the force-free case, normal diffusive behavior in the long-time limit. Further, the model can describe anomalous behavior at the intermediate times.

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1. Introduction

The continuous-time random walk (CTRW) model [1] was proved a useful tool for the description of systems out of equilibrium [2, 3]. In fact, the CTRW has been used in a wide range of applications such as earthquake modelling [4], random networks [5], self-organized criticality [6], electron tunneling [7], electron transport in nanocrystalline films [8] and financial stock market [9]. However, analyses of diffusion processes are often restricted to a long-time limit. On the other hand, informations about the initial and intermediate processes are important to distinguish different systems which may lead to the same behavior in the long-time limit. Despite some progress in simple CTRW has been made, more novel approaches need to be developed for the description of CTRW with generic waiting time probability density function (PDF) and external force. In the CTRW model, without external force, the PDF obeys the following equation in Fourier-Laplace space:

$$\rho_{ks}(k,s) = \frac{(1-g_s(s))\,\rho_{k0}(k)}{s\,(1-\psi_{ks}(k,s))}, \tag{1}$$

where $\rho_{k0}(k)$ is the Fourier transform of the initial condition $\rho_0(x)$, $\psi_{ks}(k,s)$ is the Fourier-Laplace transform of the jump PDF $\psi(x,t)$ and $g_s(s)$ is the Laplace transform of the waiting time PDF $g(t) = \int_{-\infty}^{\infty} \mathrm{d}x\psi(x,t)$. The CTRW can be simplified through the decoupled jump PDF $\psi_{ks}(k,s) = \varphi_k(k)g_s(s)$ in Fourier-Laplace space, where $\varphi(x) = \int_{-\infty}^{\infty} \mathrm{d}t\psi(x,t)$ is the jump length PDF. Under the case of finite jump length variance $\int_{-\infty}^{\infty} \mathrm{d}x x^2\varphi(x)$ [2], the PDF for CTRW can be given by

$$\rho_{ks}(k,s) = \frac{(1-g_s(s))\,\rho_{k0}(k)}{s\,(1-(1-Ck^2)\,g_s(s))} \tag{2}$$

in Laplace-Fourier space, where $\sqrt{C}$ has a dimension of length and $\rho_{k0}(k)$ is the Fourier transform of the initial condition $\rho_0(x)$. Although this equation is valid for a finite jump length variance, anomalous diffusion can be produced by it with appropriate choices of $g(t)$. However, this equation is not convenient to be used to study diffusion behavior in finite domains and/or in the presence of external forces. In particular, for a long-tailed power-law waiting time PDF $g(t) \sim (t/\tau)^{\alpha}$ the fractional diffusion equation can be used to study diffusion [2].

Recently, we have made progress in obtaining an integro-differential diffusion equation for the CTRW with any waiting time PDF and external force $F(x)$ [10, 11]:

$$\frac{\partial\rho(x,t)}{\partial t} - \int_0^t \mathrm{d}t_1\, g(t-t_1)\frac{\partial\rho(x,t_1)}{\partial t_1} = CL_{FP}\frac{\partial}{\partial t}\int_0^t \mathrm{d}t_1\, g(t-t_1)\,\rho(x,t_1), \tag{3}$$

where

$$L_{FP} = -\frac{\partial}{\partial x}\frac{F(x)}{k_BT} + \frac{\partial^2}{\partial x^2}, \tag{4}$$

k_B is the Boltzmann constant, and T is the absolute temperature. Some interesting results from (3) are also presented in [12, 13]. We note that equation (3) can also be obtained by the usage of the subordination process [14].

The aim of this work is to investigate the CTRW model with the waiting time PDF given by a combination of exponential and Mittag-Leffler function. It is well-known that the waiting time PDF, given by a pure exponential function, produces normal diffusion process for all the time. The above-mentioned waiting time PDF permits us to investigate the CTRW model with a combination of exponential and stretched exponential function at small times. In particular, we obtain analytical solutions for the first two moments and PDF for force-free and linear force cases. We show that the model describes, for force-free case, normal diffusion regimes at the small and large times, and anomalous diffusion regimes at the intermediate times; this means that the stretched exponential does not modify the normal diffusion process at small times.

2. Mean square displacement, first two moments and probability distribution

In this work we investigate the CTRW model described by equation (3), using the following waiting time PDF:

$$g(t) = \left(b + \lambda b^{1-\alpha}\right) e^{-bt} E_{\alpha,1}(-\lambda t^{\alpha}), 0 < \alpha \le 1, b > \lambda^{\frac{1}{\alpha}}, \tag{5}$$

where b and λ are positive constants and $E_{\mu,\nu}(y)$ is the generalized Mittag-Leffler function defined by [15] $E_{\mu,\nu}(y) = \sum_{n=0}^{\infty} y^n/\Gamma(\nu + \mu n)$, $\mu > 0$, $\nu > 0$. The waiting time PDF $g(t)$ interpolates approximately between the initial exponential form and intermediate power-law behavior, and with exponential behavior in the long-time limit; it is different from the functions employed in the previous works [10, 12, 13]. In those cases the functions are given by a combination of power-law and generalized Mittag-Leffler function $g_1(t) = \lambda t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^{\alpha})$, a sum of exponentials $g_2(t) = A \sum_{i=1}^{n} c_i e^{-a_i t}$ and a combination of power-law and exponential function $g_3(t) = d^{\gamma} t^{\gamma-1} e^{-dt}/\Gamma(\gamma)$, where $\Gamma(z)$ is the Gamma function; the first one has a power-law tail, then the system exhibits anomalous diffusion in the long-time limit, however, the second one contains multiple characteristic times and it may exhibit power-law behavior with logarithmic oscillation at the intermediate times and exponential behavior in the long-time limit. The third one has approximately initial and intermediate power-law behavior, then the system describes anomalous diffusion at the small and intermediate times, and it exhibits normal diffusion in the long-time limit. In the case of $g(t)$, it presents a finite characteristic waiting time given by $\int_0^{\infty} \mathrm{d}t\, t g(t) = [1 + \lambda(1-\alpha) b^{-\alpha}]/(b + \lambda b^{1-\alpha})$; this means that the system describes normal diffusion in the long-time limit.

The definition of the derivative of the q^{th} moment of PDF $\rho(x,t)$ with respect to t is:

$$\frac{\mathrm{d}\langle x^q \rangle}{\mathrm{d}t} = \int_{-\infty}^{\infty} x^q \frac{\partial \rho(x,t)}{\partial t} \mathrm{d}x, \tag{6}$$

where q is a positive integer number.

Force-free case. Substituting (3) into (6), we can obtain the first moment

$$\langle x(t) \rangle = \langle x(0) \rangle \tag{7}$$

and the derivative of the second moment with respect to t

$$\frac{d}{dt}\langle x^2(t)\rangle = \int_0^t g(t-t_1)\frac{d}{dt_1}\langle x^2(t_1)\rangle\, dt_1 + 2D\frac{\partial}{\partial t}\int_0^t g(t-t_1)\, dt_1 . \tag{8}$$

Equation (7) shows that the mean square displacement $\langle (x(t)-x(0))^2\rangle$ is identical to the variance $\langle (x(t)-\langle x(t)\rangle)^2\rangle$ with $\langle x(0)\rangle = x(0)$.

In order to obtain the mean square displacement we apply the Laplace transform to (8) and using

$$g_s(s) = \frac{b+\lambda b^{1-\alpha}}{(b+s)+\lambda(b+s)^{1-\alpha}}, \tag{9}$$

we obtain

$$s\langle \tilde{x}^2(s)\rangle_s - \langle x^2(0)\rangle = \frac{2C(b+\lambda b^{1-\alpha})}{(b+s)+\lambda(b+s)^{1-\alpha}-(b+\lambda b^{1-\alpha})}. \tag{10}$$

Now, using the binomial expansion to (10) yields

$$\langle (x(t)-x(0))^2\rangle = 2C\left(b+\lambda b^{1-\alpha}\right) \times \int_0^t e^{-bu}\sum_{n=0}^{\infty}\frac{[(b+\lambda b^{1-\alpha})u]^n}{n!}E^{(n)}_{\alpha,1+(1-\alpha)n}(-\lambda u^{\alpha})du, \tag{11}$$

where

$$E^{(n)}_{\mu,\nu}(y) = \frac{d^n}{dy^n}E_{\mu,\nu}(y) = \sum_{k=0}^{\infty}\frac{(n+k)!\,y^k}{k!\,\Gamma(\nu+\alpha(n+k))}. \tag{12}$$

It is noted that equation (11) shows a complicate form, but for $\alpha = 1$ the Mittag-Leffler function reduces to the exponential function, and the above result reduces to the one of normal diffusion from the ordinary diffusion equation or from the integro-differential diffusion equation (3) with the exponential waiting time PDF [10], $\langle x^2(t)\rangle = \langle x^2(0)\rangle + 2C(b+\lambda)t$. For short times the mean square displacement is given by

$$\langle (x(t)-x(0))^2\rangle \sim 2C\left(b+\lambda b^{1-\alpha}\right)t, \tag{13}$$

and for long times it yields

$$\langle (x(t)-x(0))^2\rangle \sim \frac{C\lambda\alpha(1-\alpha)(1+\lambda b^{-\alpha})}{b^{\alpha}[1+\lambda(1-\alpha)b^{-\alpha}]^2} + \frac{2C(b+\lambda b^{1-\alpha})}{1+\lambda(1-\alpha)b^{-\alpha}}t. \tag{14}$$

We see that the mean square displacement presents normal diffusive regime for short and large times. In general, the mean square displacement (11) begins with a normal diffusion regime, then it develops anomalous diffusion regime at the intermediate times, and eventually reaches a normal diffusion regime. These regimes can be viewed in figures 1 and 2. In these figures we also compare the analytical solution for the MSD (11) with the power-law function; the MSD is very close to a linear function.

Figure 1. Plots of $(x(t) - x(0))^2$ for $C = 1$, $b = 0.3$, $\lambda = 0.15$ and $\alpha = 0.5$. The solid line is obtained from (11). The dashed dotted and dashed lines are the asymptotic curves obtained from (13) and (14), respectively. The dotted line corresponds to the power-law function $0.1022t^{0.9415}$.

Figure 2. Plots of $(x(t) - x(0))^2$ for $C = 1$, $b = 0.03$, $\lambda = 0.05$ and $\alpha = 0.7$. The solid lines are obtained from (11). The dashed dotted and dashed lines are the asymptotic curves obtained from (13) and (14), respectively. The dotted line corresponds to the power-law function $0.0935t^{0.9715}$.

Now we consider the exact solution for the PDF $\rho(x, t)$. It can be obtained from [10]

$$\rho_s(x, s) = \frac{1}{2\sqrt{Cs}}\sqrt{\frac{1 - g_s(s)}{g_s(s)}} \exp\left(-\frac{|x|}{\sqrt{C}}\sqrt{\frac{1 - g_s(s)}{g_s(s)}}\right). \quad (15)$$

Substituting (9) into (15) yields

$$\rho(x, t) = \frac{1}{2\pi\sqrt{C(b + \lambda b^{1-\alpha})}} \int_0^\infty d\omega \Phi(\omega, x) \cos(\omega t + \theta(\omega, x)), \quad (16)$$

where

$$r_1(\omega) = \sqrt{\omega^2 + b^2}, \quad \theta_1(\omega) = \arccos\left(\frac{b}{r_1}\right), \quad (17)$$

$$r_2(\omega) = \lambda r_1^{1-\alpha}(\omega) \times \sqrt{\left(\cos((1 - \alpha)\theta_1(\omega)) - \frac{b^{1-\alpha}}{r_1^{1-\alpha}(\omega)}\right)^2 + \left(\sin((1 - \alpha)\theta_1(\omega)) + \frac{\omega b^{1-\alpha}}{\lambda r_1^{1-\alpha}(\omega)}\right)^2} \quad (18)$$

$$\theta_2(\omega) = \arccos\left(\frac{\lambda r_1^{1-\alpha} \quad \alpha}{r_2(\omega)}\right), \quad (19)$$

$$\Phi(\omega, x) = \frac{\sqrt{r_2(\omega)}}{\omega} e^{-\frac{|x|}{\sqrt{C(b+\lambda b^{1-\alpha})}}\sqrt{r_2(\omega)}\cos\frac{\theta_2(\omega)}{2}} \quad (20)$$

and

$$\theta(\omega, x) = \frac{\theta_2(\omega) - \pi}{2} - \frac{|x|}{\sqrt{C(b + \lambda b^{1-\alpha})}}\sqrt{r_2(\omega)} \sin\frac{\theta_2(\omega)}{2}. \quad (21)$$

The asymptotic expansion of $\rho(x, t)$ (for a given x and $t \gg 1$) is given by

$$\rho(x, t) \sim \frac{1}{2}\sqrt{\frac{1 + \lambda(1 - \alpha) b^{-\alpha}}{\pi C(b + \lambda b^{1-\alpha}) t}}. \quad (22)$$

Figure 3. Plots of $\rho(x, t)$ versus x coordinate with $C = 1$, $b = 0.03$, $\alpha = 0.5$, $\lambda = 0.15$, for the force-free case.

Equation (22) shows that the PDF $\rho(x, t)$ has a decay similar to $1/\sqrt{t}$ of the normal diffusion, and independently of the spatial coordinate. This is not a surprise because the waiting time PDF (5) has a finite characteristic waiting time.

Now we show the PDF $\rho(x, t)$ versus x coordinate for different times. In figure 3a, the PDF presents a cusp for $t = 9$ which is a hallmark of the CTRW model for anomalous diffusion process in x coordinate; however, the PDF shows a smooth shape for $t = 35$ due to the fact that the system describes normal regime for large times. In figure 3b, the PDF presents a smooth shape due to the normal diffusion regime for short times. It is worth mentioning that equation (16) is difficult to compute numerically for small values of x. In this case we have checked our numerical results obtained from (16) with those of a numerical inversion of Laplace transform algorithm [16]. Both results are similar, except at the short distance.

Linear force. We now study the case of a linear force $F(x) = -m\omega^2 x$ with the waiting time PDF (5). We first obtain the PDF $\rho(x, t)$; it can be obtained from (3). In order to do so, we employ the method of separation of variables $\rho_n(x, t) = X_n(x)T_n(t)$; substituting it into (3) yields

$$\frac{\mathrm{d}T_n(t)}{\mathrm{d}t} - \int_0^t g(t - t_1)\frac{\mathrm{d}T_n(t_1)}{\mathrm{d}t_1}\mathrm{d}t_1 = -\mu_n \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t g(t - t_1)\,T_n(t_1)\,\mathrm{d}t \tag{23}$$

and

$$CL_{FP}X_n(x) = -\mu_n X_n(x), \tag{24}$$

where μ_n are the eigenvalues. Then, the solution for $\rho(x, t)$ is given by the expansion of eigenfunctions

$$\rho(x, t\,|x', 0) = e^{\frac{\Phi(x')}{2} - \frac{\Phi(x)}{2}} \sum_n \psi_n(x')\,\psi_n(x)\,T_n(t), \tag{25}$$

where $\Phi(x) = V(x)/k_BT$, $V(x)$ is the potential given by $F(x) = -\mathrm{d}V(x)/\mathrm{d}x$, and $\psi_n(x) = e^{\Phi(x)/2}X_n(x)$. We note that the eigenvalue equation of the operator L_{FP}, (24), is the same as the one of eigenvalue equation of ordinary Fokker-Planck operator [17]. Now, we only need to solve equation (23) that depends only on time. Applying the Laplace transform to (23) yields

$$T_{sn}(s) = \frac{T_n(0)\,[1 - g_s(s)]}{s - (1 - n)\,s g_s(s)}\;. \tag{26}$$

Substituting $g_s(s)$ into (26) we obtain

$$T_n(t) = 1 - n\;\; b + \lambda b^{1-\alpha}$$
$$\times \int_0^t e^{-bu} \sum_{k_1=0}^{\infty} \frac{[(1 - n)\,(b + \lambda b^{1-\alpha})\,u]^{k_1}}{k_1!} E^{(k_1)}_{\alpha,1+(1-\alpha)k_1}(-\lambda u^{\alpha})\mathrm{d}u, \tag{27}$$

Figure 4. Plots of $\rho(x,t)$ versus x coordinate with $C = 1$, $b = 0.03$, $\alpha = 0.5$, $\lambda = 0.15$, for the linear force case.

where we have omitted the term $T_n(0)$. Then, the solution for $\rho(x,t\,|x',0)$ is given by

$$\rho(x,t\,|x',0) = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \sum_{n=0}^{\infty} \frac{T_n(t)}{2^n n!} H_n\left(\frac{\bar{x}}{\sqrt{2}}\right) H_n\left(\frac{\bar{x}'}{\sqrt{2}}\right) e^{-\frac{\bar{x}^2}{2}}, \tag{28}$$

where $\bar{x} = x\sqrt{m\omega^2/(k_B T)}$, $C = k_B T/m\omega^2$, $\mu_n = n$ and $H_n(y)$ denotes the Hermite polynomials. It is worth mentioning that $T_n(t)$ reduces to $T_n(t) = \exp[-(a+\lambda)nt]$ for $\alpha = 1$, which is the solution of the ordinary diffusion equation. In figure 4 we show the PDF for different times.

To obtain the first two moments we substitute (3) into (6), and we obtain the derivative of the first moment of PDF $\rho(x,t)$ with respect to t

$$\frac{\mathrm{d}\langle x(t)\rangle}{\mathrm{d}t} = \int_0^t g(t-t_1)\frac{\mathrm{d}\langle x(t_1)\rangle}{\mathrm{d}t_1}\mathrm{d}t_1 + \frac{C}{k_B T}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t g(t-t_1)\int_{-\infty}^{\infty} F(x)\rho(x,t)\mathrm{d}x\mathrm{d}t_1 \tag{29}$$

and the derivative of the second moment of PDF $\rho(x,t)$ with respect to t

$$\frac{\mathrm{d}\langle x^2(t)\rangle}{\mathrm{d}t} = \int_0^t g(t-t_1)\frac{\mathrm{d}\langle x^2(t_1)\rangle}{\mathrm{d}t_1}\mathrm{d}t_1 + 2C\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t g(t_1)\mathrm{d}t_1 + \frac{2C}{k_B T}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t g(t-t_1)\int_{-\infty}^{\infty} xF(x)\rho(x,t)\mathrm{d}x\mathrm{d}t_1. \tag{30}$$

Now we apply the Laplace transform to (29) and (30), and we arrive at

$$\langle x(s)\rangle_s = \frac{\langle x(0)\rangle[1-g_s(s)]}{s} \tag{31}$$

and

$$\langle x^2(s)\rangle_s = \frac{\langle x^2(0)\rangle[1-g_s(s)]}{s[1+g_s(s)]} + \frac{2Cg_s(s)}{s[1+g_s(s)]}. \tag{32}$$

We note that equation (31) can be solved for any waiting time PDF, and the solution is given by

$$\langle x(t)\rangle = \langle x(0)\rangle\left(1-\int_0^t g(t_1)\mathrm{d}t_1\right) \tag{33}$$

In the case of $g(t)$ (5), we have

$$\langle x(t)\rangle = \langle x(0)\rangle\left[1-\left(b+\lambda b^{1-\alpha}\right)\int_0^t e^{-bt_1}E_{\alpha,1}(-\lambda t_1^{\alpha})\mathrm{d}t_1\right] \tag{34}$$

and

$$\langle x^2(t)\rangle = \langle x^2(0)\rangle + 2\left(\frac{k_B T}{m\omega^2} - \langle x^2(0)\rangle\right) \times \left(b+\lambda b^{1-\alpha}\right)\int_0^t e^{-bt_1}\sum \frac{[-(b+\lambda b^{1-\alpha})t_1]^n}{n!}E^{(n)}_{\alpha,1}(-\lambda t_1^{\alpha})\mathrm{d}t_1. \tag{35}$$

∞ 1

0 $n=0$ $n!$ $\alpha,1+(1-\alpha)n$ 1 1

It is found that the first two moments have complicated forms associated with the Mittag-Leffler function. For $\alpha = 1$ the Mittag-Leffler function reduces to the exponential function, and all the above results reduce to those of the ordinary diffusion equation. The thermal equilibrium is reached when $t \to \infty$, then we have $\langle x^2(\infty)\rangle = k_B T/m\omega^2$. If the system satisfies the special initial spatial condition as $\langle x(0)\rangle = 0$ and $\langle x^2(0)\rangle = k_B T/m\omega^2$, $\langle x(t)\rangle = 0$ and $\langle x^2(t)\rangle = k_B T/m\omega^2$ for all the time; therefore, average of displacement and its second moment are independent of time.

3. Conclusion

We have investigated the uncoupled CTRW model with the waiting time PDF given by (5) for force-free and linear force cases. We have presented analytical solutions for the first two moments and probability distribution. We have shown, for the force-free case, the system presents normal regimes at the small and large times, but it presents a deviation from the normal regime at the intermediate times; we note that the solutions for the first two moments can be described in terms of the generalized Mittag-Leffler function. In figure 3 we show the PDF, and it presents cusp for the intermediate times which is associated with the anomalous regime; this result reinforces the fact that the cusp present in the PDF for anomalous regime is typical for the CTRW model (see the cusp present in the PDFs for other waiting time PDFs [10, 13]). For the linear force $F(x) = -m\omega^2 x$, all the solutions presented in this work are described in terms of the generalized Mittag-Leffler function.

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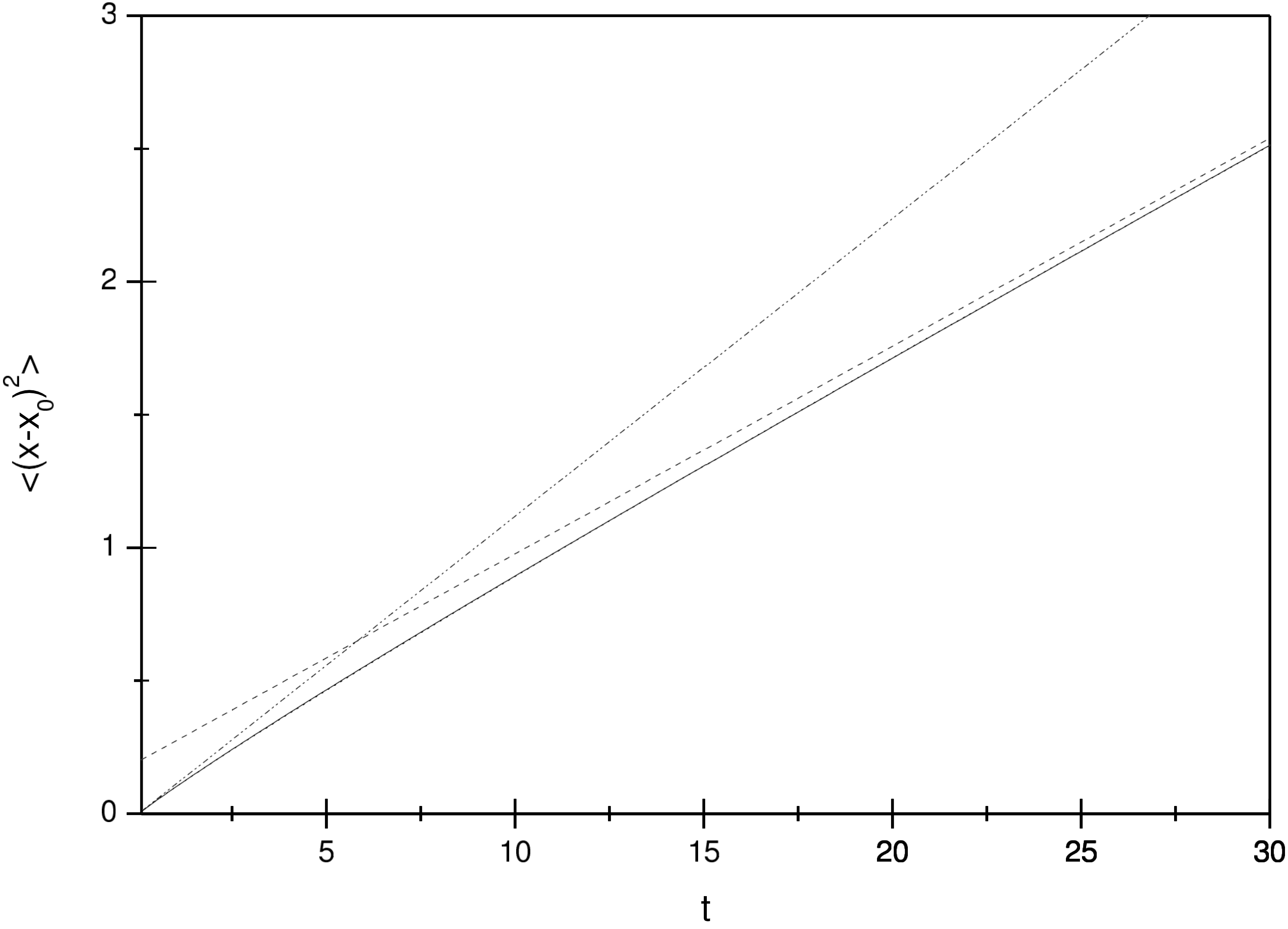

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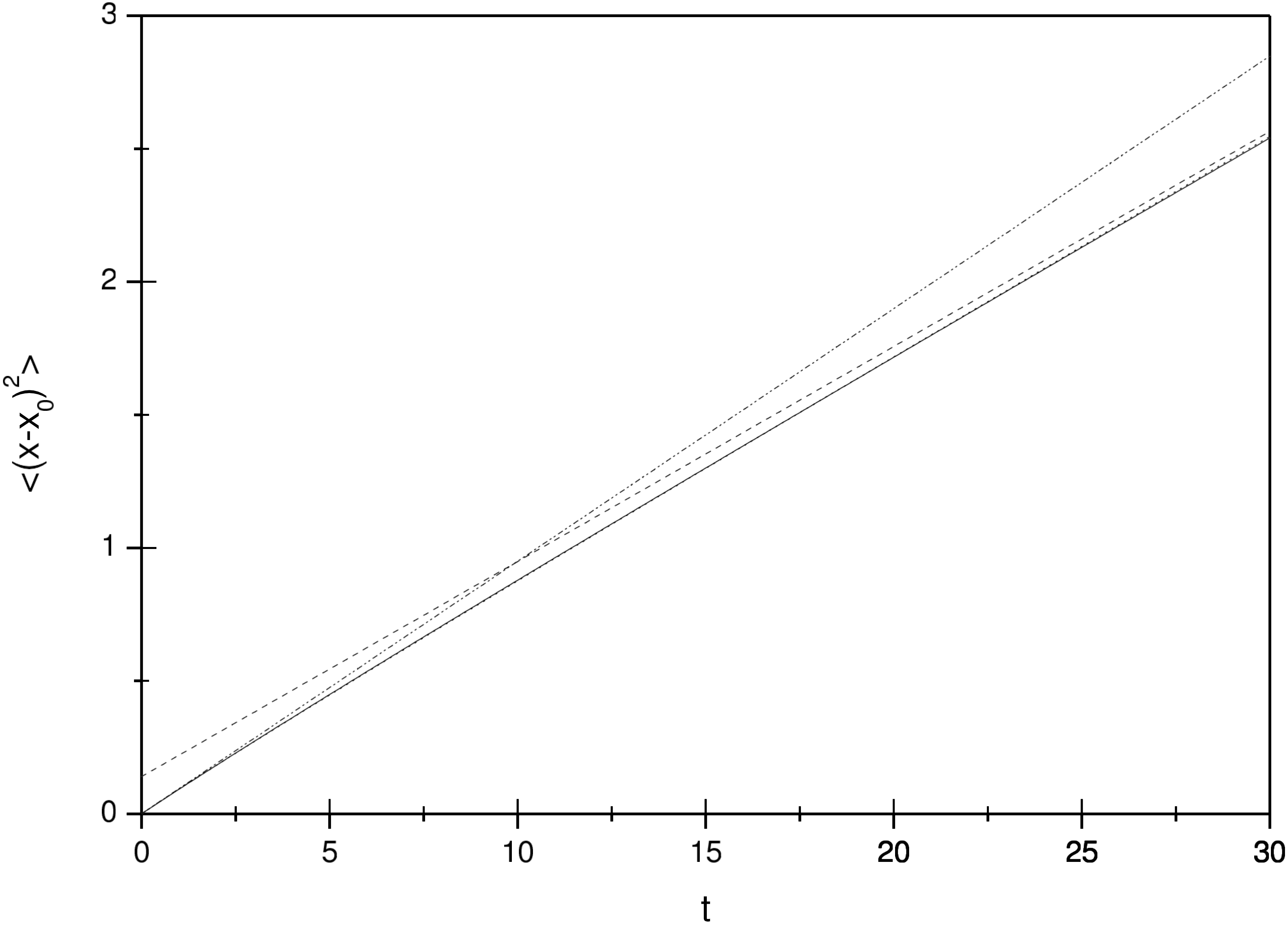
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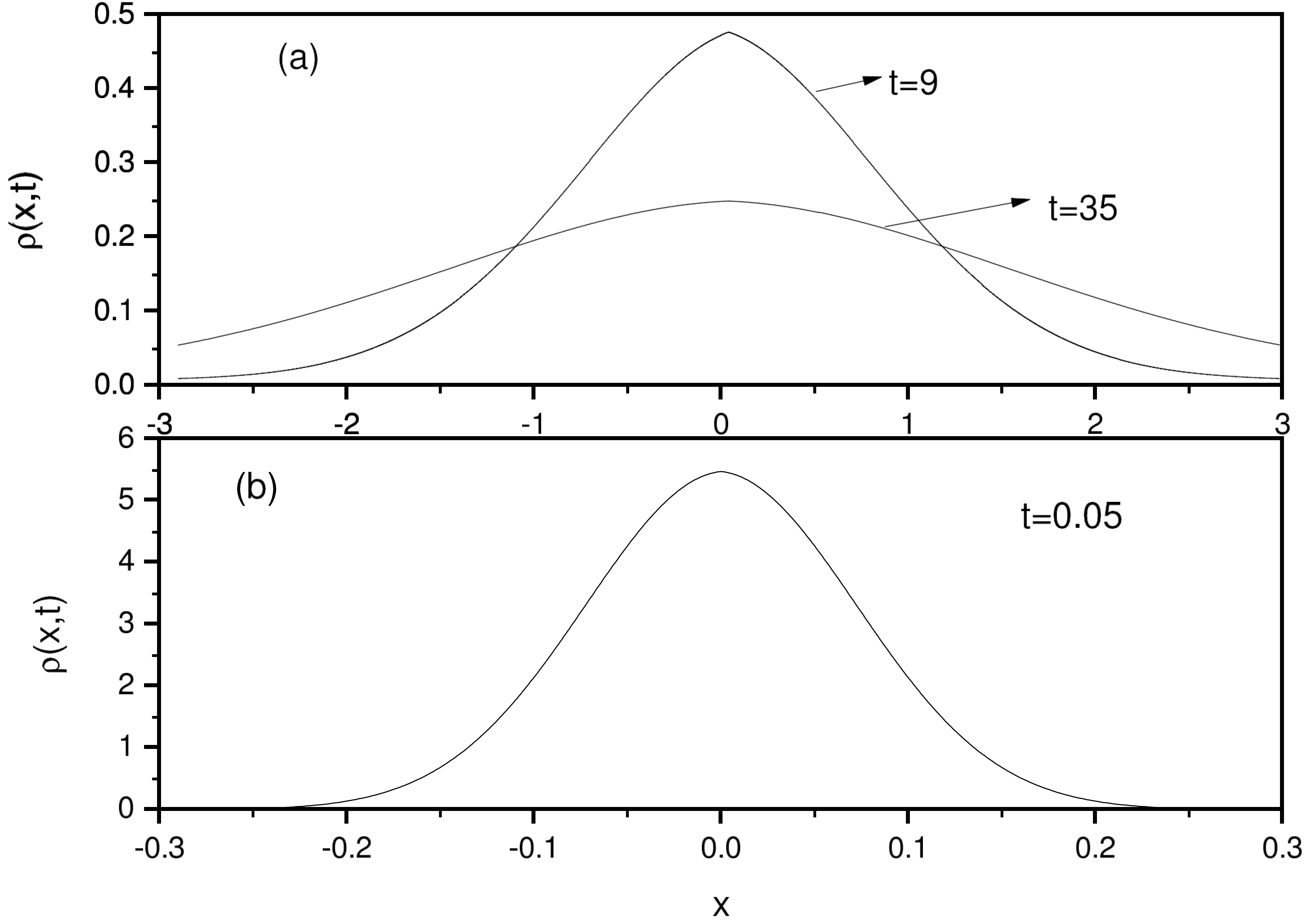
(a)
t=9
t=35
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0.4
0.3
0.2
0.1
0.0
-3
-2
-1
0
1
2
3
(b)
t=0.05
ρ(x,t)
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5
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3
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1
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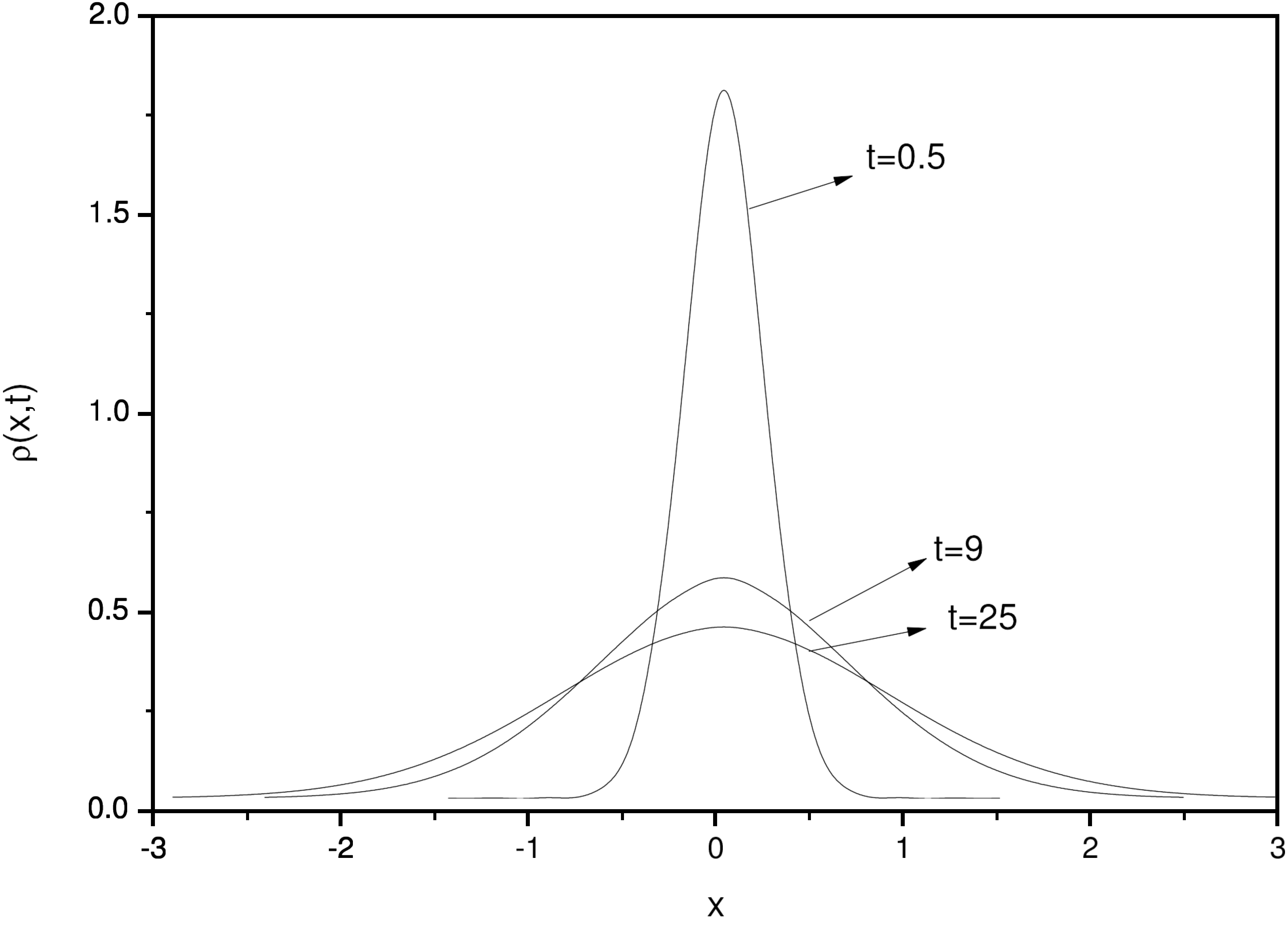
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
x



t=0.5
t=9
t=25
ρ(x,t)
x
2.0
1.5
1.0
0.5
0.0
-3
-2
-1
0
1
2
3