First-passage and first-arrival problems in continuous-time random walks: Beyond the diffusion approximation

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Some exact solutions of the first-passage and first-arrival problems for the continuous-time random-walk model are obtained. On the basis of these exact solutions, the following has been revealed. First, for some jump-length distributions with a finite variance, the approximate solutions obtained in the diffusion approximation can differ significantly from the exact solutions. Second, for some waiting time distributions with a finite mean, the times of first passage and the times of first arrival can significantly depend on the ensemble under consideration. In particular, the mean first-passage time corresponding to the stationary ensemble can be significantly greater than the mean first-passage time corresponding to the nonaged ensemble. Third, for any continuous distribution of jump lengths, the probability of first arrival is zero for a point-like target. This last result is contrary to existing opinion, but it is consistent with the fact that a single point has a probability measure equal to zero in the probability space defined by a continuous distribution of jump lengths.

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I. INTRODUCTION

The continuous-time random walk (CTRW) model developed by Montroll and Weiss [1] is one of the most popular and frequently used means of describing anomalous diffusion [2–10]. In the practical applications of this model, one usually resorts to the diffusion approximation, which allows one to pass from integral equations to differential equations, which are much easier to solve [3,4,7,10]. In this article we consider the question of the legitimacy of using the diffusion approximation when solving first-passage and first-arrival problems.

In the decoupled version of the CTRW model, the propagator [coordinate probability density function corresponding to the initial condition $P(x, t=0) = \delta(x)$] has the following form in Fourier-Laplace space [4]:

$$P(k, s) = \frac{1-\psi(s)}{s}\frac{1}{1-\psi(s)q(k)}. \quad (1)$$

Here, $\psi(s)$ is the Laplace transform of the waiting time distribution $\psi(t)$ [$\psi(s) = \int_0^\infty \exp(-st)\psi(t)\mathrm{d}t$] and $q(k)$ is the Fourier transform of the jump-length distribution $q(x)$ [$q(k) = \int_{-\infty}^{\infty} \exp(-kix)q(x)\mathrm{d}x$].

At the initial stage of development of the theory of anomalous diffusion, it was assumed that the nature of diffusion observed in experiment is completely determined by the behavior of functions $\psi(t)$ and $q(x)$ at large values of t and x, which correspond to small values of s and k [4]. So, the assumption that was previously applied to normal diffusion and which is called the diffusion approximation [11,12] was extended to anomalous diffusion. Under this assumption, functions $\psi(s)$ and $q(k)$ in expression (1) can be replaced by the leading terms of their expansions in the vicinity of $(k=0, s=0)$. If the mean waiting time ξ [$\xi = \int_0^\infty t\psi(t)\mathrm{d}t$] and the jump-length variance σ^2 [$\sigma^2 = \int_{-\infty}^{\infty} x^2 q(x)\mathrm{d}x$] are finite values then the leading terms of the expansions are

$$\psi(s) \approx 1 - \xi s, \quad (2)$$

$$q(k) \approx 1 - \frac{\sigma^2}{2}k^2. \quad (3)$$

Substituting Eqs. (2) and (3) into Eq. (1) gives the Gaussian propagator [4]

$$P(k, s) = \frac{1}{s + Dk^2}, \quad (4)$$

where $D = \sigma^2/(2\xi)$. As we see, in this approximation, CTRW reduces to normal diffusion.

The diffusion approximation excludes anomalous diffusion for finite ξ and σ^2. Within this approximation, anomalous diffusion is possible only at infinite ξ or σ^2. However, further research has shown that in many cases the assumption on which the diffusion approximation is based is violated [13–21]. In particular, the authors of Ref. [22] established through numerical modeling that the CTRW model with finite mean waiting time and finite jump-length variance meets all the paradigmatic features that belong to the anomalous diffusion as it is observed in living systems. It follows that in many cases the diffusion approximation is inapplicable and when solving specific problems it is necessary to use the exact CTRW model.

The subject of this article is the solution of some first-passage and first-arrival problems within the framework of the CTRW model without involving the diffusion approximation. A CTRW model with distinct waiting time distribution for the first jump [23,24] is considered; this allowed us to study the dependence of the results on the initial state of the system.

Previously, the integral equations of the CTRW model were solved in Refs. [25] and [26]. In Ref. [25], the survival probability P_s of an immobile target surrounded by mobile traps was calculated for one spatial dimension. For the case of a jump-length distributions with a finite variance and a waiting time distributions with a finite mean, the expression

$$P_s \approx \exp[-2\rho(\sqrt{4Dt/\pi} + K)] \quad (5)$$

was obtained in the long-time limit, where ρ is the trap concentration, D is the diffusion coefficient, and K is a constant depending on the features of the jump-length distribution. As is known, in the diffusion approximation, the constant K is equal to zero. The authors found a general expression for this constant but did not explore what values it could take. One of the results of this article is that the constant K can take any value in the interval $(-\infty, 0)$. The authors of Ref. [26] calculated the mean first-passage time for a CTRW with an exponential towards the boundary distribution of jump lengths. They found that the diffusion approximation is violated if the starting point is near the boundary. One of the results of this article is that, for some distributions of jump lengths, the diffusion approximation is violated even for a starting point far from the boundary.

The article is organized as follows: In the second section, equations are derived for the survival probability in the CTRW model with the waiting time distribution of the first jump different from the waiting time distribution of subsequent jumps. In sections from the third to the fifth, specific problems for CTRW with the jump-length distribution in the form of a sum of Laplace distributions (two-sided exponential distributions) are solved. In the third section, the first-passage problem is solved for a semi-infinite interval. In the fourth section, the first-passage problem is solved for a bounded interval. In the fifth section, the first-arrival problem is solved. In the sixth section, the case of the aged CTRW is considered.

II. EQUATIONS FOR THE SURVIVAL PROBABILITY

Let D be an arbitrary set in R^n and $\bar{D}$ its complement. The particle performs random walks, starting from point x_0, belonging to D. When it ends up in region $\bar{D}$, the particle dies. We will be interested in the survival probability, which will allow us to calculate the first-passage (first-arrival) times.

The equations of the continuous-time random walk model in the case under consideration are written as [23]

$$F(x,t) = \phi(t)q(x - x_0) + \int_0^t \int_D \psi(t-\tau)q(x-y) \times F(y,\tau)\mathrm{d}\tau\mathrm{d}y, \quad (6)$$

$$P(x,t) = \Phi(t)\delta(x - x_0) + \int_0^t \Psi(t-\tau)F(x,\tau)\mathrm{d}\tau. \quad (7)$$

Here $F(x,t)$ is the probability density that the particle arrives at the position x at time t, $P(x,t)$ is the probability density of finding the particle at position x at time t, $\psi(t)$ is the probability density to make a jump at time t after previous jump, $\Psi(t) = 1 - \int_0^t \psi(\tau)\mathrm{d}\tau$, $\phi(t)$ is the probability density of making the first jump at time t after the starting monitoring the system, $\Phi(t) = 1 - \int_0^t \phi(\tau)\mathrm{d}\tau$, $q(x)$ is the probability density of jump length, which in this article is assumed to be continuous and symmetrical: $q(x) = q(-x)$. It is assumed that the particle crosses the boundary between the two regions unhindered, so no additional conditions at the boundary are required for equations (6) and (7).

In Laplace domain, equations (6) and (7) have the form

$$F(x,s) = \phi(s)q(x - x_0) + \psi(s)\int_D q(x-y)F(y,s)\mathrm{d}y, \quad (8)$$

$$P(x,s) = \Phi(s)\delta(x - x_0) + \Psi(s)F(x,s). \quad (9)$$

In the special case when the waiting time distribution of the first jump ϕ, coincides with the waiting time distribution of the second and subsequent jumps, ψ, these equations take the form

$$F(x,s) = \psi(s)q(x - x_0) + \psi(s)\int_D q(x-y)F(y,s)\mathrm{d}y, \quad (10)$$

$$P(x,s) = \Psi(s)\delta(x - x_0) + \Psi(s)F(x,s). \quad (11)$$

A comparison of equations (8) and (10) shows that the solution of the first [we denote it by $F_\phi(x,s)$] is expressed through the solution of the second [designated $F(x,s)$] according to the formula

$$F_\phi(x,s) = (\phi/\psi)F(x,s). \quad (12)$$

From equation (11) it follows that

$$F(x,s) = P(x,s)/\Psi - \delta(x - x_0). \quad (13)$$

Substituting (13) into (12) and (12) into (9) gives the following expression for the probability density corresponding to the waiting time distribution of the first jump ϕ [we denote it by $P_\phi(x,s)$] through the probability density corresponding to the waiting time distribution of the first jump ψ [designated as $P(x,s)$]:

$$P_\phi(x,s) = \frac{\phi(s)}{\psi(s)}P(x,s) + \frac{1}{s}\left(1 - \frac{\phi(s)}{\psi(s)}\right)\delta(x - x_0). \quad (14)$$

Previously, this formula was obtained in Ref. [27] for an unbounded space, when the probability is conserved. Here it was obtained for an arbitrary set D in the presence of absorption in $\bar{D}$. Integrating this formula over area D, we obtain the relationship between the Laplace transforms of the survival probabilities:

$$Q_\phi(x_0,s) = \frac{\phi(s)}{\psi(s)}Q(x_0,s) + \frac{1}{s}\left(1 - \frac{\phi(s)}{\psi(s)}\right). \quad (15)$$

The survival probability $Q_\phi(x_0,t)$ is defined as the probability that the particle starting from x_0 in a process with a waiting-time distribution $\phi(t)$ different from $\psi(t)$ survives until time t without being absorbed into $\bar{D}$. The survival probability $Q(x_0,t)$ is defined similarly for a process with $\phi(t) = \psi(t)$. Relationship (15) is the final result of the previous calculations. It shows that $Q_\phi(x_0,s)$ can be easily calculated if $Q(x_0,s)$ is known.

It is straightforward to write down an equation for the survival probability $Q(x_0,t)$:

$$Q(x_0,t) = \Psi(t) + \int_0^t \int_D \psi(\tau)q(y - x_0)Q(y,t-\tau)\mathrm{d}\tau\mathrm{d}y. \quad (16)$$

Here we have divided the survival probability into two contributions. The first term on the right-hand side (RHS) corresponds to trajectories in which there are no jump between time $(0, t)$. The second term on the RHS takes into account trajectories in which the particle made at least one jump. The first renewal picture is used [28]. The expression $\psi(\tau)q(y - x_0)Q(y, t - \tau)$ inside the integral gives the probability of a jump from x_0 to $(y, y + dy)$ between time $(\tau, \tau + d\tau)$ and the absence of absorption from τ to t. A special case of equation (16) for set D, which is a semi-infinite interval, was considered in Ref. [26]. In the Laplace domain, equation (16) looks like

$$Q(x_0, s) = \frac{1 - \psi(s)}{s} + \psi(s) \int_D q(y - x_0)Q(y, s)\mathrm{d}y. \quad (17)$$

Formula (15) and equation (16) are valid for any set in an arbitrary space, but later in this article only problems for different types of intervals on a line will be considered.

III. FIRST-PASSAGE PROBLEM FOR A SEMI-INFINITE INTERVAL

Let us consider the case when the sets D and $\bar{D}$ are semi-infinite intervals $x \geqslant 0$ and $x < 0$. For this case, there is a general expression for the double Laplace transform of the survival probability $Q(p, s) = \int_0^\infty \int_0^\infty \exp(-px - st)Q(x, t)\mathrm{d}x\mathrm{d}t$ (hereinafter the index 0 in x_0 is omitted):

$$Q(p, s) = \frac{\sqrt{1 - \psi(s)}}{ps} \times \exp\left(-\frac{p}{\pi}\int_0^\infty \frac{\ln[1 - \psi(s)\hat{q}(\omega)]}{p^2 + \omega^2}\mathrm{d}\omega\right), \quad (18)$$

where $\hat{q}(\omega) = \int_{-\infty}^{\infty} \exp(i\omega x)q(x)\mathrm{d}x$ is the Fourier transform of the $q(x)$. This expression is obtained from the Pollaczek-Spitzer formula [29–33] using the formula connecting the Laplace transform $A(s)$ of a certain quantity for a process with continuous time with the generating function $B(u)$ of the same quantity for a process with discrete time: $A(s) = \frac{1-\psi(s)}{s}B(\psi(s))$ [25,34]. From formula (18), using the limit theorem $\lim_{p\to\infty} pQ(p, s) = Q(x = 0, s)$, the following expression is obtained for the survival probability at $x = 0$:

$$Q(x = 0, s) = \frac{\sqrt{1 - \psi}}{s}. \quad (19)$$

In the special case of exponential distribution of waiting time $\psi(t) = \exp(-\kappa t)$ we have

$$Q(x = 0, s) = \frac{1}{\sqrt{s(\kappa + s)}}. \quad (20)$$

Inverting the Laplace transform gives a continuous-time analog of the Sparre-Andersen theorem [30,35]

$$Q(x = 0, t) = \exp\left(-\frac{\kappa t}{2}\right)I_0\left(\frac{\kappa t}{2}\right), \quad (21)$$

where $I_0(x)$ is the modified Bessel function of the first kind. Since $I_0(x) \simeq \frac{1}{\sqrt{2\pi x}}\exp(x)$ at large x, we have

$$Q(x = 0, t) \simeq \frac{1}{\sqrt{\pi\kappa t}} \quad (22)$$

at large time. From formula (19) and the Tauberian theorem it follows that this relation is also valid for any waiting-time distribution with a mean waiting time equal to $1/\kappa$. Formulas (19) and (22) will be used below to control the correctness of the results obtained.

Further in this article it will be assumed that the distribution of jump lengths has the form of a weighted sum of Laplace distributions:

$$q(x) = \frac{1}{2}\sum_{i=1}^{N} \alpha_i\nu_i \exp(-\nu_i|x|), \quad (23)$$

with positive parameters ν_i and parameters α_i satisfying the condition $\sum_{i=1}^N \alpha_i = 1$. Parameters α_i, in principle, can be negative, but for simplicity they will be assumed to be positive.

In the case considered in this section, equation (17) takes the form

$$Q(x, s) = \frac{1 - \psi}{s} + \frac{\psi}{2}\sum_{i=1}^{N}\alpha_i\nu_i \times \int_x^\infty \exp[-\nu_i(\xi - x)]Q(\xi, s)\mathrm{d}\xi + \frac{\psi}{2}\sum_{i=1}^{N}\alpha_i\nu_i \times \int_0^x \exp[\nu_i(\xi - x)]Q(\xi, s)\mathrm{d}\xi. \quad (24)$$

We look for a solution to this equation in the form

$$Q(x, s) = \beta_0 + \sum_{j=1}^{N}\beta_j \exp(-\lambda_j x). \quad (25)$$

Substituting expression (25) into equation (24) shows that this equation will be satisfied if $\beta_0 = 1/s$, the parameters λ_j are N different solutions of the equation

$$\sum_{i=1}^{N}\frac{\alpha_i\nu_i^2}{\nu_i^2 - \lambda_j^2} = \frac{1}{\psi}, \quad (26)$$

and the parameters β_j for $j = 1, \dots, N$ are the components of the vector that is the solution to the linear system of equations

$$\sum_{j=1}^{N}\frac{\beta_j\nu_i}{\lambda_j - \nu_i} = \frac{1}{s}, \quad i = 1, 2, \dots, N. \quad (27)$$

For $N = 1$ and $N = 2$, equations (26) and (27) can be easily solved analytically.

A. $N = 1$

In this case, the positive solution to equation (26) is $\lambda_1 = \nu_1\sqrt{1 - \psi}$, and the solution to equation (27) is $\beta_1 = (\sqrt{1 - \psi} - 1)/s$. For the survival probability we have the expression

$$Q(x, s) = \frac{1}{s}\left\{1 - (1 - \sqrt{1 - \psi})\exp\left(-\frac{x}{l}\sqrt{1 - \psi}\right)\right\}, \quad (28)$$

where $l = 1/\nu_1$. At $x = 0$ we have $Q(x = 0, s) = (\sqrt{1 - \psi})/s$, as it should be.

Let us consider the behavior of the survival probability at long times. Assuming that the mean waiting time is finite, we represent the Laplace transform of the waiting-time distribution at small s as $\psi(s) \simeq 1 - s/\kappa$. As a result, we obtain from (28)

$$Q(x,s) \simeq \frac{1}{s}\left\{1 - \exp\left(-\frac{x}{l}\sqrt{\frac{s}{\kappa}}\right)\right\} + \frac{1}{\sqrt{s\kappa}}\exp\left(-\frac{x}{l}\sqrt{\frac{s}{\kappa}}\right). \tag{29}$$

Inverting the Laplace transform, we obtain

$$Q(x,t) \simeq \text{erf}\left\{\frac{x}{l\sqrt{4\kappa t}}\right\} + \frac{1}{\sqrt{\pi\kappa t}}\exp\left\{-\frac{x^2}{4l^2\kappa t}\right\}. \tag{30}$$

A similar expression was previously obtained for a discrete time in Ref. [29]. At $x = 0$ we have $Q(x = 0, t) = 1/\sqrt{\pi\kappa t}$, as it should be.

The first term on the right side of (30) represents the diffusion approximation. Let us find a condition under which this approximation is valid. For a fixed x and t tending to infinity, $\text{erf}\{x/(l\sqrt{4\kappa t})\}$ is approximately equal to $x/(l\sqrt{\pi\kappa t})$, and $\exp\{-x^2/(4l^2\kappa t)\}$ is close to unity. Consequently, the second term on the right side of (30) will be negligible compared with the first term under the condition $x \gg l$. The value l is approximately equal to the mean length of the jump; therefore, in the case under consideration, the diffusion approximation is valid if the distance between the starting point and the boundary of region D significantly exceeds the mean length of the jump. In particular, for the error of the diffusion approximation to be less than one percent, condition $x > 100l$ must be satisfied.

B. $N = 2$

In this case, positive solutions to equation (26) are

$$\lambda_1 = \sqrt{d - c} \tag{31}$$

and

$$\lambda_2 = \sqrt{d + c}, \tag{32}$$

where

$$d = \frac{\nu_1^2 + \nu_2^2 - \psi\left(\alpha_1\nu_1^2 + \alpha_2\nu_2^2\right)}{2}, \tag{33}$$

$$c = \sqrt{d^2 - (1-\psi)\nu_1^2\nu_2^2}. \tag{34}$$

The solutions to equation (27) are

$$\beta_1 = -\frac{\lambda_2(\lambda_1 - \nu_1)(\lambda_1 - \nu_2)}{s\nu_1\nu_2(\lambda_2 - \lambda_1)}, \tag{35}$$

$$\beta_2 = \frac{\lambda_1(\lambda_2 - \nu_1)(\lambda_2 - \nu_2)}{s\nu_1\nu_2(\lambda_2 - \lambda_1)}. \tag{36}$$

With these parameters β_1 and β_2, the survival probability (25) at $x = 0$, $Q(x = 0, s) = \beta_0 + \beta_1 + \beta_2$ is equal to $\sqrt{1 - \psi}/s$, as it should be.

The leading terms of the expansions of parameters λ_j and β_j as s tends to zero are

$$\lambda_1 = \sqrt{\frac{s}{\kappa}\frac{\nu_1^2\nu_2^2}{\alpha_1\nu_2^2 + \alpha_2\nu_1^2}}, \tag{37}$$

$$\lambda_2 = \sqrt{\alpha_1\nu_2^2 + \alpha_2\nu_1^2}, \tag{38}$$

$$\beta_1 = -\frac{1}{s} + \frac{\lambda_1}{s}\left\{\frac{1}{\nu_1} + \frac{1}{\nu_2} - \frac{1}{\lambda_2}\right\}, \tag{39}$$

$$\beta_2 = \frac{\lambda_1\lambda_2}{s\nu_1\nu_2} - \frac{\lambda_1}{s}\left\{\frac{1}{\nu_1} + \frac{1}{\nu_2} - \frac{1}{\lambda_2}\right\}. \tag{40}$$

Thus, for small s we have the following expression for the survival probability:

$$Q(x,s) \simeq \frac{1}{s}\left[1 - \exp\left\{-\frac{x}{\bar{l}}\sqrt{\frac{s}{\kappa}}\right\}\right] + \frac{A}{\sqrt{s\kappa}}\exp\left\{-\frac{x}{\bar{l}}\sqrt{\frac{s}{\kappa}}\right\} + \frac{1-A}{\sqrt{s\kappa}}\exp\left\{-\frac{\bar{l}^2}{l_1 l_2}x\right\}. \tag{41}$$

Here we introduce the notation $l_1 = 1/\nu_1$, $l_2 = 1/\nu_2$,

$$\bar{l} = \sqrt{\alpha_1 l_1^2 + \alpha_2 l_2^2}, \tag{42}$$

$$A = l_1/\bar{l} + l_2/\bar{l} - l_1 l_2/\bar{l}^2. \tag{43}$$

Inverting the Laplace transform, we obtain

$$Q(x,t) \simeq \text{erf}\left\{\frac{x}{\bar{l}\sqrt{4\kappa t}}\right\} + \frac{A}{\sqrt{\pi\kappa t}}\exp\left\{-\frac{x^2}{4\bar{l}^2\kappa t}\right\} + \frac{1-A}{\sqrt{\pi\kappa t}}\exp\left\{-\frac{\bar{l}^2}{l_1 l_2}x\right\}. \tag{44}$$

At $x = 0$ we have $Q(x = 0, t) = 1/\sqrt{\pi\kappa t}$, as it should be. This expression differs from (30) by the presence of the third term on the right side and coefficient A in the second term. The second term is negligible compared with the first term under the condition $x \gg A\bar{l}$. The third term does not play a significant role for large x. Therefore, in this case, for the error of the diffusion approximation to be less than one percent, condition $x > 100A\bar{l}$ must be satisfied.

There are distributions of the form (23) such that, for a fixed mean jump length, the parameter A will be arbitrarily large. For example, let C be an arbitrary number greater than one and let

$$l_1 = C\bar{l}, \tag{45}$$

$$l_2 = \bar{l}/C, \tag{46}$$

$$\alpha_1 = \frac{1 - 1/C^2}{C^2 - 1/C^2}, \tag{47}$$

$$\alpha_2 = \frac{C^2 - 1}{C^2 - 1/C^2}, \tag{48}$$

then the square of the mean jump length, $\alpha_1 l_1^2 + \alpha_2 l_2^2$, is equal to $\bar{l}^2$, and the constant A is equal to $C + 1/C - 1$. Since C can be arbitrarily large, A can also be arbitrarily large, regardless of $\bar{l}$.

From the previous considerations it is clear that there are distributions of jump lengths for which the diffusion approximation will be violated even at very large x. These are distributions with large values of parameter A. From formulas (45)–(48) it follows that these are the distributions with large l_1 and small l_2, with α_1 close to zero and α_2 close to one; that is, the distributions with "heavy tails." With this distribution, the particle predominantly makes short jumps, but sometimes also makes long jumps.

C. The many-particle problem

Consider the following problem, which was previously considered in Ref. [25]. Particles are randomly distributed on a line with density ρ. At the initial moment, they begin to move in accordance with the CTRW model. At point $x = 0$ there is a stationary particle that dies as soon as one of the moving particles passes through $x = 0$. We need to find the survival probability of the stationary particle as a function of time. In Ref. [25] the following solution to this problem was obtained:

$$P_s = \exp\left[-2\rho f(t)\right], \tag{49}$$

where

$$f(t) = \int_0^\infty \{1 - Q(x,t)\}\mathrm{d}x. \tag{50}$$

Using the Pollacek-Spitzer formula, the authors found the following general expression for the function $f(t)$ at large times in the case of finite mean waiting time we are considering:

$$f(t) \simeq \sqrt{\frac{4\kappa \bar{l}^2 t}{\pi}} + K. \tag{51}$$

The constant K is expressed through the jump-length distribution as

$$K = \frac{1}{\pi}\int_0^\infty \ln\left\{\frac{1-\hat{q}(\omega)}{\bar{l}^2\omega^2}\right\}\frac{\mathrm{d}\omega}{\omega^2}. \tag{52}$$

If we take (44) as the survival probability in formula (50), then we obtain (51) with the constant K equal to $-\bar{l}A$. Therefore, in this case, the survival probability (49) can be written as

$$P_s = \exp(2\rho\bar{l}A)P_s^{\mathrm{dif}}, \tag{53}$$

where $P_s^{\mathrm{dif}} = \exp[-2\rho(4\kappa\bar{l}^2 t/\pi)^{1/2}]$ is the survival probability calculated in the diffusion approximation. This shows that for large A the true survival probability will be significantly greater than the survival probability calculated in the diffusion approximation. Note that if we substitute

$$\hat{q}(\omega) = \frac{\alpha_1}{1 + l_1^2\omega^2} + \frac{\alpha_2}{1 + l_2^2\omega^2} \tag{54}$$

into formula (52), we obtain the same value for the constant K: $-\bar{l}A$. This confirms the correctness of the calculations leading to formula (44).

IV. FIRST-PASSAGE PROBLEM FOR A BOUNDED INTERVAL

This section considers the case when the sets D and $\bar{D}$ are bounded interval $[-L, L]$ and two semi-infinite intervals $x < -L$ and $x > L$. In this case, equation (17) takes the form (only positive x are considered)

$$Q(x,s) = \frac{1-\psi}{s} + \frac{\psi}{2}\sum_{i=1}^N \alpha_i\nu_i \int_x^L \exp[-\nu_i(\xi - x)]Q(\xi,s)\mathrm{d}\xi + \frac{\psi}{2}\sum_{i=1}^N \alpha_i\nu_i \int_{-L}^x \exp[\nu_i(\xi - x)]Q(\xi,s)\mathrm{d}\xi. \tag{55}$$

The solution to this equation must be a symmetric function of x, so we look for it in the form

$$Q(x,s) = \beta_0 + \sum_{j=1}^N \beta_j\{\exp(-\lambda_j x) + \exp(\lambda_j x)\}. \tag{56}$$

Substituting this expression into equation (55) shows that this equation will be satisfied if $\beta_0 = 1/s$, the parameters λ_j are N different solutions of the equation

$$\sum_{i=1}^N \frac{\alpha_i\nu_i^2}{\nu_i^2 - \lambda_j^2} = \frac{1}{\psi}, \tag{57}$$

and the parameters β_j for $j = 1, \dots, N$ are the components of the vector that is the solution to the linear system of equations

$$\sum_{j=1}^N \beta_j\left\{\frac{\nu_i\exp(\lambda_j L)}{\lambda_j - \nu_i} - \frac{\nu_i\exp(-\lambda_j L)}{\lambda_j + \nu_i}\right\} = \frac{1}{s}, \quad i = 1, 2, \dots, N. \tag{58}$$

A. $N = 1$

When $N = 1$ we find from equations (57) and (58)

$$\lambda_1 = \nu_1\sqrt{1-\psi}, \tag{59}$$

$$\beta_1 = -\frac{1}{2s}\frac{\psi}{\mathrm{ch}(\lambda_1 L) + \sqrt{1-\psi}\,\mathrm{sh}(\lambda_1 L)}. \tag{60}$$

Hence,

$$Q(x,s) = \frac{1}{s}\left\{1 - \frac{\psi\,\mathrm{ch}\left(\frac{x}{l}\sqrt{1-\psi}\right)}{\mathrm{ch}\left(\frac{L}{l}\sqrt{1-\psi}\right) + \sqrt{1-\psi}\,\mathrm{sh}\left(\frac{L}{l}\sqrt{1-\psi}\right)}\right\}. \tag{61}$$

If instead of the variable x, counted from the middle of the interval, we introduce the variable $y = L - x$, counted from the boundary of the interval, and direct L to infinity, keeping y constant, then this formula will turn into formula (28), as it should be.

We use formula (61) to calculate the mean first-passage time (MFPT) $T(x)$. As known, $T(x) = \lim_{s\to 0} Q(x,s)$. Assuming $\psi(s) \approx 1 - s/\kappa$ and calculating the limit, we obtain

$$T(x) = \frac{1}{2\kappa l^2}(L^2 - x^2 + 2Ll + 2l^2). \tag{62}$$

In the diffusion approximation we have

$$T^{\mathrm{diff}}(x) = \frac{1}{2\kappa l^2}(L^2 - x^2). \tag{63}$$

To evaluate the accuracy of the diffusion approximation, let us move in (62) to the variable $y = L - x$, counted from the boundary of the interval:

$$T(y) = \frac{1}{2\kappa l^2}(2Ly - y^2 + 2Ll + 2l^2). \tag{64}$$

If both the mean length of the jump, l, and the distance from the starting point to the boundary, y, are much smaller than the length of the interval, $2L$, then the condition for the validity of the diffusion approximation will look like $2Ly \gg 2Ll$; that is, $y \gg l$. For the error to be less than one percent, condition $y > 100l$ must be met.

B. $N = 2$

When $N > 1$, the MFPT is easier to find by directly solving the equation for $T(x)$ instead of the equation for $Q(x, s)$. The equation for $T(x)$ is obtained from (55) in the limit $s \to 0$:

$$T(x) = \frac{1}{\kappa} + \frac{1}{2}\sum_{i=1}^{N}\alpha_i\nu_i\int_x^L \exp[-\nu_i(\xi - x)]T(\xi)\mathrm{d}\xi + \frac{1}{2}\sum_{i=1}^{N}\alpha_i\nu_i\int_{-L}^{x}\exp[\nu_i(\xi - x)]T(\xi)\mathrm{d}\xi. \quad (65)$$

The solution is sought in the form

$$T(x) = \beta_0 + \sum_{j=1}^{N-1}\beta_j 2\mathrm{ch}(\lambda_j x) + \beta_N x^2. \quad (66)$$

Substituting this expression into equation (65) shows that this equation will be satisfied if

$$\beta_N = -\frac{1}{2\kappa\bar{l}^2}, \quad (67)$$

the parameters λ_j are $N-1$ different nonzero positive solutions to the equation

$$\sum_{i=1}^{N}\frac{\alpha_i\nu_i^2}{\nu_i^2 - \lambda_j^2} = 1, \quad (68)$$

and the parameters β_j for $j = 0, \dots, N-1$ are the components of the vector that is the solution to the linear system of equations

$$\sum_{j=1}^{N-1}\beta_j\left\{\frac{\nu_i\exp(\lambda_j L)}{\lambda_j - \nu_i} - \frac{\nu_i\exp(-\lambda_j L)}{\lambda_j + \nu_i}\right\} = \beta_0 + \beta_N\left\{L^2 + \frac{2L}{\nu_i} + \frac{2}{\nu_i^2}\right\}, \quad i = 1, 2, \dots, N. \quad (69)$$

For $N = 2$, solutions to equations (68) and (69) are

$$\lambda_1 = \sqrt{\alpha_1\nu_2^2 + \alpha_2\nu_1^2}, \quad (70)$$

$$\beta_0 = \beta_2\left\{\frac{d_1t_2 - d_2t_1}{t_1 - t_2} - L^2\right\}, \quad (71)$$

$$\beta_1 = \beta_2\frac{d_1 - d_2}{t_1 - t_2}, \quad (72)$$

where

$$d_i = 2Ll_i + 2l_i^2, \quad (73)$$

$$t_i = \frac{\nu_i\exp(\lambda_1 L)}{\lambda_1 - \nu_i} - \frac{\nu_i\exp(-\lambda_1 L)}{\lambda_1 + \nu_i}. \quad (74)$$

If parameters l_i and α_i are determined by formulas (45)–(48), then instead of formulas (70), (73) and (74) we will have

$$\lambda_1 = 1/\bar{l}, \quad (75)$$

$$d_1 = 2L\bar{l}C + 2\bar{l}^2C^2, \quad (76)$$

$$d_2 = 2L\bar{l}/C + 2\bar{l}^2/C^2, \quad (77)$$

$$t_1 = \frac{\exp(L/\bar{l})}{C - 1} - \frac{\exp(-L/\bar{l})}{C + 1}, \quad (78)$$

$$t_2 = \frac{\exp(L/\bar{l})}{1/C - 1} - \frac{\exp(-L/\bar{l})}{1/C + 1}. \quad (79)$$

From these formulas it follows that, if conditions $C \gg 1$ and $L \gg \bar{l}$ are satisfied, then the parameters β_0 and β_1 will be approximately equal to $-\beta_2(L^2 + d_1)$ and $\beta_2 d_1\exp(-L/\bar{l})$, respectively. From this we get the following expression for MFPT:

$$T(x) \simeq \frac{1}{2\kappa\bar{l}^2}\left\{L^2 - x^2 + d_1 - 2d_1\frac{\mathrm{ch}(x/\bar{l})}{\exp(L/\bar{l})}\right\}. \quad (80)$$

This expression is valid when the third and fourth terms in brackets do not cancel each other, in particular, at $x \ll L$, when the fourth term is negligible. Since d_1 can be arbitrarily large, the result given by expression (80) can differ significantly from the result of the diffusion approximation (63) even at $x = 0$, that is, at the maximum distance of the starting point from the boundary of the interval $[-L, L]$.

V. FIRST-ARRIVAL PROBLEM

This section considers the case when the sets D and $\bar{D}$ are two semi-infinite intervals $x < -L$ and $x > L$ and bounded interval $[-L, L]$. In this case, equation (17) takes the form (only positive x are considered)

$$Q(x,s) = \frac{1-\psi}{s} + \frac{\psi}{2}\sum_{i=1}^{N}\alpha_i\nu_i\int_x^\infty \exp[-\nu_i(\xi - x)]Q(\xi,s)\mathrm{d}\xi + \frac{\psi}{2}\sum_{i=1}^{N}\alpha_i\nu_i\int_L^x \exp[\nu_i(\xi - x)]Q(\xi,s)\mathrm{d}\xi + \frac{\psi}{2}\sum_{i=1}^{N}\alpha_i\nu_i\int_{-\infty}^{-L}\exp[\nu_i(\xi - x)]Q(\xi,s)\mathrm{d}\xi. \quad (81)$$

The solution to this equation must be a symmetric function bounded at infinity, so we look for it in the form

$$Q(x,s) = \beta_0 + \sum_{j=1}^{N}\beta_j\exp(-\lambda_j|x|). \quad (82)$$

Substituting this expression into equation (81) shows that this equation will be satisfied if $\beta_0 = 1/s$, the parameters λ_j are N different solutions of the equation

$$\sum_{i=1}^{N}\frac{\alpha_i\nu_i^2}{\nu_i^2 - \lambda_j^2} = \frac{1}{\psi}, \quad (83)$$

and the parameters β_j for $j = 1, \dots, N$ are the components of the vector that is the solution to the linear system of equations

$$\sum_{j=1}^{N}\beta_j\exp(-\lambda_j L)\left\{\frac{\nu_i\exp(-\nu_i L)}{\nu_i + \lambda_j} - \frac{\nu_i\exp(\nu_i L)}{\nu_i - \lambda_j}\right\} = \frac{\exp(-\nu_i L) - \exp(\nu_i L)}{s}, \quad i = 1, 2, \dots, N. \quad (84)$$

When $N = 1$ we find from equations (83) and (84)

$$\lambda_1 = \nu_1\sqrt{1-\psi}, \quad (85)$$

$$\beta_1 = -\frac{\psi}{s}\frac{\mathrm{sh}(\nu_1 L)\exp(\lambda_1 L)}{\mathrm{sh}(\nu_1 L) + \sqrt{1-\psi}\,\mathrm{ch}(\nu_1 L)}. \quad (86)$$

Hence,

$$Q(x,s)=\frac{1}{s}\left\{1-\frac{\psi\,\mathrm{sh}(\nu_1 L)\exp\left(\lambda_1(L-x)\right)}{\mathrm{sh}(\nu_1 L)+\sqrt{1-\psi})\mathrm{ch}(\nu_1 L)}\right\}. \tag{87}$$

If instead of the variable x we introduce the variable $y=x-L$, equal to the distance from the starting point to the boundary, and direct L to infinity, keeping y constant, then this formula will turn into formula (28), as it should be.

Formula (87) shows that the marginal survival probability $Q(x,t\to\infty)=\lim_{s\to 0}[sQ(x,s)]$ is equal to zero for any nonzero absorption interval $[-L,L]$, but when $L=0$, that is, when the interval contracts to a single point $x=0$, the marginal probability is equal to one. This is explained by the fact that the probability of a particle hitting any finite interval as a result of a jump is different from zero, but the probability of hitting a single point is zero. To demonstrate this more clearly, consider formula (87) for large s, corresponding to small times. Suppose $\psi(s)=\kappa/(\kappa+s)$, then $\psi\approx\kappa/s$ at large s and the main terms of expansion (87) in powers of $1/s$ have the form

$$Q(x,s)\approx\frac{1}{s}-\frac{\kappa}{s^2}\frac{\mathrm{sh}(\nu_1 L)\exp\left[\nu_1(L-x)\right]}{\mathrm{sh}(\nu_1 L)+\mathrm{ch}(\nu_1 L)}+\cdots. \tag{88}$$

Going to physical time gives

$$Q(x,t)\approx 1-\kappa t\frac{\mathrm{sh}(\nu_1 L)\exp\left[\nu_1(L-x)\right]}{\mathrm{sh}(\nu_1 L)+\mathrm{ch}(\nu_1 L)}+\cdots. \tag{89}$$

In the second term on the right side, the factor κt is equal to the probability that the first jump is made during time t (at $t\ll 1/\kappa$). The fraction behind this factor gives the probability that the jump from point x falls into the interval $[-L,L]$:

$$\frac{\mathrm{sh}(\nu_1 L)\exp\left[\nu_1(L-x)\right]}{\mathrm{sh}(\nu_1 L)+\mathrm{ch}(\nu_1 L)}=\frac{1}{2}\int_{-L}^{L}\exp\left[\nu_1(\xi-x)\right]\mathrm{d}\xi. \tag{90}$$

From here we see why the linear term in expansion (89) disappears at $L=0$. The reason is that the integral on the right side of (90) is equal to zero; that is, that the probability of hitting a single point is zero. Since the probability of hitting a single point is also zero at the second, third, and so on jumps, all subsequent terms of expansion (89) also disappear at $L=0$. The same reasoning is valid for any continuous distribution $q(x)$. If the particle is at point x, then the probability of it falling into the interval $[-L,L]$ as a result of a jump is equal to the integral $\int_{-L}^{L}q(\xi-x)\mathrm{d}\xi$. If the distribution is continuous, then this integral tends to zero as L tends to zero.

As is known, in the diffusion approximation, the survival probability in the first-arrival problem does not depend on the width of the absorption interval and is equal to the survival probability in the first-passage problem [36]. This also applies to an interval consisting of a single point. From the above it follows that these diffusion approximation results are completely inconsistent with the exact solutions of the first-arrival problem in the CTRW model with a continuous distribution of jump lengths. This is explained by the fact that in the diffusion approximation the particle cannot jump over intermediate points as happens in the CTRW model.

If the absorbing region $\bar{D}$ is small, then the first-arrival problem can be approximately solved by a method that is valid in a space of any dimension and for any distribution $q(x)$. This method makes it possible to find not only the survival probability, but also the coordinate PDF. The equation for the coordinate PDF has the following form in Laplace domain:

$$P(x,s)=\frac{1-\psi}{s}\delta(x-x_0)+\psi\int_D q(x-y)P(y,s)\mathrm{d}y. \tag{91}$$

In this equation, it is assumed that if a particle falls into region $\bar{D}$, then it disappears and is excluded from further consideration. But we can, without distorting the function $P(x,s)$ in region D, assume that the particle disappears not at the moment of arrival in $\bar{D}$, but at the moment of the jump following its arrival in this region. In this case, the equation for $P(x,s)$ will be written as

$$P(x,s)=\frac{1-\psi}{s}\delta(x-x_0)+\psi\int_{-\infty}^{\infty}q(x-y)P(y,s)\mathrm{d}y - \psi\int_{\bar{D}}q(x-y)P(y,s)\mathrm{d}y. \tag{92}$$

It is obtained from (91) by adding and subtracting the term $\psi\int_{\bar{D}}q(x-y)P(y,s)\mathrm{d}y$. This equation is valid for all $x\in(-\infty,\infty)$. If the region $\bar{D}$ is small, we can approximate the last integral by some quadrature formula and solve this equation using the Fourier transform method. The result will be the expression $P(x,s)=f(x,s,P_i)$, containing as unknown parameters the values $P_i=P(x_i,s)$ at some points x_i of the region $\bar{D}$. By writing the self-consistency conditions $f(x_i,s,P_i)=P_i$ for all x_i, we obtain linear equations for the parameters P_i, solving which we uniquely determine the function $f(x,s,P_i)$. In this way the coordinate PDF will be found, and therefore the survival probability can be found.

If the domain $\bar{D}$ contracts to a point, then the integral over this domain in equation (92) vanishes for any continuous distribution of jump lengths in space of any dimension, so this equation reduces to an equation that preserves probability. It follows that the probability of hitting a point target is zero for any distribution of jump lengths in space of any dimension.

Let us show that for $L\ll 1/\nu_1$ this method gives a solution that practically coincides with the exact solution (87). We use the simplest approximation of the integral $\int_{-L}^{L}q(x-y)P(y,s)\mathrm{d}y$ by the expression $2Lq(x)P(0,s)$. Solving equation (92), we find

$$P(x,s)=P_\infty(x,s|x_0)-2LP(0,s)\Phi(x,s|0), \tag{93}$$

where $P_\infty(x,s|x_0)$ is the coordinate PDF for an infinite line corresponding to the initial condition $\delta(x-x_0)$ and $\Phi(x,s|x_0)=\frac{s}{1-\psi}P_\infty(x,s|x_0)-\delta(x-x_0)$. Setting x equal to zero in equation (93), solving this equation for $P(0,s)$ and substituting the resulting expression back into (93), we obtain

$$P(x,s)=P_\infty(x,s|x_0)-\frac{2L\Phi(x,s|0)P_\infty(0,s|x_0)}{1+2L\Phi(0,s|0)}. \tag{94}$$

The survival probability is found using formula

$$Q(x_0,s)=\int_{-\infty}^{\infty}P(y,s)\mathrm{d}y-2LP(0,s), \tag{95}$$

which gives

$$Q(x_0,s)=\frac{1}{s}\left(1-\frac{2L\Phi(0,s|x_0)}{1+2L\Phi(0,s|0)}\right). \tag{96}$$

This formula is valid for any continuous distribution $q(x)$. In the special case of $q(x) = \frac{\nu_1}{2}\exp(-\nu_1|x|)$, the function $\Phi(x, s|x_0)$ is expressed as

$$\Phi(x, s|x_0) = \frac{\psi \nu_1}{2\sqrt{1-\psi}} \exp(-\lambda_1|x - x_0|). \quad (97)$$

Substituting this expression into (96), we obtain

$$Q(x_0, s) = \frac{1}{s}\left(1 - \frac{\psi \nu_1 L \exp(-\lambda_1 x_0)}{\psi \nu_1 L + \sqrt{1-\psi}}\right). \quad (98)$$

If in formula (87) we replace $\mathrm{sh}(\nu_1 L)$ with $\nu_1 L$, and $\mathrm{ch}(\nu_1 L)$ and $\exp(-\lambda_1 L)$ with units (these replacements are valid for $L \ll 1/\nu_1$), then we get an expression that practically coincides with (98). This means that formula (96) gives a good approximation to the exact solution of the first-arrival problem. The smaller the length of the interval $[-L, L]$, the better the accuracy of this approximation. In the limit when the interval is contracted to one point, it gives the exact solution $Q(x_0, s) = 1/s$.

From the above considerations it is clear that formulas similar to formula (96) can be obtained for first-arrival problems in spaces of any dimension. For example, in the case of two dimensions, a similar formula, instead of the one-dimensional density Φ, will contain the corresponding two-dimensional density and instead of the length of the interval $[-L, L]$, it will contain the area of the region $\bar{D}$.

VI. AGED CONTINUOUS-TIME RANDOM WALK

In the three previous sections, equation (17) was solved, which assumes that at the initial moment of time the system is in such a state that the distribution of the waiting time for the first jump coincides with the distribution of the waiting time for the second and subsequent jumps. This section examines the question of how the solutions found in the previous sections can change if the waiting-time distribution of the first jump differs from the waiting-time distribution of the subsequent jumps.

The correct choice of the waiting-time distribution of the first jump depends on the initial condition. If the diffusion system is created at the beginning of observation (at $t = 0$), then the distribution $\phi(t)$ coincides with $\psi(t)$ [23]. If observation begins some time after the creation of the diffusion system, then the system is said to have aged. If a time equal to t_a has passed before the start of observation, then ϕ as a function of the variables t and t_a is expressed in the Laplace domain as

$$\phi(s, u) = \frac{\psi(s) - \psi(u)}{[1 - \psi(u)](u - s)}, \quad (99)$$

where u is the Laplace variable corresponding to t_a [27,37–39]. In this case, relation (15) is written as

$$Q_\phi(x, s, u) = \frac{\phi(s, u)}{\psi(s)} Q(x, s) + P_{im}(s, u), \quad (100)$$

where

$$P_{im}(s, u) = \frac{1}{s}\left(\frac{1}{u} - \frac{\phi(s, u)}{\psi(s)}\right).$$

To move from Laplace images to physical domain, it is convenient to transform expressions $P_{im}(s, u)$ and $\Omega(s, u) \equiv \frac{\phi(s,u)}{\psi(s)}$ to the following forms:

$$P_{im} = \frac{\Theta(u)}{u(u-s)}\left[\left(\frac{1}{\Theta(s)} - \frac{1}{\Theta_\infty}\right) - \left(\frac{1}{\Theta(u)} - \frac{1}{\Theta_\infty}\right)\right], \quad (101)$$

$$\Omega = \frac{\Theta(u)}{u\Theta_\infty} + \frac{\Theta(u)}{u(u-s)}\left[u\left(\frac{1}{\Theta(u)} - \frac{1}{\Theta_\infty}\right) - s\left(\frac{1}{\Theta(s)} - \frac{1}{\Theta_\infty}\right)\right], \quad (102)$$

where

$$\Theta(s) = \frac{s\psi(s)}{1 - \psi(s)} \quad (103)$$

is the Laplace image of the memory function [40] and $\Theta_\infty = \lim_{s\to\infty} \Theta(s)$. It follows that, in physical domain, quantities P_{im} and Ω look like

$$P_{im}(t, t_a) = \int_0^{t_a} f_1(t') f_2(t + t_a - t') \mathrm{d}t', \quad (104)$$

$$\Omega(t, t_a) = \frac{f_1(t_a)}{\Theta_\infty}\delta(t) - \frac{d}{dt} P_{im}(t, t_a), \quad (105)$$

where $f_1(t_a)$ is the inverse Laplace transform of $\Theta(u)/u$ and $f_2(t)$ is the inverse Laplace transform of $1/\Theta(s) - 1/\Theta_\infty$. The survival probability (100) takes the form

$$Q_\phi(x, t, t_a) = \frac{f_1(t_a)}{\Theta_\infty} Q(x, t) - \int_0^t \frac{d}{dt'} P_{im}(t', t_a) \times Q(x, t - t')\mathrm{d}t' + P_{im}(t, t_a). \quad (106)$$

It is clear from this that in an aged system, at the initial moment of time, a particle with probability $f_1(t_a)/\Theta_\infty$ is in a mobile state and with probability $P_{im}(0, t_a) = 1 - f_1(t_a)/\Theta_\infty$ is in an immobile state. If particle is in a mobile state, then over time the probability of its survival changes in the same way as in a nonaged system [such as $Q(x, t)$]. If it is in an immobile state, then over time it passes at rate $-\frac{d}{dt}P_{im}(t, t_a)$ into a mobile state and further the probability of its survival changes in the same way as in a nonaged system.

In the simple case, when the waiting-time distribution has the form of a weighted sum of two exponentials,

$$\psi(t) = p\frac{\exp(-t/\tau_1)}{\tau_1} + (1-p)\frac{\exp(-t/\tau_2)}{\tau_2}, \quad (107)$$

functions $P_{im}(t, t_a)$ and $\frac{\phi}{\psi}(t, t_a)$ are calculated explicitly. In this case, function $\Theta(s)$ takes the form

$$\Theta(s) = \frac{1}{\xi}\frac{1 + a\gamma s}{1 + \gamma s}, \quad (108)$$

and from formulas (104) and (105) the following expressions follow:

$$P_{im}(t, t_a) = \frac{a-1}{a}\exp\left(-\frac{t}{a\gamma}\right)\left[1 - \exp\left(-\frac{t_a}{\gamma}\right)\right], \quad (109)$$

$$\frac{\phi}{\psi}(t, t_a) = \left[\frac{1}{a} + \frac{a-1}{a}\exp\left(-\frac{t_a}{\gamma}\right)\right]\delta(t) + \frac{a-1}{a^2\gamma}\exp\left(-\frac{t}{a\gamma}\right)\left[1 - \exp\left(-\frac{t_a}{\gamma}\right)\right], \quad (110)$$

where

$$\xi = p\tau_1 + (1-p)\tau_2, \tag{111}$$

$$\gamma = \tau_1\tau_2/\xi, \tag{112}$$

$$a = \xi[p/\tau_1 + (1-p)/\tau_2]. \tag{113}$$

In Ref. [22] it is shown that the CTRW with waiting-time distribution (107) is capable of describing the anomalous diffusion observed in experiment. Therefore formulas (109) and (110) can be used to describe real physical systems. One important property of aged systems should be noted, which follows from formula (109). Expression $1-\exp(-t_a/\gamma)$ in this formula describes the transition of an ensemble of particles from a mobile state to an immobile state. The rate of this transition is characterized by the constant $1/\gamma$. The expression $\exp(-t/a\gamma)$ describes the reverse transition from the immobile state to the mobile state. The rate of this transition is characterized by the constant $1/a\gamma$. Since the parameter a is always greater than one [41,42], the reverse transition is always slower than the forward transition. At large values of parameter a, the time of the reverse transition will be significantly longer than the time of the forward transition.

We now compare the survival probabilities for the aged and nonaged systems. As an aged system, we take a stationary system, i.e., system corresponding to an infinite delay time $t_a \to \infty$. Stationary systems deserves special attention because the first-passage time often needs to be known just for the stationary (or equilibrium) state. In particular, the rate constant of a diffusion-controlled bimolecular reaction (Smoluchowski problem) is calculated for the steady state [43] and the mean escape time from the potential well (Kramers problem) is calculated for the equilibrium state [44]. Formula (15) in the stationary case looks like

$$Q_\phi(x,s) = \frac{\Theta_0}{\Theta(s)}Q(x,s) + \frac{1}{s}\left(1-\frac{\Theta_0}{\Theta(s)}\right), \tag{114}$$

where $\Theta_0/\Theta(s) = \lim_{u\to 0}\phi(s,u)/\psi(s)$. Next, we take formula (28) as a specific expression for $Q(x,s)$ and compare the behavior of $Q(x,t)$ and $Q_\phi(x,t)$ defined by expression (114) at small and large times.

First, let us find the behavior of $Q(x,t)$ at small t. To do this, let us represent ψ as $\Theta/(s+\Theta)$ in formula (28) and expand $Q(x,s)$ in powers of $1/s$ as s tends to infinity:

$$Q(x,s) = \frac{1}{s} - \frac{\Theta_\infty}{2s^2}\exp\left(-\frac{x}{l}\right) + \cdots . \tag{115}$$

Inverting the Laplace transform gives

$$Q(x,t) = 1 - \Theta_\infty t\frac{1}{2}\exp\left(-\frac{x}{l}\right) + \cdots . \tag{116}$$

Here, in the second term on the right, the factor $\Theta_\infty t$ is the probability that the first jump is made in time t. Factor $\exp[-(x/l)]/2$ is the probability that a jump from point x brings the particle to region $x<0$.

Now let us find $Q_\phi(x,t)$ at small times. Substituting (28) into (114), we obtain

$$Q_\phi(x,s) = \frac{1}{s}\left\{1 - \frac{\Theta_0}{\Theta(s)}\left(1-\sqrt{\frac{s}{s+\Theta(s)}}\right)\right.$$
$$\left.\times\exp\left(-\frac{x}{l}\sqrt{\frac{s}{s+\Theta(s)}}\right)\right\}. \tag{117}$$

Expanding this expression in powers of $1/s$ as s tends to infinity gives

$$Q_\phi(x,s) = \frac{1}{s} - \frac{\Theta_0}{2s^2}\exp\left(-\frac{x}{l}\right) + \cdots . \tag{118}$$

Hence

$$Q_\phi(x,t) = 1 - \Theta_0 t\frac{1}{2}\exp\left(-\frac{x}{l}\right) + \cdots . \tag{119}$$

This expression differs from (116) in that Θ_∞ is replaced by Θ_0. Θ_∞ is the frequency of jumps in the newly created ensemble in which each particle is at the beginning of the waiting period. Θ_0 is the frequency of jumps in a stationary ensemble. The ratio Θ_∞/Θ_0 is equal to the ratio of the diffusion coefficients D_0/D_∞, where D_0 and D_∞ are the diffusion coefficients found from the dependence of the mean-square displacement on time [45]. D_0 is the diffusion coefficient at t equal to zero, and D_∞ is the diffusion coefficient at t tending to infinity. In real physical systems, the ratio D_0/D_∞ can be very large [9], therefore, at short times, $Q(x,t)$ can decrease much faster than $Q_\phi(x,t)$.

The behavior of $Q(x,t)$ given by (28) at large times was discussed above; as t tends to infinity, it tends to zero according to the law (here κ is equal to $1/\xi$)

$$Q(x,t) \approx \frac{x/l+1}{\sqrt{\pi\kappa t}}. \tag{120}$$

Let us show that, at times when $Q(x,t)$ is close to zero, $Q_\phi(x,t)$ can remain close to one. To do this, let us take (107) as the distribution of the waiting time. Then the second term in (114) takes the form

$$\frac{(a-1)\gamma}{1+a\gamma s} \tag{121}$$

and for $Q_\phi(x,t)$ we have inequalities

$$1 > Q_\phi(x,t) > \frac{a-1}{a}\exp\left(-\frac{t}{a\gamma}\right). \tag{122}$$

Parameters a and γ can be arbitrarily large [41,42], so the right side of the second inequality can be close to one for any t. In addition, these parameters do not depend on the parameters included in formula (120). Consequently, $Q_\phi(x,t)$ can be close to unity even at times at which $Q(x,t)$ is close to zero.

The physical meaning of parameters a and γ is as follows: Parameter a is equal to the ratio of diffusion coefficients D_0/D_∞, that is, it characterizes the degree of diffusion slowdown. Parameter γ characterizes the length of the time interval during which the slowdown occurs. Large values of these parameters are present in the case of pronounced transient anomalous diffusion. Consequently, a strong dependence of the survival probability on the initial state of the system in the first-passage and first-arrival problems will occur for systems with pronounced anomalous diffusion.

It is clear that if the survival probability depends strongly on the initial state of the system, then the first-passage time will also depend strongly. Let us demonstrate this using the example of a system described by the memory function (108).

In the case of a stationary initial state, the MFPT is found from formula (114) as s tends to zero:

$$T_\phi(x) = T(x) + \frac{d}{ds}\ln[\Theta(s)]\Big|_{s=0}. \tag{123}$$

When $\Theta(s)$ is defined by formula (108) the second term on the right is equal to $(a-1)\gamma$. Since a and γ can be arbitrarily large, MFPT for a stationary initial state can be significantly larger than MFPT for a nonstationary initial state.

VII. DISCUSSION

When solving specific problems within the framework of the CTRW model, the diffusion approximation is usually used. This article examines the question of the legality of using this approximation when solving first-passage and first-arrival problems. Exact solutions obtained under the assumption that the distribution of jump lengths has the form of a weighted sum of Laplace distributions are compared with approximate solutions obtained in the diffusion approximation. In particular, in the case of the first-passage problem a two-term distribution was considered, the Fourier image of which has the form

$$q(k) = \frac{1}{C^2 - 1/C^2}\left(\frac{1 - 1/C^2}{1 + C^2\bar{l}^2k^2} + \frac{C^2 - 1}{1 + \bar{l}^2k^2/C^2}\right). \tag{124}$$

It is shown that at large C the diffusion approximation gives satisfactory results only in cases where the starting point is located sufficiently far from the boundary of the absorbing region. If C tends to infinity, then for the diffusion approximation to remain valid, the distance from the starting point to the boundary must tend to infinity. This fact is explained as follows: The series expansion of distribution (124) at small k has the form

$$q(k) = 1 - \bar{l}^2k^2 + \frac{C^4 - C^2 - 1/C^4 + 1/C^2}{C^2 - 1/C^2}\bar{l}^4k^4 + \cdots. \tag{125}$$

In order for the diffusion approximation to be valid, it is necessary that the third term of this expansion be significantly less than the second term, i.e., that the following condition must be met:

$$k^2 \ll \frac{C^2 - 1/C^2}{\bar{l}^2(C^4 - C^2 - 1/C^4 + 1/C^2)}. \tag{126}$$

From this it can be seen that, as C increases, the range of values of k for which the diffusion approximation is valid narrows. Accordingly, the range of x values narrows. But since small k corresponds to large x, the range of values of x does not shrink to zero but shifts towards infinity.

The above reasoning were applied to distributions with finite variance, but they can also be applied to distributions with infinite variance. For example, if we take the weighted sum of two Lévy distributions,

$$q(k) = \frac{(1 - 1/C)\exp(-C\bar{l}^\alpha k^\alpha)}{C - 1/C} + \frac{(C-1)\exp(-\bar{l}^\alpha k^\alpha/C)}{C - 1/C}, \tag{127}$$

the expansion of which into a series in small k has the form

$$q(k) = 1 - \bar{l}^\alpha k^\alpha + \frac{C^2 - C - 1/C^2 + 1/C}{2(C - 1/C)}\bar{l}^{2\alpha}k^{2\alpha} + \cdots, \tag{128}$$

then we can see that as C increases, the range of values of k in which the third term is negligible compared with the second one narrows. Accordingly, the range of x values narrows. Thus, although for any C the approximate expression for the distribution of jump lengths, $q(k) \approx 1 - \bar{l}^\alpha k^\alpha$, remains the same, its range of validity narrows with increasing C. Consequently, the range of validity of the equation with a fractional derivative with respect to a spatial variable, which is a consequence of this approximation [4], also narrows.

This paper shows that for any continuous distribution of jump lengths, the probability of first arrival is zero for a point-like target. This seems to contradict the results of works that obtained nonzero distribution of the first-arrival time to a point-like target for Lévy flights [46–48]. The apparent contradiction is explained by the fact that in Refs. [46–48] the diffusion approximation was used. If we abandon the diffusion approximation, then the method of finding the distribution of the first-passage time used in Refs. [46–48] will give the result obtained in this article. In Refs. [46–48], the distribution of the first-passage time was found using the well-known formula

$$\rho_{fp}(s) = \frac{W(0, s|x_0)}{W(0, s|0)}, \tag{129}$$

where

$$W(0, s|x_0) = \int_{-\infty}^{\infty} \exp(ikx_0)P(k, s)\mathrm{d}k, \tag{130}$$

and $P(k, s)$ is the propagator given by formula (1). The authors of Refs. [46–48] used an equation with the fractional derivative with respect to the spatial variable which leads to the following expression for the propagator: $P(k, s) = 1/(s + K_\alpha|k|^\alpha)$. As a result, they obtained a nonzero density $\rho_{fp}(s)$ for $1 < \alpha \leqslant 2$. However, if we take the exact expression for the Lévy flights propagator $[P(k, s) = 1/[s + \kappa(1 - \exp(\bar{l}^\alpha|k|^\alpha)]]$, then in the denominator of formula (129) we get infinity and the density $\rho_{fp}(s)$ will be equal to zero for any α. It is clear from this that using an equation with a fractional derivative with respect to a spatial variable to solve the first-arrival problem is unlawful.

This paper considers only distributions with two terms in sum (23) that can be analyzed analytically. However, the resulting equations for parameters α_i and ν_i are valid for any number of terms. Therefore, the method used here can be applied to solve problems with real distributions of jump lengths encountered in practice, including truncated Lévy flights. This is possible since any continuous distribution can be approximated with any accuracy by the sum of exponentials (23) [49,50]. The effectiveness of this approach is confirmed by its use in solving similar problems in other branches of science

[51,52]. This approach also works in cases where the distribution of $q(x)$ is asymmetrical and when among the parameters α_i there are negative ones [51,52].

The main conclusion of this article is the following: When solving a specific practical problem of the first passage or first arrival within the framework of the CTRW model, it is necessary to know the exact form of the distributions $\psi(t)$ and $q(x)$ and solve not the diffusion equation or equation with the fractional derivative with respect to the spatial variable but the original integral equation. In addition, it is necessary to take into account the dependence of the solutions on the aging. If the problem is solved in the diffusion approximation without taking aging into account, then in each case it is necessary to confirm the compliance of the obtained solutions with the characteristics of the physical system under consideration.

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