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Research Article

Fractional Diffusion Equations for Lattice and Continuum: Grünwald-Letnikov Differences and Derivatives Approach

Vasily E. Tarasov

Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia

Correspondence should be addressed to Vasily E. Tarasov; tarasov@theory.sinp.msu.ru

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Fractional diffusion equations for three-dimensional lattice models based on fractional-order differences of the Grünwald-Letnikov type are suggested. These lattice fractional diffusion equations contain difference operators that describe long-range jumps from one lattice site to another. In continuum limit, the suggested lattice diffusion equations with noninteger order differences give the diffusion equations with the Grünwald-Letnikov fractional derivatives for continuum. We propose a consistent derivation of the fractional diffusion equation with the fractional derivatives of Grünwald-Letnikov type. The suggested lattice diffusion equations can be considered as a new microstructural basis of space-fractional diffusion in nonlocal media.

1. Introduction

Fractional calculus and differential equation of noninteger orders [1-5] have a long history that is connected with the names of famous scientists such as Liouville, Riemann, Grünwald, Letnikov, Marchaud, and Riesz. Derivatives and integrals of noninteger orders have a lot of applications in different areas of physics [6-10]. Fractional calculus is a powerful tool to describe processes in continuously distributed media with nonlocal properties. As it was shown in [11, 12], the continuum equations with fractional derivatives are directly connected [7] to lattice models with long-range interactions. The lattice equations for fractional nonlocal media and the correspondent continuum equations have been considered recently in [13-15]. Fractional-order differences and the correspondent derivatives have been first proposed by Grünwald [16] and by Letnikov [17]. At the present time these generalized differences and derivatives are called the Grünwald-Letnikov fractional differences and derivatives [1-3, 18]. One-dimensional lattice models with long-range interactions of the Grünwald-Letnikov type and the correspondent fractional differential and integral continuum equations have been suggested in [19]. The suggested form of long-range interaction is based on the form of the left-sided and right-sided Grünwald-Letnikov fractional differences. A possible form of lattice vectors calculus based on the fractional-order differences of the Grünwald-Letnikov type has been suggested in [20]. In this paper, we apply this approach to describe diffusion on lattices with long-range jumps and to derive fractional diffusion equations for nonlocal continuum with power-law nonlocality.

The diffusion equations describe the change of probability of a random function in space and time in transport processes, and they usually have the form of second-order partial differential equation of parabolic type. Unfortunately, for complex nonlocal media, the usual second-order diffusion equation cannot adequately describe real processes. For example, the diffusion processes with the Poissonian waiting time and the Lévy distribution for the jump length cannot be described by equation with second-order derivatives with respect to coordinates. The Lévy distribution describes the Lévy flights [21, 22] that are random walks, where the jump lengths have probability distributions with heavy tails. The Lévy motion can be described by equation with spatial derivatives of noninteger orders μ , [22]. In this case, the moment of order δ for the Lévy motion has the form $\langle |x(t)|^{\delta} \rangle \sim t^{\delta/\mu}$, where $0 < \delta < \mu \le 2$. Usually the spacefractional diffusion equations are obtained from the secondorder differential equations by replacing the second-order space derivatives by fractional-order derivatives. Fractional diffusion equations with coordinate derivatives of noninteger order have been suggested in [23]. The solutions and properties of these equations are considered in [24–26]. The diffusion equations with fractional coordinate derivatives were also considered in [8, 9, 27].

In this paper we propose a consistent derivation of the space-fractional diffusion equation with Grünwald-Letnikov derivatives of noninteger orders by using lattice models with long-range jumps that is considered new microstructural basis to describe fractional diffusion processes in nonlocal media. In this paper, we suggest a lattice equation for probability density of particle in unbounded homogeneous three-dimensional lattice with long-range jumps between lattice sites. We prove that continuous limit for the suggested lattice diffusion equation gives the space-fractional diffusion equation for nonlocal continuum. The fractional differential equation for continuum contains the Grünwald-Letnikov derivatives on noninteger orders. Continuum models can be considered as a continuous limit of lattice models, where the length-scales of a continuum element are much larger than the distances between the lattice sites. The suggested approach to derive the space-fractional diffusion equations can serve as a microstructural basis to describe the spatialfractional diffusion processes.

2. Fractional Diffusion Equation for Lattice

The differences of fractional order and the correspondent fractional derivatives have been introduced by Grünwald in 1867 and independently by Letnikov in 1868.

Differences of noninteger orders are defined as a generalization of the integer order difference

$$\nabla_{a,\pm}^{m} f(x) = \sum_{n=1}^{m} \frac{(-1)^{n} m!}{n! (m-n)!} f(x \mp na), \quad (a \in \mathbb{R}_{+}, m \in \mathbb{N}).$$

The Fourier transformation F of the fractional-order differences of Grünwald-Letnikov type (see Section 20 of [1,2]) has the form

$$\mathscr{F}\left\{\nabla_{a,\pm}^{\alpha}f\left(x\right)\right\}\left(k\right) = \left(1 - e^{\pm ak}\right)^{\alpha}\mathscr{F}\left\{f\right\}\left(k\right). \tag{2}$$

The differences of integer orders (1) are defined by the finite series. The differences of noninteger order $\alpha \in \mathbb{R}_+$ are defined as infinite series (see Section 20 of [1, 2]). Fractional-order differences of Grünwald-Letnikov type are defined by

$$\nabla_{a,\pm}^{\alpha} f(x) = \sum_{n=0}^{\infty} \frac{(-1)^n \Gamma(\alpha+1)}{\Gamma(n+1) \Gamma(\alpha-n+1)} f(x \mp na), \quad (a > 0).$$
(3)

The difference $\nabla_{a,+}^{\alpha}$ is called left-sided fractional difference, and $\nabla_{a,-}^{\alpha}$ is called the right-sided fractional difference. We note that the series in (3) converges absolutely and uniformly for every bounded function f(x) and $\alpha > 0$.

Using the fractional-order differences (3), we can consider the derivatives of noninteger orders. The left- and right-sided Grünwald-Letnikov derivatives of fractional order $\alpha > 0$ are defined by

$$^{\mathrm{GL}}D_{x,\pm}^{\alpha}f\left(x\right) = \lim_{a \to 0+} \frac{\nabla_{a,\pm}^{\alpha}f\left(x\right)}{\left|a\right|^{\alpha}}.\tag{4}$$

For integer values of $\alpha = m \in \mathbb{N}$ the Grünwald-Letnikov derivatives (4) are equal to the usual integer order derivatives up to the sign in the form

$$^{GL}D_{x,\pm}^{m}f(x) = (\pm 1)^{m} \frac{d^{m}f(x)}{dx^{m}}.$$
 (5)

We can note that the Grünwald-Letnikov fractional derivatives coincide with the Marchaud fractional derivatives for the functions from $L_r(\mathbb{R})$, where $1 \le r < \infty$ (see Theorem 20.4 in [1, 2]).

Let us consider three-dimensional unbounded and bounded lattices. Physical lattices are characterized by space periodicity. For unbounded lattices we can use three noncoplanar vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_2 that are the shortest vectors by which a lattice can be displaced and be brought back into itself. Sites of this lattice can be characterized by the number vector $\mathbf{n}=(n_1,n_2,n_3)$, where n_j (j=1,2,3) are integer. For simplification, we consider a lattice with mutually perpendicular primitive lattice vectors \mathbf{a}_j (j=1,2,3). We choose directions of the axes of the Cartesian coordinate system that coincide with the vector \mathbf{a}_j . In this case $\mathbf{a}_j=a_j\mathbf{e}_j$, where $a_j=|\mathbf{a}_j|>0$ and \mathbf{e}_j are the basis vectors of the Cartesian coordinate system. This means that we use a primitive orthorhombic Bravais lattice. Then the vector \mathbf{n} can be represented as $\mathbf{n}=n_1\mathbf{e}_1+n_2\mathbf{e}_2+n_3\mathbf{e}_3$.

Choosing a coordinate origin at one of the lattice sites, the positions of all other sites with $\mathbf{n} = (n_1, n_2, n_3)$ are described by the vector $\mathbf{r}(\mathbf{n}) = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. The lattice sites are numbered by \mathbf{n} , so that vector \mathbf{n} can be considered as a number vector of the corresponding particle. We assume that the positions of particles in the lattice coincide with the lattice sites. The distribution function, which describes probability density for lattice site \mathbf{n} , will be denoted by $f(\mathbf{n},t) = f(n_1,n_2,n_3,t)$. This function satisfies the conditions

$$\sum_{n_{1}=-\infty}^{+\infty} \sum_{n_{2}=-\infty}^{+\infty} \sum_{n_{3}=-\infty}^{+\infty} f(n_{1}, n_{2}, n_{3}, t) = 1,$$

$$f(n_{1}, n_{2}, n_{3}, t) \ge 0 \quad (t \ge 0).$$
(6)

To describe dynamics of the distribution function $f(\mathbf{n},t)$ in the lattice models with long-range jumps between sites, we define fractional-order difference operators of the Grünwald-Letnikov type in the direction $\mathbf{e}_j = \mathbf{a}_j/|\mathbf{a}_j|$ of the lattice. Fractional-order difference operators of the Grünwald-Letnikov type for unbounded lattice are the operators $\mathrm{GL}_{\mathbb{D}_L^\pm}\left[\begin{smallmatrix}\alpha_j\\i\end{smallmatrix}\right]$ that act on the function $f(\mathbf{m},t)$ as

$$\mathbb{GL} \mathbb{D}_{L}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix} f(\mathbf{m}, t) = \frac{1}{a_{j}^{\alpha}} \sum_{m_{j} = -\infty}^{+\infty} \mathbb{GL} K_{\alpha_{j}}^{\pm} (n_{j} - m_{j}) f(\mathbf{m}, t)
\left(\alpha_{j} > 0, \ j = 1, 2, 3\right),$$
(7)

where the kernels ${}^{\rm GL}K_{\alpha}^{\pm}(n)$ are defined by the equation

$$^{\mathrm{GL}}K_{\alpha_{j}}^{\pm}(n) = \frac{(-1)^{n} \Gamma\left(1 + \alpha_{j}\right) (H[n] \pm H[-n])}{2\Gamma\left(|n| + 1\right) \Gamma\left(1 + \alpha_{j} - |n|\right)}, \qquad (8)$$
$$\left(\alpha_{j} > 0, \ n \in \mathbb{Z}\right),$$

and $\Gamma(z)$ is the gamma function, H[n] is the discrete variable Heaviside step function that is defined as H[n] = 1 for $n \ge 0$, and H[n] = 0 for n < 0, where $n \in \mathbb{Z}$. The parameter α_j is called the order of the operator. It should be noted that the definition of H[0] = 1 for discrete variable Heaviside function is significant for us, since it allows us to write the kernels ${}^{GL}K_{\alpha}^{+}(n)$ in the simple form without allocating repeated zero terms. Fractional-order difference operators (7) can be called a lattice fractional partial derivative in the direction $\mathbf{e}_i = \mathbf{a}_i/|\mathbf{a}_i|$.

It should be noted that one-dimensional lattice models with the long-range interaction of the form ${}^{GL}K_{\alpha}^{\dagger}(n)$ and correspondent fractional nonlocal continuum models have been suggested in [19]. The lattice operators (7) recently have been proposed in [20].

It is easy to see that kernels ${}^{GL}K_{\alpha}^{+}(n)$ and ${}^{GL}K_{\alpha}^{-}(n)$ are even and odd functions such that ${}^{GL}K_{\alpha}^{\pm}(-n) = \pm {}^{GL}K_{\alpha}^{\pm}(n)$. The form of the lattice operators (7) can be defined by the addition and subtraction of the Grünwald-Letnikov fractional differences

$$\mathbb{GL} \mathbb{D}_{L}^{\pm} \begin{bmatrix} \alpha \\ j \end{bmatrix} f(\mathbf{m}, t)
= \frac{1}{|a_{j}|^{\alpha}} \sum_{m_{j}=0}^{\infty} \frac{(-1)^{m_{j}} \Gamma(1+\alpha)}{2\Gamma(m_{j}+1)\Gamma(1+\alpha-m_{j})}
\times \left(f(\mathbf{n} - m_{j}\mathbf{e}_{j}, t) \pm f(\mathbf{n} - m_{j}\mathbf{e}_{j}, t) \right).$$
(9)

We should note that in (9) the summation is realized over nonnegative values m_j , in contrast to the sum over all integer values in (7).

For bounded physical lattice models the fractional-order difference operators also can be defined. Fractional-order difference operators of the Grünwald-Letnikov type for bounded lattice with $m_j^1 \leq m_j \leq m_j^2$ are the operators ${}^{\mathrm{GL}}_B \mathbb{D}_L^{\pm} \left[\begin{smallmatrix} \alpha_j \\ j \end{smallmatrix} \right]$ that act on the function $f(\mathbf{m},t)$ as

$$GL_{B} \mathcal{D}_{L}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix} f(\mathbf{m}, t) = \frac{1}{a_{j}^{\alpha}} \sum_{m_{j}=m_{j}^{1}}^{m_{j}^{2}} GL_{\alpha_{j}}^{\pm} \left(n_{j} - m_{j} \right) f(\mathbf{m}, t)$$

$$\left(j = 1, 2, 3 \right), \tag{10}$$

where kernels ${}^{\rm GL}K^{\pm}_{\alpha_j}(n)$ are defined by (8). The suggested forms of fractional difference operators for bounded physical lattice models are based on the Grünwald-Letnikov fractional differences on finite intervals (see Section 20.4 of [1, 2]). For the finite interval $[x_j^1, x_j^2]$, the integer values m_j^1, m_j^2 , and m_j are defined by the equations

$$m_j^1 = \begin{bmatrix} \frac{x_j^1}{a_j} \end{bmatrix}, \qquad m_j^2 = \begin{bmatrix} \frac{x_j^2}{a_j} \end{bmatrix}, \qquad m_j = \begin{bmatrix} \frac{x_j}{a_j} \end{bmatrix}, \quad (11)$$

where the brackets $[\cdot]$ of (11) mean the floor function that maps a real number to the largest previous integer number.

Using the semigroup property for fractional differences of nonnegative orders (see Property 2.29 in [3]), it is easy to show that the semigroup property holds for the fractional operators (7) in the form

$$^{\mathrm{GL}}\mathbb{D}_{L}^{\pm}\begin{bmatrix}\alpha\\j\end{bmatrix}^{\mathrm{GL}}\mathbb{D}_{L}^{\pm}\begin{bmatrix}\beta\\j\end{bmatrix} = {^{\mathrm{GL}}\mathbb{D}_{L}^{\pm}\begin{bmatrix}\alpha+\beta\\j\end{bmatrix}}, \quad (\alpha > 0, \ \beta > 0).$$
(12)

Using this equation, it is easy to prove the commutativity and the associativity of the lattice operator (7) of the Grünwald-Letnikov type. The commutativity and associativity of the fractional operators (7) of the Grünwald-Letnikov type for different directions are obvious.

To describe isotropic physical lattices we should use the difference operators $\mathbb{GL} \mathbb{D}_L^{\pm} \left[\begin{smallmatrix} \alpha_j \\ j \end{smallmatrix} \right]$ and $\mathbb{GL} \mathbb{D}_L^{\pm} \left[\begin{smallmatrix} \alpha_j \\ j \end{smallmatrix} \right]$ with orders $\alpha_i = \alpha$ for all j = 1, 2, 3.

Let us give possible equations for distribution function $f(\mathbf{n},t)$ on unbounded and bounded lattices. For unbounded homogeneous lattice the diffusion equation for probability density can be considered in the form

$$\frac{\partial f(\mathbf{n}, t)}{\partial t} = -\sum_{i=1}^{3} g_{i}^{\text{GL}} \mathbb{D}^{\pm} \begin{bmatrix} \alpha_{i} \\ i \end{bmatrix} f(\mathbf{m}, t)
+ \sum_{i, j=1}^{3} g_{ij}^{\text{GL}} \mathbb{D}^{\pm, \pm} \begin{bmatrix} \alpha_{i} & \beta_{j} \\ i & j \end{bmatrix} f(\mathbf{m}, t).$$
(13)

For bounded lattice we should use the fractional difference operators (10), and the correspondent analog of (13) has the form

$$\frac{\partial f(\mathbf{n},t)}{\partial t} = -\sum_{i=1}^{3} g_{i}^{\text{GL}}_{B} \mathbb{D}^{\pm} \begin{bmatrix} \alpha_{i} \\ i \end{bmatrix} f(\mathbf{m},t)
+ \sum_{i,j=1}^{3} g_{ij}^{\text{GL}}_{B} \mathbb{D}^{\pm,\pm} \begin{bmatrix} \alpha_{i} & \beta_{j} \\ i & j \end{bmatrix} f(\mathbf{m},t).$$
(14)

Equations (13) and (14) are the three-dimensional lattice diffusion equations that describe fractional diffusion processes with the lattice jumps. Here $f(\mathbf{n},t)$ is the probability density function to find the test particle at site \mathbf{n} at time t. The italics $i, j \in \{1; 2; 3\}$ are the coordinate indices, and g_i and g_{ij} are lattice coupling constants.

The first and second terms of the right-hand side of (13) and (14) describe the particle drift and diffusion on the lattice. These correspondent kernels describe the longrange drift and diffusion to **n**-site from all other **m**-sites. Parameters α_i and β_j in the kernels are positive real numbers that characterize how quickly the intensity of the drift and diffusion processes in the lattice decrease with increasing the value $\mathbf{n} - \mathbf{m}$. Kernels $K_{\alpha_j}^{\pm}(n_j - m_j)$, where j = 1, 2, 3, describe long-range jumps in direction \mathbf{a}_j with lattice step length $|n_j - m_j|$ in the lattice. In (13), we use the combination of the lattice operators

$${}^{\mathrm{GL}}\mathbb{D}^{\pm,\pm}\begin{bmatrix}\alpha_{i} & \beta_{j} \\ i & j\end{bmatrix} = {}^{\mathrm{GL}}\mathbb{D}^{\pm}\begin{bmatrix}\alpha_{i} \\ i\end{bmatrix} {}^{\mathrm{GL}}\mathbb{D}^{\pm}\begin{bmatrix}\beta_{j} \\ j\end{bmatrix}, \tag{15}$$

where i, j take values from the set $\{1; 2; 3\}$. The action of the operator (15) on the lattice probability density $f(\mathbf{m}, t)$ is

$$GL_{\mathbb{D}}^{\pm,\pm} \begin{bmatrix} \alpha_{i} & \beta_{j} \\ i & j \end{bmatrix} f(\mathbf{m}, t)$$

$$= \sum_{m_{i}=-\infty}^{+\infty} \sum_{m_{j}=-\infty}^{+\infty} K_{\alpha_{i}}^{\pm} (n_{i} - m_{i}) K_{\beta_{j}}^{\pm} (n_{j} - m_{j}) f(\mathbf{m}, t) .$$
(16)

Equations (13) and (14) describe fractional diffusion processes on the physical lattices, where long-range jumps can be realized. The lattice diffusion equations (13) and (14) can be considered as lattice analogs of the fractional diffusion equations for the processes with the Poissonian waiting time and the Lévy distribution for the jump length.

Suggested lattice equations (13) and (14) can be considered as master equations that allow us to describe time-evolution of particles and quasiparticles on lattice since evolution is modelled as being in exactly one of the countable numbers of lattice sites at any given time, where switching between sites is treated probabilistically. These equations are differential equations for the variation over time of the probabilities that the particle occupies each of the lattice sites.

3. Fractional Diffusion Equation for Continuum

To describe fractional diffusion in the nonlocal continua, we should use fractional derivatives with respect to space coordinates instead of the lattice operators. Continuum analogs of the fractional-order difference operators of the Grünwald-Letnikov type are the fractional derivatives of Grünwald-Letnikov type.

Fractional-order difference operators ${}^{GL}\mathbb{D}_L^{\pm}\left[\begin{smallmatrix}\alpha_j\\j\end{smallmatrix}\right]$ defined by (7) are transformed by the continuous limit operation into the fractional derivative of Grünwald-Letnikov type with respect to coordinate x_j in the form

$$\lim_{a_{j}\to 0+} \left({}^{GL}\mathbb{D}_{L}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix} f(\mathbf{m}, t) \right) = {}^{GL}\mathbb{D}_{C}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix} f(\mathbf{r}, t), \quad (17)$$

where ${}^{\text{GL}}\mathbb{D}_{\text{C}}^{\pm}\left[\begin{smallmatrix} \alpha_j \\ j \end{smallmatrix} \right]$ are the continuum fractional derivatives of the Grünwald-Letnikov type that are defined by

$${}^{\mathrm{GL}}\mathbb{D}_{C}^{\pm}\begin{bmatrix}\alpha\\j\end{bmatrix} = \frac{1}{2}\left({}^{\mathrm{GL}}D_{x_{j,+}}^{\alpha} \pm {}^{\mathrm{GL}}D_{x_{j,-}}^{\alpha}\right),\tag{18}$$

which contain the Grünwald-Letnikov fractional derivatives ${}^{\mathrm{GL}}D^{\alpha}_{x_j,\pm}$ with respect to space coordinate x_j that can be written as

$$^{\mathrm{GL}}D_{x_{j},\pm}^{\alpha}f\left(\mathbf{r},t\right) = \lim_{a_{j}\to0+} \frac{1}{\left|a_{j}\right|^{\alpha}} \sum_{m_{j}=0}^{\infty} \frac{\left(-1\right)^{m_{j}} \Gamma\left(\alpha+1\right)}{\Gamma\left(m_{j}+1\right) \Gamma\left(\alpha-m_{j}+1\right)} \times f\left(\mathbf{r}\mp m_{j}\mathbf{a}_{j},t\right), \quad (\alpha>0).$$

$$\tag{19}$$

This statement can be proved by analogy with the proof for lattice model with long-range interaction of the Grünwald-Letnikov type suggested in [19].

It is important to note that the Grünwald-Letnikov fractional derivatives coincide with the Marchaud fractional derivatives (see Section 20.3 in [1, 2]) for the functions from space $L_r(\mathbb{R})$, where $1 \leq r < \infty$ (see Theorem 20.4 in [1, 2]). Moreover both the Grünwald-Letnikov and Marchaud derivatives have the same domain of definition. The Marchaud fractional derivative is defined by the equation

$${}^{M}D_{x_{j}}^{\alpha,\pm}f(\mathbf{r},t) = \frac{1}{a(\alpha,s)} \int_{0}^{\infty} \frac{\Delta_{z_{j}}^{s,\pm}f(\mathbf{r},t)}{z_{j}^{\alpha+1}} dz_{j}, \quad (0 < \alpha < s),$$
(20)

where $\Delta_{z_i}^{s,\pm}$ is the finite difference of integer order s,

$$\Delta_{z_j}^{s,\pm} f(\mathbf{r},t) = \sum_{k=0}^{s} \frac{(-1)^k s!}{(s-k)!k!} f(\mathbf{r} - kz_j \mathbf{e}_j, t), \qquad (21)$$

and $a(\alpha, s)$ is

$$a(\alpha, s) = \frac{s}{\alpha} \int_{0}^{1} \frac{(1 - \xi)^{s-1}}{(\ln(1/\xi))^{\alpha}} d\xi.$$
 (22)

Using (5), we can note that derivatives (18) for integer orders $\alpha = n \in \mathbb{N}$ have the forms

$${}^{\mathrm{GL}}\mathbb{D}_{C}^{+} \begin{bmatrix} n \\ j \end{bmatrix} = \frac{1 \pm (-1)^{n}}{2} \frac{\partial^{n}}{\partial x_{j}^{n}}.$$
 (23)

Therefore the continuum fractional derivatives ${}^{\mathrm{GL}}\mathbb{D}_{C}^{+}\left[\begin{smallmatrix}n\\j\end{smallmatrix}\right]$ are the usual derivatives of integer order n for even values α only, and the continuum operators ${}^{\mathrm{GL}}\mathbb{D}_{C}^{-}\left[\begin{smallmatrix}n\\j\end{smallmatrix}\right]$ are the derivatives of integer order n for odd values α only.

For bounded lattices, the fractional-order difference operators ${}_{B}^{\text{GL}} \mathbb{D}_{L}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix}$ defined by (10) are transformed by the continuous limit

$$\lim_{a_{j}\to0+} \begin{pmatrix} GL \mathbb{D}_{L}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix} f(\mathbf{m},t) \end{pmatrix} = {}_{B}^{GL} \mathbb{D}_{C}^{\pm} \begin{bmatrix} \alpha_{j} \\ j \end{bmatrix} f(\mathbf{r},t), \quad (24)$$

into the continuum fractional derivatives of the Grünwald-Letnikov type with respect to space coordinate x_j ,

$${}_{B}^{\mathrm{GL}}\mathbb{D}_{C}^{\pm}\begin{bmatrix}\alpha\\j\end{bmatrix} = \frac{1}{2}\left({}_{x_{j}^{1}}^{\mathrm{GL}}D_{x_{j},+}^{\alpha} \pm {}_{x_{j}^{2}}^{\mathrm{GL}}D_{x_{j},-}^{\alpha}\right),\tag{25}$$

which contain the Grünwald-Letnikov fractional operators defined on the finite interval $[x_j^1, x_j^2]$ with $x_j^1 = m_j^1 a_j$ and $x_j^1 = m_j^2 a_j$, in the form

$${}_{B}^{GL}D_{x_{j},\pm}^{\alpha}f(\mathbf{r},t) = \lim_{a_{j}\to0+} \frac{1}{\left|a_{j}\right|^{\alpha}} \sum_{m_{j}=0}^{M_{j}^{\pm}} \frac{(-1)^{m_{j}} \Gamma(\alpha+1)}{\Gamma(m_{j}+1) \Gamma(\alpha-m_{j}+1)} \times f(\mathbf{r} \mp m_{j}\mathbf{a}_{j},t),$$
(26)

where

$$M_j^+ = \left[\frac{x_j - x_j^1}{a_j}\right], \qquad M_j^- = \left[\frac{x_j^2 - x_j}{a_j}\right].$$
 (27)

The suggested forms of continuum fractional derivatives of the Grünwald-Letnikov type allow us to consider diffusion processes on bounded areas of nonlocal continuum.

The lattice diffusion equation (13) in the continuum limit gives the fractional diffusion equation with derivatives of noninteger orders with respect to space coordinates. This space-fractional diffusion equation for the probability density $f(\mathbf{r},t)$ has the form

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = -\sum_{i=1}^{3} D_{i}(\alpha)^{\mathrm{GL}} \mathbb{D}_{C}^{-} \begin{bmatrix} \alpha_{i} \\ i \end{bmatrix} f(\mathbf{r},t)
+ \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} D_{ij}(\alpha,\beta)^{\mathrm{GL}} \mathbb{D}_{C}^{-,-} \begin{bmatrix} \alpha_{i} & \beta_{j} \\ i & j \end{bmatrix} f(\mathbf{r},t),$$
(28)

where $D_i(\alpha)$ is the drift vector and $D_{ij}(\alpha,\beta)$ is the diffusion tensor for the continuum that are defined by the lattice coupling constants g_i and g_{ij} by the relations $D_i(\alpha) = g_i$, $D_{ij}(\alpha,\beta) = 2g_{ij}$. Similarly, the diffusion equation for bounded lattice gives the fractional diffusion equation for bounded region of continua

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = -\sum_{i=1}^{3} D_{i}(\alpha) {}_{B}^{GL} \mathbb{D}_{C}^{-} \begin{bmatrix} \alpha_{i} \\ i \end{bmatrix} f(\mathbf{r},t)
+ \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} D_{ij}(\alpha,\beta) {}_{B}^{GL} \mathbb{D}_{C}^{-,-} \begin{bmatrix} \alpha_{i} & \beta_{j} \\ i & j \end{bmatrix} f(\mathbf{r},t).$$
(29)

It should be noted that coincidence of orders of fractional derivatives in the first and second terms allows us to represent the fractional diffusion equation (28) in the form of the spacefractional continuity equation

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = -\sum_{i=1}^{3} {}_{GL} \mathbb{D}_{C}^{-} \begin{bmatrix} \alpha_{i} \\ i \end{bmatrix} J_{i}(\mathbf{r},t), \qquad (30)$$

where J_i is the probability flow

$$J_{i}(\mathbf{r},t) = D_{i}(\alpha) f(\mathbf{r},t) - \frac{1}{2} \sum_{j=1}^{3} D_{ij}(\alpha,\beta)^{\mathrm{GL}} \mathbb{D}_{C}^{-} \begin{bmatrix} \beta_{j} \\ j \end{bmatrix} f(\mathbf{r},t).$$
(31)

Equation (31) can be considered as the fractional phenomenological Fick first law for nonlocal media. If $\alpha_i = 1$ for all i = 1, 2, 3, the continuity equation (30) can be represented as the standard form of the well-known continuity equation

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = -\sum_{i=1}^{3} \frac{\partial J_i(\mathbf{r},t)}{\partial x_i},$$
(32)

where $J_i(\mathbf{r}, t)$ is defined by (31) with $\beta_i \neq 1$ in general.

For one-dimensional case with $D_i(\alpha) = 0$ and $f(\mathbf{r}, t) = f(x, t)$, (28) can be represented in the form

$$\frac{\partial f(x,t)}{\partial t} = K(\mu) \nabla^{\mu} f(x,t), \qquad (33)$$

where $K(\mu)$ is the generalized diffusion constant,

$$K(\mu) = \frac{1}{2}D_{11}(\alpha, \beta), \qquad (34)$$

and ∇^{μ} is the fractional derivative of order μ ,

$$\nabla^{\mu} = {}^{\mathrm{GL}} \mathbb{D}_{C}^{-} \begin{bmatrix} \alpha_{1} \\ x \end{bmatrix} {}^{\mathrm{GL}} \mathbb{D}_{C}^{-} \begin{bmatrix} \beta_{1} \\ x \end{bmatrix} = {}^{\mathrm{GL}} \mathbb{D}_{C}^{-} \begin{bmatrix} \alpha_{1} + \beta_{1} \\ x \end{bmatrix}, \qquad (35)$$

$$\mu = \alpha_{1} + \beta_{1}.$$

Here we use the semigroup property of fractional derivatives of the Grünwald-Letnikov type. Equation (33) describes the fractional diffusion processes with the Poissonian waiting time and the Lévy distribution for the jump length (see Section 3.5 of [22]). In [22] the space-fractional diffusion equation (33) contains the Weyl fractional derivative ∇^{μ} of order μ , of one-dimensional case. The solution of (33) can be obtained analytically by using the Fox function $H_{2,2}^{1,1}$ (for details see Section 3.5 of [22] and [28]). The exact calculation of fractional moments [22] gives

$$\left\langle \left| x\left(t\right) \right| ^{\delta} \right\rangle = \frac{2\left(K\left(\mu\right) \right) ^{\delta/\mu} \Gamma\left(-\delta/\mu\right) \Gamma\left(1+\delta\right) }{\mu\Gamma\left(-\delta/2\right) \Gamma\left(1+\delta/2\right) } t^{\delta/\mu}, \tag{36}$$

where $0 < \delta < \mu \le 2$.

Using (2), it is possible to demonstrate that the space-fractional diffusion equations are connected with continuous time random walk processes with diverging second moment of the jump length distribution [22].

If $\alpha_j = \beta_j = 1$ for all j = 1, 2, 3, then (28) and (29) give the well-known second-order diffusion equation

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = -\sum_{i=1}^{3} D_{i} \frac{\partial f(\mathbf{r},t)}{\partial x_{i}} + \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} D_{ij} \frac{\partial^{2} f(\mathbf{r},t)}{\partial x_{i} \partial x_{j}}, \quad (37)$$

where $D_i = D_i(1)$ is the drift vector and $D_{ij} = D_{ij}(1, 1)$ is the diffusion tensor for local continuum.

4. Conclusion

Lattice analog of the fractional-order differential equations for bounded and unbounded three-dimensional lattices with long-range jumps of particles is suggested. These lattice equations can be considered as a new microscopic basis to describe the fractional diffusion in nonlocal continua. In the lattice diffusion equations, we use the fractional-order difference analogs of fractional derivatives, which are represented by kernels that describe long-range jumps of lattice particles. The proposed kernels of long-range jumps on the lattice can be considered for integer and fractional orders of suggested difference operators. The continuous limits for these diffusion equations with fractional-order differences

give the continuum fractional derivatives of the Grünwald-Letnikov type with respect to space coordinates. The obtained fractional diffusion on nonlocal continua can be considered as a continuous limit of the suggested lattice diffusion, where the sizes of continuum elements are much larger than the distances between sites of the lattice. The main advantage of the suggested approach is a possibility to consider fractional-order difference diffusion equations as tools for formulation of a microstructural basic model of fractional diffusion in nonlocal continua. The proposed three-dimensional lattice diffusion equations can play an important role in formulating discrete models of nonlocal processes in microscale and nanoscale.

It is interesting to generalize the suggested lattice approach to consider lattice Lévy flights subject to external force fields and the Galilean invariance. This transport process on lattice can be described by lattice fractional diffusion equations. We assume that the lattice Lévy flights in a constant force field are similar to lattice fractional diffusion in a constant velocity field by analogy with diffusion processes in continuum models [29].

We assume that the proposed lattice approach to the lattice fractional diffusion can be generalized to different types of Bravais lattices such as monoclinic, triclinic, hexagonal, and rhombohedral lattices. We also assume that the suggested approach to the fractional diffusion can be generalized for lattice models with the fractal spatial dispersion, which are suggested in [30] (see also [31, 32]), and the continuum limits of these fractal lattice models can give continuum models of fractal media [33, 34] that are described by non-integer-dimensional space approach [35, 36].

Conflict of Interests

The author declares that there is no conflict of interests regarding the publication of this paper.

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