# NORMAL AND ANOMALOUS DIFFUSION OF GRAINS

**S.A. TRIGGER, G.J.F. VAN HEIJST [1], G.M.W. KROESEN [1], P.P.J.M. SCHRAM [1], E. STOFFELS [1], W.W. STOFFELS [1]**

**Joint Institute for High Temperatures, Russian Acad. Sci.**
*(Moscow 127412, Russia; e-mail: strig@gmx.net)*

[1]**Eindhoven University of Technology**
*(P.O. Box 516, 5600 MB Eindhoven, The Netherlands)*

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The problem of normal and anomalous space diffusion is formulated on the basis of the appropriate probability transition function for diffusion (PTD function). The method of fractional differentiation with respect to spatial coordinates is avoided to construct the correct probability distributions for arbitrary distances, which is important for applications to different stochastic problems. A general integral equation for a particle distribution, which contains the time-dependent PTD function with two times, is formulated and discussed. On this basis, the fractional differentiation with respect to time is also avoided and a wide class of time dependent PTD functions can be investigated.

Under usual conditions, the stochastic motion of grains leads to the second moment of the mass distribution that is linear in time. Such a type of diffusion processes plays a crucial role in plasmas, nuclear physics, and in many other problems. At the same time, a deviation from the linear dependence of the mean square displacement on time has been experimentally observed in many systems. The average square separation of a pair of particles passively moving in a turbulent flow grows, according to Richardson's law, with the third power of time [1]. For the diffusion typical of glasses and related complex systems [2], a dependence slower than a linear one is observed. These two types of anomalous diffusion obviously are characterized as superdiffusion and subdiffusion. For the description of these two diffusion regimes, various effective models and methods have been suggested. The continuous time random walk (CTRW) model of Scher and Montroll [3], leading to a strongly subdiffusive behavior, is a basis for understanding the photoconductivity in strongly disordered and glassy semiconductors. The Levy-flight models [4], leading to superdiffusion, describe such various phenomena as self-diffusion in micelle systems [5], reaction and transport in polymer systems [6], etc. For both cases, the so-called fractional differential equations in coordinate and time spaces are applied as an effective approach [7].

In this paper, we show that all known regimes of diffusion, as well as some new ones, can be effectively considered on basis of the appropriate probability transition function for diffusion (PTD function) $W_D(\mathbf{r}-\mathbf{r}',\mathbf{t},\mathbf{t}')$. Depending on the specific structure of this function, the usual diffusion, superdiffusion, and subdiffusion can be described without fractional differentiation with respect to coordinates and time.

The relation between diffusion in the coordinate and velocity spaces has been considered recently in [8] on the basis of a probability transition function $W_V(V,t)$ for the velocity space (PTV) [9]. However, this approach is not applicable for the calculation of some special types of spatial diffusion in the coordinate space, when the PTD function has slowly decreasing tails in the coordinate space. Anomalous diffusion can be related not only to coordinate-, but also, in general, to time-dependent PTD functions. To describe all interesting cases, we suggest to use the approach of the PTD function. We also formulate a general integral equation for the distribution function of particles $f_g(\mathbf{r},t)$, which gives the most general description of normal and anomalous diffusions.

Let us consider diffusion in the coordinate space on the basis of a master equation, which describes the balance of grains coming in and out the point $\mathbf{r}$ at the moment $t$. The structure of this equation is formally similar to the master equation in the momentum space. Of course, for the coordinate space, there is no conservation law similar to that in the momentum space:

$$\frac{df_g(\mathbf{r},t)}{dt}=\int d\mathbf{r}'\left\{W(\mathbf{r},\mathbf{r}')f_g(\mathbf{r}',\mathbf{t})-W(\mathbf{r}',\mathbf{r})f_g(\mathbf{r},t)\right\}.\quad(1)$$

Here and below, we use the simplified notation $W$ for a PTD function $W_D$. The probability transition $W(\mathbf{r},\mathbf{r}')$ describes the probability for a grain to transfer from the point $\mathbf{r}'$ to the point $\mathbf{r}$ per unit time. We can rewrite this equation in the coordinates $\mathbf{u}=\mathbf{r}'-\mathbf{r}$ and $\mathbf{r}$ as

$$\frac{df_g(\mathbf{r},t)}{dt}=$$


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$$= \int d\mathbf{u} \left\{ W(\mathbf{u}, \mathbf{r} + \mathbf{u}) f_g(\mathbf{r} + \mathbf{u}, \mathbf{t}) - W(\mathbf{u}, \mathbf{r}) f_g(\mathbf{r}, t) \right\}. \quad (2)$$

Assuming that the characteristic displacements are small, one may expand Eq. (2) and arrive at the Fokker—Planck form of the equation for the density distribution $f_g(\mathbf{r}, t)$

$$\frac{df_g(\mathbf{r}, t)}{dt} = \frac{\partial}{\partial r_\alpha} \left[ A_\alpha(\mathbf{r}) f_g(\mathbf{r}, t) + \frac{\partial}{\partial r_\beta} \left( B_{\alpha\beta}(\mathbf{r}) f_g(\mathbf{r}, t) \right) \right]. \quad (3)$$

The coefficients $A_\alpha$ and $B_{\alpha\beta}$ describing the acting force and diffusion, respectively, can be written as functionals of the probability function (PTD) in the coordinate space $W$ in the form

$$A_\alpha(\mathbf{r}) = \int d^s u u_\alpha W(\mathbf{u}, \mathbf{r}) \quad (4)$$

and

$$B_{\alpha\beta}(\mathbf{r}) = \frac{1}{2} \int d^s u \, u_\alpha u_\beta W(\mathbf{u}, \mathbf{r}), \quad (5)$$

where $s$ is the dimension of the coordinate space.

This consideration cannot be applied to specific situations in which the integral in Eq. (5) is infinite. In this case, we have to examine the general transport equation (1). We will now consider the problem for the homogeneous and isotropic case where the PTD function depends only on $|\mathbf{u}|$. By Fourier-transformation, we arrive at the following form of Eq. (1):

$$\frac{df_g(\mathbf{k}, t)}{dt} = \int d^s u \left[ \exp(i\mathbf{k} \cdot \mathbf{u}) - 1 \right] W(u) f_g(\mathbf{k}, t) \equiv$$

$$\equiv X(\mathbf{k}) f_g(\mathbf{k}, t). \quad (6)$$

Here, $X(\mathbf{k}) \equiv X(k)$ and $W(u) \equiv W(|\mathbf{u}|)$. Let us assume a simple form of the PTD function with a power dependence on the distance $W(u) = C/|\mathbf{u}|^\alpha$, where $C$ is a constant and $\alpha > 0$. Such singular dependence is typical of the jump diffusion probability in heteropolymers in a solution (see, e.g., [10], where the different applications of anomalous diffusion are considered on the basis of the fractional differentiation method). In the one-dimensional case, we find

$$X(k) \equiv -4 \int_0^\infty du \, \sin^2 \left( \frac{k u}{2} \right) W(u) =$$

$$= -2^{3-\alpha} C |k|^{\alpha-1} \int_0^\infty d\zeta \frac{\sin^2 \zeta}{\zeta^\alpha}. \quad (7)$$

For $1 < \alpha < 3$, this function is finite and is equal to

$$X(k) = -\frac{C \, \Gamma[(3-\alpha)/2] \, |k|^{\alpha-1}}{2^\alpha \sqrt{\pi} \, \Gamma(\alpha/2)(\alpha - 1)}, \quad (8)$$

where $\Gamma$ is the gamma-function. At the same time, integral (5) for such a type of PTD functions is infinite, because usual diffusion is absent. The considered procedure for the simplest cases of a power dependence of the PTD function is equivalent to the equation with fractional space differentiation [7, 10]

$$\frac{df_g(x, t)}{dt} = \tilde{D} \Delta^{\mu/2} f_g(x, t), \quad (9)$$

where $\tilde{D}$ is the diffusion coefficient for (in general) the processes of a non-Fokker-Planck type. The linear operator $\Delta^{\mu/2}$ is a fractional Laplacian, whose action $\Delta^{\mu/2} f(x)$ on a function $f(x)$ in the Fourier space is described by the relation $-(k^2)^{\mu/2} \tilde{f}(k) = -|k|^\mu \tilde{f}(k)$, where $\tilde{f}(k)$ is the Fourier transform of a function $f(x)$. In the case considered above, $\mu \equiv (\alpha - 1)$, where $0 < \mu < 2$, and $\tilde{D}$ is proportional to $C$. For more general PT functions which (for arbitrary values of $u$) are not proportional to the $\alpha$-th power of $u$, the method described above is also applicable, although the fractional derivative does not exist.

For the case of a pure power dependence of the PT, the non-stationary solution for the density distribution describes the so-called super-diffusion (or Levy flights). The solution of Eq. (9) in the Fourier space reads

$$\tilde{f}_g(k, t) = \exp(-\tilde{D} |k|^\mu t), \quad (10)$$

which corresponds in the coordinate space to the so-called symmetric Levy stable distribution:

$$f_g(x, t) = \frac{1}{(\tilde{D}t)^{1/\mu}} L \left[ \frac{x}{(\tilde{D}t)^{1/\mu}}; \mu, 0 \right]. \quad (11)$$

In the general case, it follows from Eq. (6) that

$$f_g(k, t) = C_1 \exp[X(k)t] \quad (12)$$

with some constant $C_1$.

In the same way, we can consider the three-dimensional case.

Of course, the consideration on the basis of the PTD function given above allows one to avoid the fractional differentiation method and to consider more general physical situations of the non-power probability transitions. Let us consider that for a simple example.

Taking (in the one-dimensional case) the PT function $W(u)$ in the form

$$W(u) = C\frac{1-\exp[-\sigma u^p]}{u^\alpha} \tag{13}$$

with $p > 0$, we arrive at the function

$$X(k) = -2^{3-\alpha}C|k|^{\alpha-1}T(\sigma/|k|^p,\alpha), \tag{14}$$

where

$$T(\sigma/|k|^p,\alpha) = \int_0^\infty d\zeta \frac{\{1-\exp[-\sigma(2\zeta/|k|)^p\,]\}\sin^2\zeta}{\zeta^\alpha}. \tag{15}$$

It is easy to see that the function $T(\sigma/|k|^p,\alpha)$ is finite for $1 < \alpha < p+3$, because, for small values of the distance for $p > 0$, the divergence is suppressed also for some powers $\alpha > 3$. A simple calculation for $\alpha = 2$ and $p = 1$ leads to the following result, which cannot be found by the usual fractional differentiation method:

$$T(\sigma/|k|,2) = \frac{\pi}{2} - \arctan(|k|/\sigma) + \frac{\sigma}{2|k|}\ln\left[1+k^2/\sigma^2\right]. \tag{16}$$

The asymptotic behavior of the function $X(k)$ for $k \to \infty$ is similar, as follows from Eq. (16), to the case $W(u) = C/u^\alpha$. Therefore, the universal behavior of $X(k)$ is provided by the asymptotical properties of the PTD function for $1 < \alpha < 3$.

It should be noted in connection with the problem of a generalized description of diffusion that not only the space dependence, but also the time dependence of the PTD function can be very different from the case of classical diffusion. This kind of problems is related to the class of stochastic transport, which describes the so-called subdiffusive behavior [3].

Let us formulate a more general transport equation for the density distribution:

$$f_g(\mathbf{r},t) = f_g(\mathbf{r},t=0) + \int_0^t d\tau \int d\mathbf{r}'\{W(\mathbf{r},\mathbf{r}',\tau,t-\tau)f_g(\mathbf{r}',\tau) - W(\mathbf{r}',\mathbf{r},\tau,t-\tau)f_g(\mathbf{r},\tau)\}. \tag{17}$$

For the case of a stationary PTD function, we return to Eq. (1). In the absence of memory effects, but with the PT function being a function of the current time $\tau$, we arrive at an equation that is more general than Eq. (1), which describes the density evolution with a prescribed time-dependence of the PTD function.

If the system possesses memory and the function $W$ can be expanded in the coordinate space in the spirit of the Fokker—Planck approximation, we arrive at the generalized Fokker—Planck equation with time integration.

If the function $W$ possesses memory and depends only on the difference $t-\tau$, but cannot be expanded in the coordinate space, we can use the Laplace-transformation in time to find

$$f_g(\mathbf{r},z) = \frac{f_g(\mathbf{r},t=0)}{z} + \int d\mathbf{r}'\left\{W(\mathbf{r},\mathbf{r}',z)f_g(\mathbf{r}',z) - W(\mathbf{r}',\mathbf{r},z)f_g(\mathbf{r},z)\right\}. \tag{18}$$

The function $W(\mathbf{r}',\mathbf{r},z)$ is determined by the equality

$$W(\mathbf{r}',\mathbf{r},z) = \int_0^\infty d\tau W(\mathbf{r}',\mathbf{r},\tau)\exp(-z\tau). \tag{19}$$

For the spatially homogeneous case, Eq. (18) can be Fourier-transformed as

$$\tilde f_g(\mathbf{k},z) = \frac{\tilde f_g(\mathbf{k},t=0)}{z\left[1-X(\mathbf{k},z)\right]}, \tag{20}$$

where

$$X(\mathbf{k},z) = \int d^s u\left[\exp(i\mathbf{k}\cdot\mathbf{u})-1\right]W(|\mathbf{u}|,z). \tag{21}$$

If the PT function is time-independent, $W(|\mathbf{u}|,z) = W(|\mathbf{u}|)/z$ and $\tilde f_g(\mathbf{k},t=0)$ =const, we return to the case of anomalous diffusion considered above in Eqs. (6)-(16). For a general multiplicative form of the PT function $W(|\mathbf{u}|,\tau) = W_1(|\mathbf{u}|)W_2(\tau)$ (generalized Levy flights), the function

$$X(\mathbf{k},z) \equiv X_1(k)X_2(z) = \int d^s u\left[\exp(i\mathbf{k}\cdot\mathbf{u})-1\right]\times W_1(|\mathbf{u}|)\int_0^\infty d\tau W_2(\tau)\exp(-z\tau). \tag{22}$$

We arrive at the following result for the distribution $\tilde f_g(k,z)$:

$$\tilde f_g(\mathbf{k},z) = \frac{\tilde f_g(\mathbf{k},t=0)}{z\left[1-X_1(\mathbf{k})X_2(z)\right]}. \tag{23}$$

Avoiding the fractional differentiation with respect to both coordinates and time, we essentially extend and simplify the description of anomalous diffusion for PTD functions being more general than power-type ones.



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To consider the particular case of the general equation (17), in which both the retardation and prescribed time dependence are present in the kernel $W$, we can choose the simplest form of a multiplicative PTD function with exponential retardation:

$$W(\mathbf{r},\mathbf{r}',\tau,t-\tau) \equiv W_1(\mathbf{r},\mathbf{r}')W_2(\tau,t-\tau) =$$

$$= W_1(\mathbf{r},\mathbf{r}')\hat{W}_2(\tau)\exp\left[-\frac{(t-\tau)}{\tau_0}\right]. \quad (24)$$

For a homogeneous case, Eq. (17) can be analytically solved after the Fourier-transformation with respect to the space variable $u$.

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## НОРМАЛЬНА Й АНОМАЛЬНА ДИФУЗІЯ ЧАСТИНОК ПИЛУ

*С.А. Тріггер, Г.Я.Ф. ван Хейст, Г.М.В. Кроузен, П.П.Я.М. Шрам, Е. Стоффелс, В.В. Стоффелс*

Р е з ю м е

Сформульовано задачу аномальної та нормальної дифузії на основі відповідної функції імовірності транспорту частинок. Із коректної побудови розподілу імовірностей для довільних інтервалів вилучено метод дробових похідних по координатах, що важливо для різних стохастичних задач. Сформульовано й обговорюється загальне інтегральне рівняння для розподілу частинок, яке містить функцію імовірності, що залежить від часу. Завдяки цьому також виключено дробову похідну по часу і можна досліджувати широкий клас часових функцій імовірності.