## Mysteries of diffusion and labyrinths of destiny

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<u>Abstract.</u> The role of prominent Soviet physicist B I Davydov in the development of our understanding of diffusion is briefly reviewed, with emphasis on the ideas he put forward in the 1930s: introducing additional partial derivatives into diffusion equations and extending diffusion concepts to phase space.

Davydov Boris Iosifovich (1908–1963) is one of the classic scientists of Soviet physics. His paper entitled "On the velocity distribution of electrons moving in an electric field" was inserted in the anniversary issue of *Sov. Phys. Usp.* in 1967 [1]. That issue of *Sov. Phys. Usp.* was dedicated to the fifty years of Soviet physics and included the best papers of scientists of our country, as selected by the Editorial Board.

B I Davydov belonged to the Leningrad school of physics. In the mid-30s, he carried out his most famous works concerned with the development of diffusion concepts [4-7]. During the next 10 years he actively pursued semiconductor physics research [9-19]. The significance of his work in this field was emphasized by Zh I Alferov at a conference held at the Russian Research Centre 'Kurchatov Institute'. Davydov concerned himself about the problems of irreversibility in statistical physics and quantum mechanics [22-25]. From the early 50s he was actively engaged in controlled thermonuclear fusion (CTF) research. B I Davydov was the scientific supervisor of S I Braginskiĭ who deduced particle and heat fluxes in a fully ionized plasma [36]. Davydov himself took then an interest in the effect of plasma oscillations on its thermal and electrical conduction [27]. The name of B I Davydov as a leader of the works is repeatedly mentioned in the Annex No. 1 to the historic USSR Council of Ministers Resolution of May 5, 1951 entitled "Program of Theoretical Investigations to Elucidate the Feasibility of a Magnetic Thermonuclear Reactor" [37].

However, information on B I Davydov is missing from the reference book on Soviet and Russian physicists [38]. This surprising fact is not merely the result of an accidental blunder in his personal file in which his initials were confused. The time wherein he lived and worked left its tragic imprint on his scientific career. In 1952, he was dismissed from the Kurchatov Institute as a 'suspect', but was able to resume working at the Institute of Physics of the Earth (Moscow) on the problems of hydrodynamic turbu-

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Davydov Boris Iosifovich (1908-1963)

lence [29-32]. Today his ideas enjoy wide application to the description of strongly nonequilibrium systems. The amazing physical clarity of his papers is particularly appealing nowadays, when the number of publications in scientific journals is huge and the meaning quite often concealed by a multitude of details. Here we briefly discuss only four of Davydov's papers, but give the complete list of his publications.

In 1934, Davydov published a short article [5] in which he came up with the idea of modifying the conventional diffusion equation

$$\frac{\partial n}{\partial t} = D \, \frac{\partial^2 n}{\partial x^2} \,. \tag{1}$$

His idea involved the incorporation of additional partial derivatives in the classical equation with the aim of describing fast transfer processes. This problem was topical in connection with the investigation of turbulent diffusion, performed by L Richardson in 1926 [39], who discovered a significant departure of diffusion laws from the classical one:

$$R^2 \propto t^3 \gg t$$
 or  $D \approx \frac{R^2}{t} \propto R^{4/3}$ . (2)

Davydov invoked a phenomenological system of equations for the particle number density n(x, t):

$$\frac{\partial n}{\partial t} + \frac{\partial q}{\partial x} = 0, \quad \frac{\partial q}{\partial t} = \frac{q_0 - q}{\tau}, \quad (3)$$

where  $\tau$  is the scale of time, and  $q_0 = -D(\partial n/\partial x)$ . Formal calculations lead to the telegraph equation

$$\frac{\partial n}{\partial t} + \tau \frac{\partial^2 n}{\partial t^2} = D \frac{\partial^2 n}{\partial x^2}.$$
(4)

This is an equation of the hyperbolic type, which opens up additional possibilities of using characteristics to describe nonlocal effects. Davydov suggested that it be used to allow for the finite particle velocity v in molecular diffusion. The classical diffusion equation of the parabolic type would result from the telegraph equation in passing to the limit  $\tau \to 0$ , when  $D \approx v^2 \tau \to \text{const.}$  As one would expect, in the ordinary case

$$v \propto \sqrt{\frac{D}{\tau}}$$
 or  $R^2 \propto t$ , and  $v \propto \frac{1}{\sqrt{\tau}} \to \infty$ .

More recently, Cattaneo [40], Goldstein [41], Davies [42], Lyapin [43], and Monin [44] took advantage of the telegraph equation to describe diffusion.

The physical significance of Davydov's representation for the particle flux q is easily comprehended in writing down the formal solution

$$q = \int_0^t q_0(x, t') \exp\left[-\frac{t-t'}{\tau}\right] \frac{\mathrm{d}t'}{\tau} \,. \tag{5}$$

Evidently, the expression for the flux includes 'memory' effects. Subsequently, this formula was repeatedly generalized with the use of an arbitrary memory function M(t - t') in lieu of the exponential one:

$$q = \int_0^t q_0(x, t') M(t - t') \frac{dt'}{\tau}.$$
 (6)

Performing the Fourier transform with respect to the coordinate we obtain for the general case

$$\frac{\partial \tilde{n}_k(t)}{\partial t} = -k^2 \int_0^t \tilde{n}_k(t) M(t-t') \frac{\mathrm{d}t'}{\tau} = -k^2 M(t) * \tilde{n}_k(t) \,.$$
(7)

Here, we perceive an intimate relationship between Davydov's ideas and the Einstein – Smoluchowski functional. In its simplest form, the functional is of the form

$$\frac{\partial n}{\partial t} = \int_{-\infty}^{+\infty} G(x - x') \, n(x', t) \, \mathrm{d}x' \,. \tag{8}$$

The Fourier representation of this nonlocal functional with respect to the *x*-variable leads to the expression

$$\frac{\partial \tilde{n}_k(t)}{\partial t} = \tilde{G}(k) \, \tilde{n}_k(t) \,, \tag{9}$$

which is indicative of the absence of memory effects for the Fourier harmonics. To the classical diffusion equation, with regard to the Laplace transform, herein there corresponds

$$\tilde{G}(k,\omega)\tilde{n}_{k,\omega} = -Dk^2\tilde{n}_{k,\omega}.$$
(10)

In Davydov's case, the memory effects are retained, so that

$$\widetilde{G}(k,\omega)\widetilde{n}_{k,\omega} = -\frac{Dk^2}{1-i\omega\tau}\,\widetilde{n}_{k,\omega}\,. \tag{11}$$

This form of writing was undoubtedly familiar to Davydov in connection with Kolmogoroff's research [45] devoted to the Fokker–Planck equations, in which Davydov also took an interest at that time [4], as well as owing to his activity as a scientific editor [33-35]. As early as 1937, the idea of modifying the diffusion equation received impetus in the papers of Khintchine and Levy [46]. They resorted to an approximation of the form

$$\frac{\partial \tilde{n}_k(t)}{\partial t} = -k^{\alpha} \tilde{n}_k(t), \quad 0 < \alpha \le 2.$$
(12)

Monin's work in this field [44] anticipated the modern-day development of the ideas of employing additional fractional partial derivatives in diffusion equations. Leaning upon Kolmogoroff's ideas of universal turbulence properties, he obtained the following relationship from similarity considerations for turbulent diffusion:

$$\widetilde{G}(k) \propto \widetilde{G}(\varepsilon, k) = \varepsilon^{1/3} k^{2/3},$$
(13)

where  $\varepsilon$  is the rate of energy dissipation. This representation in fact satisfies Richardson's results obtained in 1926 [39], which were the subject of Davydov's analysis. If it is assumed that  $\tilde{G}(k) = -D(k)k^2$ , then one obtains

$$D(k) \approx \frac{R^2}{t} \propto R^{4/3} \propto k^{-4/3} \,. \tag{14}$$

Furthermore, according to present-day nomenclature [47], the equation

$$\frac{\partial \tilde{n}_k(t)}{\partial t} = -k^{2/3} \tilde{n}_k(t) \tag{15}$$

is an equation with a fractional derivative with respect to x:

$$\frac{\partial^{\alpha} n}{\partial x^{\alpha}} \propto \frac{n}{\left(\Delta x\right)^{\alpha}} \propto k^{\alpha} n \,,$$

where  $\alpha = 2/3$ . However, Monin did not content himself with this form. Endeavoring to arrive at an equation as clear as the telegraph one, he resorted to double differentiation with respect to time to bring his equation to the form

$$\frac{\partial^3 n}{\partial t^3} = \varepsilon \frac{\partial^2 n}{\partial x^2} \,. \tag{16}$$

We now see that after a lapse of many years following Davydov's theoretical paper the diffusion equations would repeatedly be 'complemented' with various partial derivatives

$$\frac{\partial^2 n}{\partial t^2}, \quad \frac{\partial^3 n}{\partial t^3}, \quad \frac{\partial^{\alpha} n}{\partial t^{\alpha}}, \quad \frac{\partial^{\beta} n}{\partial x^{\beta}}$$
(17)

with the aim of describing the effects of nonlocality and memory. Both cases are easily generalized by representing the memory and nonlocality effects in a common equation

$$\frac{\partial \tilde{n}_k(t)}{\partial t} = -k^2 \int_0^t \tilde{n}_k(t) \widetilde{D}(k, t-t') \frac{\mathrm{d}t'}{\tau} = -k^2 \widetilde{D}(k, t) * \tilde{n}_k(t) ,$$
(18)

or, having regard to the Laplace transform with respect to time, one has

$$-k^2 D \to -k^2 \widetilde{D}(k,\omega)$$
. (19)

Undoubtedly, Davydov was aware of the 'formal character' of employing the telegraph equation for the description of complex diffusion processes. The physics of strongly nonequilibrium systems should be closely related to the particle velocity distribution function which deviates widely from the Maxwellian function. An excellent case in point was the Druyvesteyn distribution function. It was precisely this distribution function which was the concern of Davydov's classical paper published in 1936 [6]. In this paper he considered the kinetic equation for electrons moving in stationary conditions in a weakly ionized plasma:

$$-\frac{e\mathbf{E}}{m_{\rm e}}\frac{\partial f}{\partial \mathbf{v}} = \mathrm{St}_{\mathrm{e}-\mathrm{a}}[f], \qquad (20)$$

where  $St_{e-a}[f]$  is the electron – atom collision integral.

Unlike his predecessors, Davydov included in the collision integral not only the electron energy loss due to 'friction' on atoms, but the diffusive gain of energy as well. For the symmetric part of the electron distribution function he derived the expression

$$St_{e-a}[f] = \frac{1}{v^2} \frac{\partial}{\partial v} \left[ \frac{m_e}{M} v^3 v(v) \left( \frac{T_a}{m_e v} \frac{\partial f}{\partial v} + f \right) \right].$$
(21)

Indeed, elementary estimates indicate that both processes are of the same order of magnitude. However, another important point is that the condition  $St_{e-a}[f] = 0$  should lead to the Maxwellian electron distribution function with a temperature  $T_a$ . Davydov derived this condition without phenomenological assumptions by solving the kinetic equation with the use of expansion of the distribution function in terms of Legendre polynomials:

$$f(\mathbf{v}) = F_0(v) + F_1(v)\cos\theta.$$
(22)

On rearrangement (22), Davydov represented the divergent type equation for the fluxes in the velocity space as

$$\frac{1}{v^2} \frac{\mathrm{d}}{\mathrm{d}v} \left[ v^2 J(v) \right] = 0.$$
<sup>(23)</sup>

From the condition that the particle source is nonexistent for a momentum  $p \rightarrow 0$ , Davydov derived a diffusive type equation for the particle flux:

$$J(v) = \frac{2}{3} \frac{e^2 E^2}{m_e^2 v_T^2} \frac{dF_0}{dv} + \chi_{e-a} \left( vF_0 + \frac{T_a}{m_e} \frac{dF_0}{dv} \right) = 0.$$
 (24)

Davydov managed not only to transfer the diffusion concepts from ordinary space to phase space, but also to obtain an elegant solution of the Fokker–Planck equation for the symmetric part of the electron distribution function:

$$F_0(v) = A \exp\left\{-\int_0^v \frac{m_e v \,\mathrm{d}v}{T_a + 2e^2 E^2 / 3\chi_{e-a} v_T^2 m_e}\right\}.$$
 (25)

Here, the nature underlying the disparity between the electron and atomic temperatures is readily apparent. This solution formed the firm basis for the study of nonequilibrium phenomena in a weakly ionized plasma.

In his next paper [7], Davydov employed the clear concepts of sources and outflows in phase space for the kinetic description of atomic ionization by electrons. In particular, when the average electron temperature is far greater than the atomic temperature, for the electrons with energies below the ionization threshold we have

$$-\frac{1}{3v^2} \frac{d}{dv} \left( \frac{e^2 E^2}{m_e^2 v_T} v^2 \frac{dF_0}{dv} \right)$$
$$= \frac{1}{2v^2} \frac{d}{dv} (\chi_{e-a} v_T v^3 F_0) + \frac{Q}{4\pi v^2} \delta(v) .$$
(26)

Here,  $\delta$  is the symbol of the Dirac function, and Q is the total number of inelastic collisions per unit time. Davydov accomplished the matching of solutions obtained in different velocity ranges by taking advantage of the 'flux' concepts in the phase space. His papers thereby laid the foundations for the methods of solution of specific Fokker–Planck equations.

The most prominent embodiment of Davydov's concepts is in the papers of Gurevich [48, 49] concerned with runaway electrons. These papers report the construction of the solution of the kinetic equation for fast electrons moving in a strongly ionized plasma in the presence of a stationary electric field:

$$-\frac{eE}{m_{\rm e}} \left( \mu \frac{\partial f}{\partial v} + \frac{1-\mu^2}{v} \frac{\partial f}{\partial \mu} \right) = \frac{1}{v^2} \frac{\partial}{\partial v} \left[ v^2 v_{\rm e}(v) \left( vf + \frac{T_{\rm e}}{m} \frac{\partial f}{\partial v} \right) \right] + \beta v_{\rm e}(v) \frac{\partial}{\partial \mu} \left[ (1-\mu^2) \frac{\partial f}{\partial \mu} \right].$$
(27)

Here, the following notation was used:

$$\beta = \frac{1 + Z_{\text{eff}}}{2}, \quad Z_{\text{eff}} = \frac{1}{n_{\text{e}}} \sum_{i} Z_{i} n_{i},$$
$$v_{\text{e}}(v) = \frac{4\pi e^{4} \Lambda n_{\text{e}}(x)}{m_{e}^{2} v^{3}}, \quad \mu = \cos \theta.$$

The ideas of diffusion in the phase space allowed the derivation of the analytical solution for the distribution function and the runaway particle flux. In doing this, recourse was made to arduous asymptotic expansions. The solutions were constructed in several domains of definition and matched with the aim of estimating the total runaway electron flux. This approach, which can be traced back to Davydov's papers, has now come to be the classics.

Being fully aware of the necessity of linking the kinetic description to the diffusion equation in ordinary coordinate space, in 1937 Davydov considered a spatially nonuniform kinetic problem [8]:

$$\mathbf{v} \,\frac{\partial f}{\partial \mathbf{r}} - \frac{e\mathbf{E}}{m} \,\frac{\partial f}{\partial \mathbf{v}} = \mathbf{St}_{\mathrm{e-a}}[f]\,. \tag{28}$$

However, the result he obtained was only a partial solution to the problem posed. In 1940, Kramers [50] pointed to the difficulties encountered in an attempt to obtain the diffusion equation in ordinary coordinate space:

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x} \left( Un \right) + D \frac{\partial^2 n}{\partial x^2} , \qquad (29)$$

from the simplest kinetic equation which includes the spatial nonuniformity, viz.

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F(x)}{m} \frac{\partial f}{\partial v} = \frac{1}{\tau} \frac{\partial}{\partial v} \left( vf + \frac{kT}{m} \frac{\partial f}{\partial v} \right).$$
(30)

Here U is the mean velocity, and F(x) is the force. Even here a demand arose for a 'smart trick' with integration over trajectory in lieu of 'conventional averaging'. However, this did not become a forcible argument for the introduction of heuristic corrections to the kinetic equation at that time. Kramers in fact pointed to the conventional character of the diffusion equation in use and to its intimate linkage to the notions of the behavior of correlation functions.

During the 1950s - 1990s, a huge volume of research was carried out with the aim of deriving hydrodynamic equations as well as refining the kinetic equations themselves [58-61]. The work of Albritton et al. [51] came to be an interesting outgrowth of the problem of describing the kinetics of fast electrons in a spatially nonuniform plasma. Taking advantage of conventional techniques and a variable  $W = mv^2/2$ , they considered the equation for the symmetric part of the electron distribution function in the form

$$\frac{\partial^2 F_0}{\partial x^2} + \frac{1}{W^3} \frac{\partial}{\partial W} \left( F_0 + T_c(x) \frac{\partial F_0}{\partial W} \right) = 0.$$
(31)

The aspiration to make the equation recognizable led to a simplification:

$$\frac{\partial F_0}{\partial W} \to \frac{\partial F_{\text{Maxwell}}}{\partial W} \,. \tag{32}$$

These rearrangements resulted in a parabolic diffusion equation with a source wherein the parameter  $\xi = W^4$  appears as time:

$$\frac{\partial^2 F_0}{\partial x^2} + \beta \, \frac{\partial F_0}{\partial \xi} = Q(\xi(W), x) = -\frac{T_e(x)}{W^3} \, \frac{\partial^2 F_{\text{Maxwell}}}{\partial W^2} \,. \tag{33}$$

This equation is solved with the aid of the Green function. However, despite the integral form of its solution, the nonlocal effects in this parabolic equation were largely lost, because the contribution from fast electrons was underrated.

Endeavors to improve the kinetic description of strongly nonequilibrium systems has recently led to the 'transfer' of the techniques worked out for describing anomalous diffusion in ordinary space to phase space. In the 1980s and 1990s, an increasing number of authors persist in the opinion that the equations, which had come to be regarded as classical, should be modified. For instance, in Ref. [52] it was proposed to complement the kinetic equation with the term  $\partial^2 f/\partial t^2$ . This, like the telegraph equation mentioned above, would conceivably afford the description of 'fast processes' in kinetics. It was proposed in Ref. [37] to complement the kinetic equation with a term of the form  $\partial^2 f/\partial x^2$  for the description of spatial nonlocality [53, 54]. The possibility to complement the kinetic equation with the terms

$$\frac{\partial^2 f}{\partial x^2}, \quad \frac{\partial^3 f}{\partial x^2 \partial t}, \quad \frac{\partial^3 f}{\partial x^3}$$

was considered in the book [55]. Conceivably, this might allow a description of non-Gaussian random sources in the Langevin equations. Under active examination [56, 57] is the employment of the 'arsenal' of fractional derivatives

$$\frac{\partial^{\alpha} f}{\partial v^{\alpha}}, \quad \frac{\partial^{\alpha} f}{\partial x^{\alpha}}, \quad \frac{\partial^{\alpha} f}{\partial t^{\alpha}}$$

In reality, this is merely an 'approximation of nonlocal terms' using various types of partial derivatives of the distribution function. The examples considered in our paper testify to the topicality of the approaches developed by B I Davydov in the 1930s and to his intuition.

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