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Local immobilization of particles in mass transfer described by a Jeffreys-type equation

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We consider the Jeffreys-type equation as the foundation in three different models of mass transfer, namely, the Jeffreys-type and two-phase models and the D_1 approximation to the linear Boltzmann equation. We study two classic $(1 + 1)$-dimensional problems in the framework of each model. The first problem is the transfer of a substance initially confined at a point. The second problem is the transfer of a substance from a stationary point source. We calculate the mean-square displacement (MSD) for the solutions of the first problem. The temporal behavior of the MSD in the framework of the first and third models is found to be the same as that in the Brownian motion described by the standard Langevin equation. In addition, we find a remarkable phenomenon when a portion of the substance does not move.

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I. INTRODUCTION

The classic diffusion equation, based on Fick's law, is widely used for the approximate description of nonanomalous diffusion (dispersion of a substance or species) [1,2] and Brownian motion [3–5]. However, Fick's law neglects the mass (inertia) of moving particles (molecules) and therefore the diffusion equation gives an appropriate and accurate model for diffusion phenomena only in weakly inhomogeneous media and/or for slow processes when relaxation time is short compared to a characteristic time scale. Otherwise, the description of diffusion by the diffusion equation may fail [6]. Many biological media, e.g., cellular cytoplasm, are strongly inhomogeneous, therefore, diffusion in them is not Fickian and its description by the diffusion equation is questionable.

Note that the counterpart of Fick's law is Fourier's law in the theory of heat conduction [1,2,7]. The latter leads to the heat equation, similar to the diffusion equation. Fick's law was postulated by analogy with Fourier's law, which was proposed first [2].

The simplest modification of Fick's law, taking into account the inertia of moving particles, is Cattaneo's equation [8–10]. Strictly speaking, Cattaneo's equation modifies Fourier's law since Cattaneo considered heat conduction; however, one can apply this to mass transfer as well. The modification leads to the telegraph equation, providing the finite speed of propagation [8,9,11–14]. The telegraph equation was proposed to be a substitute for the diffusion and heat equations. However, both two- and three-dimensional telegraph equations meet formal obstacles since solutions to the initial-value problem for them may become negative [15,16].

Long before Cattaneo, Jeffreys proposed a relation for the rheological description of the earth's core [17,18] that can be considered as a combination of Fick's (or Fourier's) law and Cattaneo's equation. We define this law (relation) as being of the Jeffreys type. This law leads to a partial differential equation of third order, called a Jeffreys-type equation [8,9], also known as the simplest equation of the dual-phase-lag model of heat conduction [10,19,20]. We call this a Jeffreys-type model. This model was used to describe viscoelastic fluids [8,21,22], Taylor dispersion [22,23], and heat transfer [8–10,14,19,20,24–28].

There is another two-temperature [10,14,19,20,24] or two-phase [29–32] model that also leads to a Jeffreys-type equation. This model is qualitatively different from the Jeffreys-type one. Nevertheless, there is no clear distinction between cases when the Jeffreys-type equation describes the Jeffreys-type model and the two-temperature (two-phase) model [14,20,24]. Moreover, in Ref. [24] the behavior of the two-temperature model is illustrated by that of the Jeffreys-type model. In Ref. [33] the authors erroneously state that the two models are equivalent.

The diffusion equation is known to be the simplest approximation to the linear Boltzmann equation [34] and the latter can be considered as a mesoscopic model of the former. It is notable that the telegraph equation is the P_1 approximation (the next after the diffusion one) to the linear Boltzmann equation [34]. Recently, D_N approximations to the linear Boltzmann equation were proposed [35]. They generalize the classic diffusion approximation, which corresponds to $N = 0$. We have found that the $D_{N=1}$ approximation (the next after the telegraph one) leads to the Jeffreys-type equation, the model being qualitatively different from both the Jeffreys type and two-phase ones. Note that this model is similar to the one of Guyer and Krumhansl in the theory of second sound [10,14,36,37].

The primary motivation of this study was to investigate the Jeffreys-type equation as a substitute for the diffusion equation instead of the telegraph one for the description of mass transfer. We study and compare eventually the three models (the Jeffreys-type and two-phase models and the $D_{N=1}$ approximation to the linear Boltzmann equation) as models of mass transfer. We study two classic $(1 + 1)$-dimensional problems, typical for mass transfer, in the framework of each model, where studies of the problems are lacking. The first problem is the transfer of a substance initially confined to a point. The second problem is the transfer of a substance from a stationary point source. We calculate the mean-square displacement (MSD) for the solutions of the first problem because the MSD is an integral quantity whose temporal dependence characterizes diffusion and Brownian motion. The temporal behavior of the MSD in the framework of the first and

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third models is found to be the same as that in the Brownian motion described by the standard Langevin equation. We recall here that the behavior of the MSD in the framework of the diffusion equation is wrong for short times, where it must be ballistic. Further, we find a remarkable phenomenon when a portion of the substance does not move.

The rest of the paper is organized as follows. In Sec. II we briefly recall the phenomenological derivation of the diffusion equation. In Sec. III we briefly recall some facts about the telegraph equation. In Sec. IV we describe the models of mass transfer related to the Jeffreys-type equation. In Sec. V we study the diffusion of a substance initially confined at a point in the framework of the three models. In Sec. VI we calculate the mean-square displacement for the solutions of the problems considered in Sec. V. In Sec. VII we study the diffusion of a substance from a stationary point source also in the framework of the three models. Section VIII contains concluding remarks.

II. DIFFUSION EQUATION

The macroscopic law of mass balance for a substance is expressed by the continuity equation [38]

$$\frac{\partial u}{\partial t} + \operatorname{div} \boldsymbol{J} = f, \tag{2.1}$$

where $u \equiv u(\boldsymbol{x},t)$ is the concentration of the substance, $\boldsymbol{x} = (x_1,x_2,x_3)$ is a point, t is time, $\boldsymbol{J} \equiv \boldsymbol{J}(\boldsymbol{x},t)$ is the flux of the substance, and $f \equiv f(\boldsymbol{x},t,u)$ is the net rate of production or absorption (degradation) of the substance. In the simplest approximation the flux is related to the concentration by Fick's phenomenological (first) law [1,2,38]

$$\boldsymbol{J} = -D\nabla u, \tag{2.2}$$

where D is the diffusion coefficient. The continuity equation (2.1) and Fick's law lead to the reaction diffusion equation

$$\frac{\partial u}{\partial t} - D\Delta u = f. \tag{2.3}$$

To determine a unique solution of the diffusion equation one imposes the initial condition

$$u|_{t=0} = u_0, \tag{2.4}$$

where $u_0 \equiv u_0(\boldsymbol{x})$ is the distribution of the concentration at time $t = 0$. Note that the diffusion equation is the simplest approximation to the linear Boltzmann equation [34] [see Eq. (A4)].

III. TELEGRAPH EQUATION

Fick's law neglects the inertia of moving particles. Cattaneo's equation [8–10]

$$\tau\frac{\partial \boldsymbol{J}}{\partial t} + \boldsymbol{J} = -D\nabla u, \tag{3.1}$$

where τ is the relaxation time, modifies Fick's law, taking the inertia into account. Indeed, Cattaneo's equation can be written in the equivalent integral form

$$\boldsymbol{J} = -\frac{D}{\tau}\int_0^t e^{-(t-t')/\tau}\nabla u(\boldsymbol{x},t')dt' + e^{-t/\tau}\boldsymbol{J}_0, \tag{3.2}$$

where $\boldsymbol{J}_0 \equiv \boldsymbol{J}_0(\boldsymbol{x})$ is the distribution of flux at time $t = 0$. Equation (3.2) shows that Cattaneo's equation takes into account the prehistory of a process since flux depends on the gradient of the concentration at earlier time, the dependence being exponentially decreasing with time. If the relaxation time τ in Cattaneo's equation tends to zero, one obtains in the limit Fick's law.

The continuity equations (2.1) and (3.2) lead to the integro-differential equation

$$\frac{\partial u}{\partial t} - \frac{D}{\tau}\int_0^t e^{-(t-t')/\tau}\Delta u(\boldsymbol{x},t')dt' + e^{-t/\tau}\operatorname{div}\boldsymbol{J}_0 = f.$$

This equation, with the initial condition (2.4), is equivalent to the reaction telegraph (or damped wave) equation [39,40]

$$\tau\frac{\partial^2 u}{\partial t^2} + \left(1 - \tau\frac{\partial f}{\partial u}\right)\frac{\partial u}{\partial t} - D\Delta u = f + \tau\frac{\partial f}{\partial t}, \tag{3.3}$$

with the initial conditions

$$u|_{t=0} = u_0, \qquad \left.\frac{\partial u}{\partial t}\right|_{t=0} = -\operatorname{div}\boldsymbol{J}_0 + f_0, \tag{3.4}$$

where $f_0 \equiv f_0(\boldsymbol{x},u_0) = f|_{t=0}$ is the distribution of sources at time $t = 0$. If $\tau = 0$, the telegraph equation (3.3) becomes the diffusion equation (2.3). The telegraph equation can also be obtained as the P_1 approximation to the linear Boltzmann equation [34] [see Eq. (A6)].

The telegraph equation is hyperbolic, providing the finite speed of signal propagation, and was proposed to be a substitute for the parabolic diffusion and heat equations [8,9,12–14]. However, two- and three-dimensional telegraph equations have a formal flaw since their solutions may take negative values even if the initial values are positive [15,16]. Besides, the applicability of the telegraph equation to the description of heat transfer is doubtful [16,41,42].

IV. JEFFREYS-TYPE EQUATION

A. Jeffreys-type model

The relation combining Fick's law and Cattaneo's equation has the form [8,9]

$$\begin{aligned}\tau\frac{\partial \boldsymbol{J}}{\partial t} + \boldsymbol{J} &= -\tau D_1\frac{\partial\nabla u}{\partial t} - (D_1 + D_2)\nabla u\\ &\equiv -(D_1 + D_2)\left[\tau_2\frac{\partial\nabla u}{\partial t} + \nabla u\right],\end{aligned} \tag{4.1}$$

where $D_1 > 0$, $D_1 + D_2 > 0$, and

$$\tau_2 = \frac{\tau D_1}{D_1 + D_2}$$

is another relaxation time or, equivalently, the integro-differential form

$$\begin{aligned}\boldsymbol{J} = -D_1\nabla u - \frac{D_2}{\tau}\int_0^t e^{-(t-t')/\tau}\nabla u(\boldsymbol{x},t')dt'\\ + e^{-t/\tau}(D_1\nabla u_0 + \boldsymbol{J}_0),\end{aligned} \tag{4.2}$$

where $u_0 \equiv u_0(\boldsymbol{x})$ and $\boldsymbol{J}_0 \equiv \boldsymbol{J}_0(\boldsymbol{x})$ are the distributions of the concentration and flux, respectively, at time $t = 0$. We call relations (4.1) and (4.2) the Jeffreys-type law after Jeffreys, who proposed similar relations for the rheological description of the earth's core [17,18]. Fick's law and Cattaneo's equation are particular cases of the Jeffreys-type law. Indeed, if τ in Eqs. (4.1) and (4.2) tends to zero, one obtains in the limit Fick's law with $D = D_1 + D_2$, while $D_1 = 0$ leads to Cattaneo's equation.

The Jeffreys-type law (4.1) includes two different cases, $\tau > \tau_2$ and $\tau < \tau_2$, depending on whether the relaxation time τ is higher or lower than τ_2. Both cases are considered in the literature; see, e.g., [19,25–27]. The first inequality $\tau > \tau_2$ is equivalent to $D_2 > 0$. In this case the relation (4.2) means that flux is determined by the concentration gradient both at the same moment and preceding time, the dependence on the past being exponentially decreased. The second inequality $\tau < \tau_2$ is equivalent to $D_2 < 0$. In this case the Jeffreys-type law can be written in the equivalent form

$$\nabla u = \frac{1}{D_1}\left[-\boldsymbol{J} + \frac{D_2}{\tau D_1}\int_0^t e^{-(t-t')/\tau_2}\boldsymbol{J}(\boldsymbol{x},t')dt' + e^{-t/\tau_2}(D_1\nabla u_0 + \boldsymbol{J}_0)\right], \tag{4.3}$$

which means that the gradient of the concentration is determined by flux both at the same moment and preceding time, the dependence on the past being exponentially decreased. Note that the relation (4.3) can be used for setting boundary conditions for u if mass transfer is considered in a finite domain.

The continuity equation (2.1) and the Jeffreys-type integro-differential law (4.2) lead to the integro-differential equation

$$\frac{\partial u}{\partial t} - D_1\Delta u - \frac{D_2}{\tau}\int_0^t e^{-(t-t')/\tau}\Delta u(\boldsymbol{x},t')dt' + e^{-t/\tau}(D_1\Delta u_0 + \operatorname{div}\boldsymbol{J}_0) = f.$$

This equation with the initial condition (2.4) is equivalent to the equation of third order

$$\tau\frac{\partial^2 u}{\partial t^2} + \left(1 - \tau\frac{\partial f}{\partial u}\right)\frac{\partial u}{\partial t} - \tau D_1\frac{\partial \Delta u}{\partial t} - (D_1 + D_2)\Delta u = f + \tau\frac{\partial f}{\partial t}, \tag{4.4}$$

with the initial conditions (3.4). We call Eq. (4.4) the Jeffreys-type equation [8]. The diffusion equation (2.3) and the telegraph equation (3.3) are particular cases of the Jeffreys-type equation for $\tau = 0$ and $D_1 = 0$, respectively.

Equation (4.1) can also be derived formally in the framework of the dual-phase-lag model [10,19,20]. The model applies heat transfer and Fourier's law, however, one can extend this to mass transfer and Fick's law as well. In this framework Fick's law is replaced by the relation

$$\boldsymbol{J}(\boldsymbol{x},t+\tau) = -D\nabla u(\boldsymbol{x},t+\tau_2), \tag{4.5}$$

where τ and τ_2 are the time lags of the flux and the gradient of the concentration, respectively. Both sides of the relation are expanded with the use of Taylor's formula. If only terms up to first order are retained one obtains the relation

$$\tau\frac{\partial \boldsymbol{J}}{\partial t} + \boldsymbol{J} = -D\left(\tau_2\frac{\partial \nabla u}{\partial t} + \nabla u\right),$$

which is nothing but Eq. (4.1) with $D_1 + D_2 = D$. Note that if $\tau_2 = 0$ one obtains the single-phase-lag model and Cattaneo's equation.

However, Eq. (4.5) (for both $\tau_2 > 0$ and $\tau_2 = 0$) together with the continuity equation yields delay equations leading to ill-posed initial-value problems (with unstable solutions) [43,44]. Therefore, the phase-lag models cannot be considered as sensible physical ones. At the same time the formal approximations to the phase-lag models lead to well-posed initial-value problems.

B. Two-phase (two-temperature) model

In this model two phases of a substance (or species) are considered: free (mobile) and bound (immobile) (see, e.g., [29–32]). The concentrations of these substances are denoted by $u \equiv u(\boldsymbol{x},t)$ and $v \equiv v(\boldsymbol{x},t)$, respectively, and satisfy the reaction diffusion system

$$\frac{\partial u}{\partial t} - D_1\Delta u + k_1 u - k_2 v = f, \tag{4.6a}$$

$$\frac{\partial v}{\partial t} + k_2 v - k_1 u = 0, \tag{4.6b}$$

with the initial conditions

$$u|_{t=0} = u_0, \quad v|_{t=0} = v_0, \tag{4.7}$$

where D_1 is the diffusion coefficient of the free substance, k_1 and k_2 are the coefficients of interphase mass transfer, $f = f(\boldsymbol{x},t,u)$ is the net rate of production and absorption (degradation) of the free substance, and $v_0 \equiv v_0(\boldsymbol{x})$ is the the distribution of the concentration of the immobile substance at time $t = 0$. The coefficients k_1 and k_2 are evidently positive in this model.

The concentration v can be expressed through u from Eq. (4.6b) by

$$v = k_1\int_0^t e^{-k_2(t-t')}u(\boldsymbol{x},t')dt' + e^{-k_2 t}v_0.$$

Then Eq. (4.6a) leads to the equation

$$\frac{\partial u}{\partial t} - D_1\Delta u + k_1 u - k_1 k_2\int_0^t e^{-k_2(t-t')}u(\boldsymbol{x},t')dt' - k_2 e^{-k_2 t}v_0 = f.$$

This equation, with the first of the conditions (4.7), is equivalent to the Jeffreys-type equation

$$\frac{\partial^2 u}{\partial t^2} + \left(k_1 + k_2 - \frac{\partial f}{\partial u}\right)\frac{\partial u}{\partial t} - D_1\frac{\partial \Delta u}{\partial t} - k_2 D_1\Delta u = k_2 f + \frac{\partial f}{\partial t}, \tag{4.8}$$

with the initial conditions

$$u|_{t=0} = u_0, \quad \left.\frac{\partial u}{\partial t}\right|_{t=0} = D_1\Delta u_0 - k_1 u_0 + k_2 v_0 + f_0. \tag{4.9}$$

The equation for v is

$$\frac{\partial^2 v}{\partial t^2} + (k_1 + k_2)\frac{\partial v}{\partial t} - D_1\frac{\partial \Delta v}{\partial t} - k_2 D_1\Delta v = k_1 f\left(\boldsymbol{x},t,\frac{1}{k_1}\left(\frac{\partial v}{\partial t} + k_2 v\right)\right), \tag{4.10}$$

which is different from Eq. (4.8), if $f \neq 0$. The initial conditions for v are

$$v|_{t=0} = v_0, \quad \left.\frac{\partial v}{\partial t}\right|_{t=0} = k_1 u_0 - k_2 v_0. \tag{4.11}$$

The counterpart of the two-phase model in the field of heat transfer is the two-temperature model [19,24,41,45].

C. Relation between the coefficients of the two models

If sources and sinks (absorption) are absent, i.e., $f = 0$, then the Jeffreys-type equations (4.4) and (4.8) are identical and the coefficients are related by

$$\tau = \frac{1}{k_1 + k_2}, \quad D_2 = -\frac{k_1}{k_1 + k_2} D_1 \tag{4.12a}$$

or, vice versa,

$$k_1 = -\frac{1}{\tau}\frac{D_2}{D_1} \equiv \frac{1}{\tau} - \frac{1}{\tau_2}, \quad k_2 = \frac{1}{\tau}\left(1 + \frac{D_2}{D_1}\right) \equiv \frac{1}{\tau_2}, \tag{4.12b}$$

the diffusion coefficient D_1 being the same in the two models. At the same time, the initial conditions (3.4) and (4.9) for the equations concerning the time derivative are different. In Sec. V it will be shown that this leads to qualitatively different behavior of the solutions to the initial-value problems for the Jeffreys-type equations.

It is necessary to emphasize here that the positive coefficient k_1 in the two-phase model (4.6) corresponds to the negative coefficient D_2 in the Jeffreys-type law (4.1)–(4.3). Conversely, the positive coefficient D_2 corresponds to the negative coefficient k_1.

D. The $D_{N=1}$ approximation to the linear Boltzmann equation

We consider here an approximation to the linear Boltzmann equation (also referred to as the linear transport or radiative transfer equation) [34,46,47], which describes, e.g., neutron transport and radiative heat transfer (transport of thermal energy by photons) (see Appendix A 3). We use the notation $D_{N=1}$ instead of D_1 since the latter stands for the coefficient.

Consider the monoenergetic (one-speed) linear Boltzmann equation

$$\begin{aligned}\frac{\partial \psi}{\partial t} &+ c\boldsymbol{\Omega}\cdot\nabla\psi + (\kappa + \sigma)\psi \\ &= \sigma \int_{\mathbb{S}^2} K(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\psi(\boldsymbol{x},\boldsymbol{\Omega}',t)d\boldsymbol{\Omega}' + \frac{1}{4\pi}F,\end{aligned} \tag{4.13}$$

where $\psi \equiv \psi(\boldsymbol{x},\boldsymbol{\Omega},t)$ is the particle phase space density, i.e., the density of particles at the point $\boldsymbol{x}$ and at time t moving along the direction $\boldsymbol{\Omega} \in \mathbb{S}^2$, $\mathbb{S}^2$ is the unit sphere in $\mathbb{R}^3$, c is the velocity of particles, κ and σ are the absorption and scattering rates, respectively, K is the collision (or scattering) kernel, and $F \equiv F(\boldsymbol{x},t)$ is the source density (due to isotropic sources for simplicity).

Integration of the linear Boltzmann equation over the unit sphere, together with the normalization $\int_{\mathbb{S}^2} K(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')d\boldsymbol{\Omega} = 1$, gives the continuity equation

$$\frac{\partial u}{\partial t} + \operatorname{div}\boldsymbol{J} + \kappa u = F, \tag{4.14}$$

where

$$u(\boldsymbol{x},t) = \int_{\mathbb{S}^2} \psi(\boldsymbol{x},\boldsymbol{\Omega},t)d\boldsymbol{\Omega} \tag{4.15}$$

is the particle density and

$$\boldsymbol{J}(\boldsymbol{x},t) = c\int_{\mathbb{S}^2} \boldsymbol{\Omega}\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d\boldsymbol{\Omega} \tag{4.16}$$

is flux. In the $D_{N=1}$ approximation [35] the particle density and flux are related by Eq. (A7), which can be written as

$$\tau\frac{\partial \boldsymbol{J}}{\partial t} + \boldsymbol{J} = -(D_1 + D_2)\nabla u + \frac{\tau D_1}{4}(3\Delta\boldsymbol{J} + \nabla\operatorname{div}\boldsymbol{J}), \tag{4.17}$$

where

$$\tau = \frac{1}{\kappa + \sigma_1}, \quad D_1 = \frac{4c^2}{15(\kappa + \sigma_2)},$$
$$D_2 = \left[\frac{1}{\kappa + \sigma_1} - \frac{4}{5(\kappa + \sigma_2)}\right]\frac{c^2}{3}, \quad \gamma = \kappa$$

(see Appendix A) (the parameter γ will be used elsewhere).

The continuity equation (4.14) and relation (4.17) imply that the particle density satisfies the Jeffreys-type equation

$$\begin{aligned}\tau\frac{\partial^2 u}{\partial t^2} &+ (1 + \tau\gamma)\frac{\partial u}{\partial t} - \tau D_1\frac{\partial \Delta u}{\partial t} \\ &- [(1 + \tau\gamma)D_1 + D_2]\Delta u + \gamma u \\ &= F + \tau\frac{\partial F}{\partial t} - \tau D_1\Delta F,\end{aligned} \tag{4.18}$$

which is the same as Eq. (A8). The initial conditions for this equation are

$$u|_{t=0} = u_0, \quad \left.\frac{\partial u}{\partial t}\right|_{t=0} = -\gamma u_0 - \operatorname{div}\boldsymbol{J}_0 + F_0, \tag{4.19}$$

where $F_0 \equiv F_0(\boldsymbol{x}) = F|_{t=0}$ is the distribution of sources at time $t = 0$. In the absence of sources and absorption, i.e., if $F = 0$ and $\kappa \equiv \gamma = 0$, Eq. (4.18) takes the form

$$\tau\frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} - \tau D_1\frac{\partial \Delta u}{\partial t} - (D_1 + D_2)\Delta u = 0, \tag{4.20}$$

which is the same as Eq. (4.4) with $f = 0$. In a steady state the relation (4.17) takes the form

$$\boldsymbol{J} = -(D_1 + D_2)\nabla u + \frac{\tau D_1}{4}(3\Delta\boldsymbol{J} + \nabla\operatorname{div}\boldsymbol{J}), \tag{4.21}$$

which differs qualitatively from Fick's law.

It is necessary to emphasize that the relation (4.17) is similar to but not the same as the equation of Guyer and Krumhansl (B4). The reason is that Guyer and Krumhansl considered the linearized Boltzmann equation rather than the linear one; the difference is explained in Ref. [46].

V. INITIAL-VALUE PROBLEMS FOR THE HOMOGENEOUS JEFFREYS-TYPE EQUATION WITH ABSORPTION

In this section we study the classic one-dimensional transport problem for a substance initially confined at a point. We suppose that sources are absent and the substance is absorbed (degraded); therefore, we set $f = -\gamma u$, where

γ is the absorption (degradation) rate. The study reveals a remarkable phenomenon when a finite portion of the substance does not move, though this portion diminishes exponentially with time.

There is also a qualitative difference between the two cases $D_2 > 0$ and $D_2 < 0$. In the first case the solution is wavelike because the characteristic values take complex values. In the second case the characteristic values are real and hence the solution is not wavelike.

A. Jeffreys-type model

In the one-dimensional case the problem (3.4) and (4.4) with $f = -\gamma u$ takes the form

$$\tau \frac{\partial^2 u_{\text{Je}}}{\partial t^2} + (1+\tau\gamma)\frac{\partial u_{\text{Je}}}{\partial t} - \tau D_1 \frac{\partial^3 u_{\text{Je}}}{\partial x^2 \partial t} - (D_1 + D_2)\frac{\partial^2 u_{\text{Je}}}{\partial x^2} + \gamma u_{\text{Je}} = 0, \quad x \in \mathbb{R}, \quad t > 0, \tag{5.1}$$

$$u_{\text{Je}}|_{t=0} = u_0, \quad \left.\frac{\partial u_{\text{Je}}}{\partial t}\right|_{t=0} = -\gamma u_0 - \frac{\partial J_0}{\partial x}. \tag{5.2}$$

The one-dimensional continuity equation (2.1) implies that if and only if $\gamma = 0$, i.e., absorption is absent, mass is conserved: $\int_{-\infty}^{\infty} u_{\text{Je}}(x,t)dx = \int_{-\infty}^{\infty} u_0(x)dx \equiv \text{const}$.

Consider the particular initial conditions

$$u_0(x) = \delta(x), \quad J_0(x) = 0. \tag{5.3}$$

The Fourier transform of the problem (5.1)–(5.3) yields

$$\tau \frac{\partial^2 \mathcal{F}u_{\text{Je}}}{\partial t^2} + [1 + \tau(D_1\xi^2 + \gamma)]\frac{\partial \mathcal{F}u_{\text{Je}}}{\partial t} + [(D_1 + D_2)\xi^2 + \gamma]\mathcal{F}u_{\text{Je}} = 0, \quad \xi \in \mathbb{R}, \quad t > 0, \tag{5.4}$$

$$\mathcal{F}u_{\text{Je}}|_{t=0} = 1, \quad \left.\frac{\partial \mathcal{F}u_{\text{Je}}}{\partial t}\right|_{t=0} = -\gamma, \tag{5.5}$$

where

$$\mathcal{F}u(\xi,\cdot) = \int_{-\infty}^{\infty} u(x,\cdot)e^{i\xi x}dx$$

defines the Fourier transform. The solution to the original problem is therefore given by

$$u(x,\cdot) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathcal{F}u(\xi,\cdot)e^{-ix\xi}d\xi.$$

The characteristic values of Eq. (5.4) are

$$\lambda_{1,2}(\xi) = \frac{1}{2\tau}\{-[1 + \tau(D_1\xi^2 + \gamma)] \pm \sqrt{[1 - \tau(D_1\xi^2 + \gamma)]^2 - 4\tau D_2\xi^2}\}, \tag{5.6}$$

where the plus sign corresponds to λ_1. Note that if $-D_1 < D_2 \leqslant 0$, the characteristic values are real; otherwise, if $D_2 > 0$, there are two intervals on the real line, symmetric with respect to the origin, where the characteristic values are complex conjugate.

The solution to the problem (5.4) and (5.5) is

$$\mathcal{F}u_{\text{Je}}(\xi,t) = \frac{1}{\lambda_1(\xi) - \lambda_2(\xi)}\{[\lambda_1(\xi)e^{\lambda_2(\xi)t} - \lambda_2(\xi)e^{\lambda_1(\xi)t}] - \gamma[e^{\lambda_1(\xi)t} - e^{\lambda_2(\xi)t}]\}. \tag{5.7}$$

The asymptotic behavior of the characteristic values is described by

$$\lambda_1(\xi) = -\frac{1}{\tau}\left(1 + \frac{D_2}{D_1}\right) + O\left(\frac{1}{\xi^2}\right) \equiv -k_2 + O\left(\frac{1}{\xi^2}\right), \tag{5.8a}$$

$$\lambda_2(\xi) = -D_1\xi^2 + \frac{D_2}{\tau D_1} - \gamma + O\left(\frac{1}{\xi^2}\right) \equiv -(D_1\xi^2 + k_1 + \gamma) + O\left(\frac{1}{\xi^2}\right) \tag{5.8b}$$

as $\xi \to \pm\infty$, where we have used the relations (4.13) between the coefficients of the two models. Therefore, the asymptotic behavior of the Fourier transform (5.7) with respect to ξ is

$$\mathcal{F}u_{\text{Je}}(\xi,t) = e^{-k_2 t} + O\left(\frac{1}{\xi^2}\right) \quad \text{as} \quad \xi \to \pm\infty. \tag{5.9}$$

This means that the solution u_{Je} has the form

$$u_{\text{Je}}(x,t) = u_{\text{Je}}^s(x,t) + u_{\text{Je}}^r(x,t), \tag{5.10}$$

where

$$u_{\text{Je}}^s(x,t) = e^{-k_2 t}\delta(x) \tag{5.11}$$

is the singular term, while the regular term u_{Je}^r is a continuous function [48]. The presence of the singular term means that in the Jeffreys-type model a finite portion of the substance does not move, though this portion diminishes exponentially with time.

If $\tau\gamma < 1$ the asymptotic behavior of the regular term with respect to t is

$$e^{\gamma t}\mathcal{F}u_{\text{Je}}^r\left(\frac{\xi}{\sqrt{t}},t\right) \to e^{-D_{\text{Je}}\xi^2} \quad \text{as} \quad t \to +\infty,$$

with

$$D_{\text{Je}} = D_1 + \frac{D_2}{1 - \tau\gamma},$$

which leads to the asymptotic behavior

$$e^{\gamma t}\sqrt{t}u_{\text{Je}}^r(\sqrt{t}x,t) \to \frac{1}{2\sqrt{\pi D_{\text{Je}}}}\exp\left(-\frac{x^2}{4D_{\text{Je}}}\right)$$

as $t \to +\infty$. This means that if $\tau\gamma < 1$ the solution u_{Je} behaves asymptotically as $t \to +\infty$ as the solution

$$u_{\text{DE}}(x,t) = \frac{1}{2\sqrt{\pi D_{\text{Je}}t}}\exp\left(-\frac{x^2}{4D_{\text{Je}}t} - \gamma t\right) \tag{5.12}$$

of the diffusion equation

$$\frac{\partial u_{\text{DE}}}{\partial t} - D_{\text{Je}}\frac{\partial^2 u_{\text{DE}}}{\partial^2 x} + \gamma u_{\text{DE}} = 0, \quad x \in \mathbb{R}, \quad t > 0,$$

with the initial condition

$$u_{\text{DE}}|_{t=0} = \delta(x). \tag{5.13}$$

Figures 1–3 show two solutions u_{Je}. In both cases absorption is absent, i.e., $\gamma = 0$, and therefore the mass of the substance is conserved. The solution, shown in Figs. 1 and 2, is obtained with the parameters $\tau = 1$, $D_1 = 1$, and $D_2 = 4$. The solution, shown in Fig. 3, is obtained with the parameters

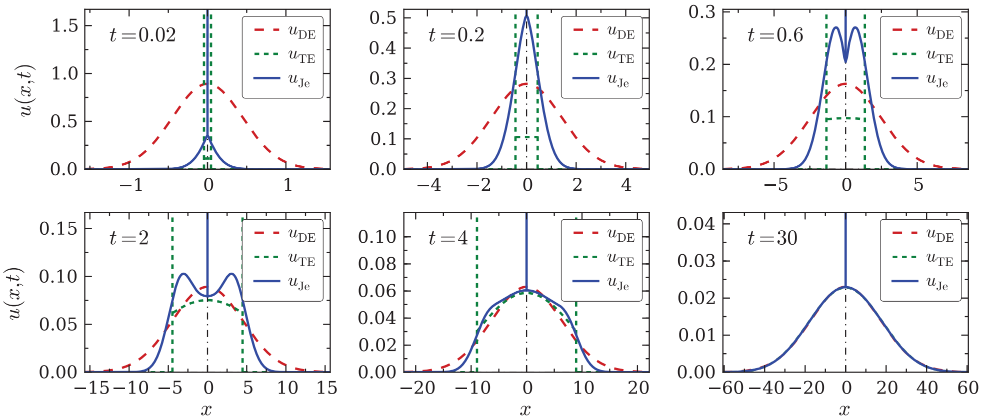

FIG. 1. (Color online) Solution u_{Je} to the problem (5.1)–(5.3) with $\tau = 1$, $D_1 = 1$, $D_2 = 4$, and $\gamma = 0$ in comparison with those of the diffusion and telegraph equations (see the text). The vertical lines stand for the singular terms u^s_{TE} and u^s_{Je}. The portions of the regular term are $\int_{-\infty}^{\infty} u^r_{\mathrm{Je}}(x,0.02)dx \approx 0.10$, $\int_{-\infty}^{\infty} u^r_{\mathrm{Je}}(x,0.2)dx \approx 0.63$, $\int_{-\infty}^{\infty} u^r_{\mathrm{Je}}(x,0.6)dx \approx 0.95$, and $\int_{-\infty}^{\infty} u^r_{\mathrm{Je}}(x,2)dx \approx 1.0000$.

$\tau = 1$, $D_1 = 1$, and $D_2 = -0.5$ (which corresponds to $k_1 = 0.5$ and $k_2 = 0.5$). The solution, shown in Fig. 1, is wavelike because the characteristic values (5.6) take complex values due to $D_2 > 0$. In the second case $D_2 < 0$, therefore the characteristic values are real and for this reason the solution, shown in Fig. 3, is not wavelike. All the figures show also the diffusion asymptotics (5.12) with $\gamma = 0$, in this case $D_{\mathrm{Je}} = D_1 + D_2$.

Figure 1 shows also the solution of the telegraph equation

$$\tau \frac{\partial^2 u_{\mathrm{TE}}}{\partial t^2} + \frac{\partial u_{\mathrm{TE}}}{\partial t} - (D_1 + D_2)\frac{\partial^2 u_{\mathrm{TE}}}{\partial x^2} = 0, \quad x \in \mathbb{R}, \quad t > 0$$

[this is Eq. (5.1) with $\partial_{xxt} u_{\mathrm{Je}} = 0$ and $\gamma = 0$] with the initial conditions

$$u_{\mathrm{TE}}|_{t=0} = \delta(x), \quad \left.\frac{\partial u_{\mathrm{TE}}}{\partial t}\right|_{t=0} = 0.$$

This solution is given by [11,12]

$$u_{\mathrm{TE}}(x,t) = u^s_{\mathrm{TE}}(x,t) + u^r_{\mathrm{TE}}(x,t),$$

where

$$u^s_{\mathrm{TE}}(x,t) = \frac{e^{-t/2\tau}}{2v}\left[\delta\left(\frac{x}{v} - t\right) + \delta\left(\frac{x}{v} + t\right)\right]$$

is the singular term and

$$\begin{aligned} u^r_{\mathrm{TE}}(x,t) = \frac{e^{-t/2\tau}}{2v}\frac{1}{2\tau}\Bigg[& I_0\left(\frac{1}{2\tau}\sqrt{t^2 - \frac{x^2}{v^2}}\right) \\ & + t\left(\sqrt{t^2 - \frac{x^2}{v^2}}\right)^{-1} I_1\left(\frac{1}{2\tau}\sqrt{t^2 - \frac{x^2}{v^2}}\right)\Bigg] \\ & \times H\left(t - \frac{|x|}{v}\right) \end{aligned}$$

is the regular term, where $v = \sqrt{(D_1 + D_2)/\tau}$ is the velocity, I_0 and I_1 are the modified Bessel functions, and $H(\cdot)$ is the Heaviside step function. The regular term is discontinuous at $x = \pm vt$.

The solution (5.7) and the one-dimensional continuity equation (2.1) with $f = 0$ imply that the Fourier transform of flux is

$$\mathcal{F}J(\xi,t) = \frac{i}{\xi}\frac{\lambda_1(\xi)\lambda_2(\xi)}{\lambda_1(\xi) - \lambda_2(\xi)}[e^{\lambda_1(\xi)t} - e^{\lambda_2(\xi)t}].$$

The asymptotic behavior of the Fourier transform of flux is described by

$$\left(\mathcal{F}\frac{\partial J}{\partial x}\right)(\xi,t) \equiv -i\xi\mathcal{F}J(\xi,t) \to k_2 e^{-k_2 t}$$

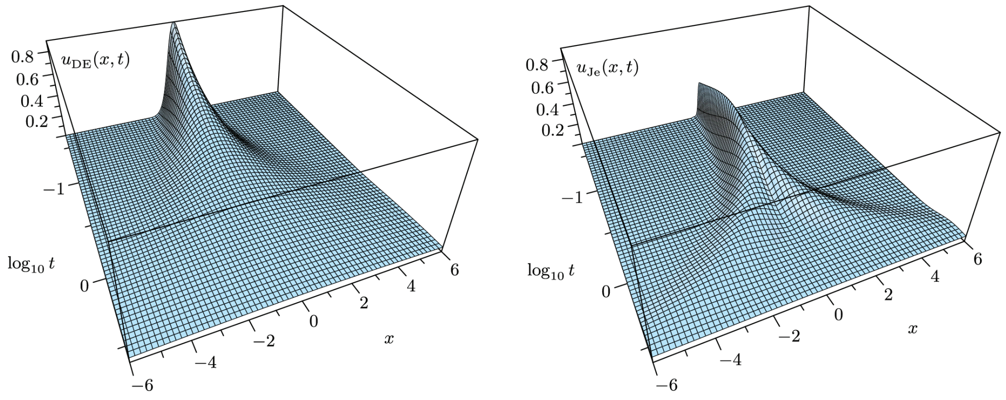

FIG. 2. (Color online) Spatiotemporal images of solutions u_{DE} and u^r_{Je} as in Fig. 1 with $t \in [0.02,4]$.

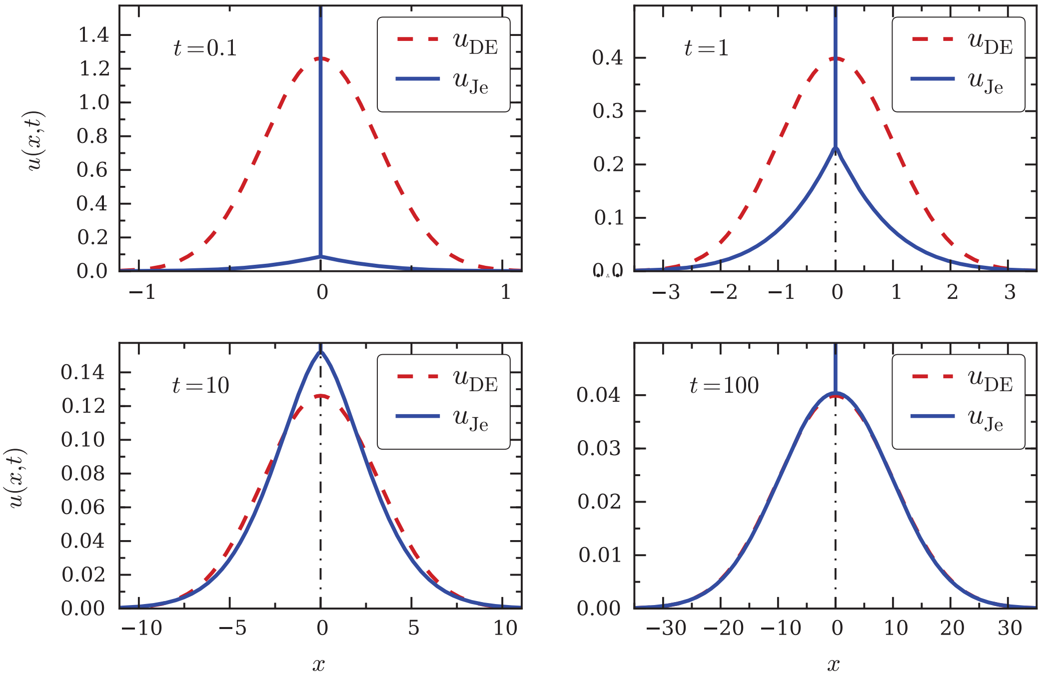

FIG. 3. (Color online) Solution $u_{\rm Je}$ to the problem (5.1)–(5.3) with $\tau = 1$, $D_1 = 1$, $D_2 = -0.5$, and $\gamma = 0$ in comparison with that of the diffusion equation (see the text). The vertical lines stand for the singular term $u^s_{\rm Je}$. The portions of the regular term are $\int_{-\infty}^{\infty} u^r_{\rm Je}(x,0.1)dx \approx 0.05$, $\int_{-\infty}^{\infty} u^r_{\rm Je}(x,1)dx \approx 0.39$, and $\int_{-\infty}^{\infty} u^r_{\rm Je}(x,10)dx \approx 0.99$.

as $\xi \to \pm\infty$, which means that flux $J(x,t)$ has a finite discontinuity at $x = 0$, equal to $k_2 e^{-k_2 t}$, which tends to zero as $t \to +\infty$. Note that flux $J(x,t)$ is an odd function with respect to x.

B. Two-phase model

Here we study the behavior of the net concentration $w_{\rm TP} = u_{\rm TP} + v_{\rm TP}$, where $u_{\rm TP}$ and $v_{\rm TP}$ are the concentrations of the free and bound phases, respectively. In the one-dimensional case the problem (4.8) and (4.9) and the problem (4.10) and (4.11) with $f = -\gamma u$ lead to the problem

$$\frac{\partial^2 w_{\rm TP}}{\partial t^2} + (k_1 + k_2 + \gamma)\frac{\partial w_{\rm TP}}{\partial t} - D_1 \frac{\partial^3 w_{\rm TP}}{\partial x^2 \partial t} - k_2 D_1 \frac{\partial^2 w_{\rm TP}}{\partial x^2} + k_2 \gamma w_{\rm TP} = 0, \quad x \in \mathbb{R}, \quad t > 0, \tag{5.14}$$

$$w_{\rm TP}|_{t=0} = u_0 + v_0, \quad \left.\frac{\partial w_{\rm TP}}{\partial t}\right|_{t=0} = D_1 \frac{\partial^2 u_0}{\partial x^2}. \tag{5.15}$$

The total mass of the free and bound phases is conserved if and only if $\gamma = 0$, i.e., absorption is absent: $\int_{-\infty}^{\infty} w_{\rm TP}(x,t)dx = \int_{-\infty}^{\infty}[u_0(x) + v_0(x)]dx \equiv \text{const}$. Indeed, Eqs. (4.7) imply that the total mass obeys the equation $\partial_t w_{\rm TP} - D_1 \Delta u_{\rm TP} = -\gamma u_{\rm TP}$, or in Fourier space $\partial_t \mathcal{F} w_{\rm TP} + \xi^2 D_1 \mathcal{F} u_{\rm TP} = -\gamma \mathcal{F} u_{\rm TP}$.

Consider the particular initial conditions

$$u_0(x) = \alpha\delta(x), \quad v_0(x) = (1-\alpha)\delta(x), \quad 0 \leqslant \alpha \leqslant 1. \tag{5.16}$$

The Fourier transform of the problem (5.14)–(5.16) yields

$$\frac{\partial^2 \mathcal{F} w_{\rm TP}}{\partial t^2} + (k_1 + k_2 + \gamma + D_1\xi^2)\frac{\partial \mathcal{F} w_{\rm TP}}{\partial t} + k_2(D_1\xi^2 + \gamma)\mathcal{F} w_{\rm TP} = 0, \quad \xi \in \mathbb{R}, \quad t > 0, \tag{5.17}$$

$$\mathcal{F} w_{\rm TP}|_{t=0} = 1, \quad \left.\frac{\partial \mathcal{F} w_{\rm TP}}{\partial t}\right|_{t=0} = -\alpha D_1 \xi^2. \tag{5.18}$$

The characteristic values of Eq. (5.17) are

$$\lambda_{1,2}(\xi) = \tfrac{1}{2}[-(k_1 + k_2 + \gamma + D_1\xi^2) \pm \sqrt{(k_1 - k_2 + \gamma + D_1\xi^2)^2 + 4k_1k_2}], \tag{5.19}$$

where the plus sign corresponds to λ_1. These values differ from the characteristic values (5.6) if $\gamma \neq 0$, however, their asymptotic behavior is the same [see (5.8)].

The solution to the problem (5.17) and (5.18) is

$$\mathcal{F} w_{\rm TP}(\xi,t) = \frac{1}{\lambda_1(\xi) - \lambda_2(\xi)}\{[\lambda_1(\xi)e^{\lambda_2(\xi)t} - \lambda_2(\xi)e^{\lambda_1(\xi)t}] - \alpha[e^{\lambda_1(\xi)t} - e^{\lambda_2(\xi)t}]D_1\xi^2\}. \tag{5.20}$$

Taking into account the asymptotic behavior of the characteristic values, one can conclude that the asymptotic behavior of the Fourier transform of the solution is

$$\mathcal{F} w_{\rm TP}(\xi,t) = (1-\alpha)e^{-k_2 t} + O\left(\frac{1}{\xi^2}\right) \quad \text{as} \quad \xi \to \pm\infty$$

[cf. with the asymptotics (5.9)]. This means that the solution $w_{\rm TP}$ has the form

$$w_{\rm TP}(x,t) = w^s_{\rm TP}(x,t) + w^r_{\rm TP}(x,t), \tag{5.21}$$

where

$$w^s_{\rm TP}(x,t) = (1-\alpha)e^{-k_2 t}\delta(x) \tag{5.22}$$

is the singular term, while the regular term $w^r_{\rm TP}$ is a continuous function [48]. The presence of the singular term means that if $\alpha < 1$ in the two-phase model a finite portion of the substance does not move, though this portion diminishes exponentially with time.

The asymptotic behavior of the Fourier transform (5.20) with respect to t is

$$e^{\gamma_{\rm TP}t}\mathcal{F}w^r_{\rm TP}\left(\frac{\xi}{\sqrt{t}},t\right) \to \frac{1}{2}\left(1+\frac{k_+}{s}\right)e^{-D_{\rm TP}\xi^2}$$

as $t \to +\infty$, where

$$D_{\rm TP} = \frac{1}{2}\left(1-\frac{k_-}{s}\right)D_1, \quad \gamma_{\rm TP} = \frac{k_+ - s}{2},$$
$$k_\pm = k_1 + \gamma \pm k_2, \quad s = \sqrt{k_-^2 + 4k_1k_2}.$$

This means that as $t \to +\infty$ the solution $u_{\rm TP}$ behaves asymptotically as

$$w^\infty_{\rm TP} \equiv \frac{1}{2}\left(1+\frac{k_+}{s}\right)u_{\rm DE}(x,t), \tag{5.23}$$

where

$$u_{\rm DE}(x,t) = \frac{1}{2\sqrt{\pi D_{\rm TP}t}}\exp\left(-\frac{x^2}{4D_{\rm TP}t} - \gamma_{\rm TP}t\right)$$

is the solution of the diffusion equation

$$\frac{\partial u_{\rm DE}}{\partial t} - D_{\rm TP}\frac{\partial^2 u_{\rm DE}}{\partial^2 x} + \gamma_{\rm TP}u_{\rm DE} = 0, \quad x \in \mathbb{R}, \quad t > 0,$$

with the initial condition (5.13). If $\gamma = 0$ then $k_+ = s$ and

$$D_{\rm TP} = \frac{k_2}{k_1 + k_2}D_1 \equiv D_1 + D_2.$$

Figure 4 shows the solution $w_{\rm TP}$ with $\alpha = 1$, i.e., $u_0 = \delta(x)$ and $v_0 = 0$. The parameters are $D_1 = 1$, $k_1 = 0.5$, $k_2 = 0.5$ (which corresponds to $\tau = 1$ and $D_2 = -0.5$; cf. Fig. 3), and $\gamma = 0$. The total mass of $w_{\rm TP}$ is conserved. The figure shows also the diffusion asymptotics (5.23) with $\gamma = 0$, which is the same as the asymptotics (5.12) with $\gamma = 0$. For comparison the figure shows the solution $u^0_{\rm DE}$ to the problem for the diffusion equation (4.6a) with $k_1 = k_2 = 0$, $f = -\gamma u$, and the initial condition $u_0 = \delta(x)$, i.e., this would be the concentration of the free substance if interphase mass transfer were absent. Note that the solution $w_{\rm TP}$ with $\alpha = 0$, i.e., $u_0 = 0$ and $v_0 = \delta(x)$, is the same as the solution $u_{\rm Je}$ to the problem (5.1)–(5.3) with the same parameters (see Fig. 3).

C. The $D_{N=1}$ approximation to the linear Boltzmann equation

In the one-dimensional case Eq. (4.18) with $F = 0$ takes the form

$$\tau\frac{\partial^2 u_{\rm Bo}}{\partial t^2} + (1+\tau\gamma)\frac{\partial u_{\rm Bo}}{\partial t} - \tau D_1\frac{\partial^3 u_{\rm Bo}}{\partial x^2 \partial t}$$
$$-(D_1 + D_2')\frac{\partial^2 u_{\rm Bo}}{\partial x^2} + \gamma u_{\rm Bo} = 0, \quad x \in \mathbb{R}, \quad t > 0,$$

with $D_2' = D_2 + \tau\gamma D_1$. The initial conditions (4.19) in this case are

$$u_{\rm Bo}|_{t=0} = u_0, \quad \left.\frac{\partial u_{\rm Bo}}{\partial t}\right|_{t=0} = -\gamma u_0 - \frac{\partial J_0}{\partial x}.$$

This problem is similar to the problem (5.1) and (5.2) in the framework of the Jeffreys-type model.

VI. MEAN-SQUARE DISPLACEMENT

The MSD is an integral quantity whose temporal dependence characterizes diffusion and Brownian motion. It is of interest to calculate the MSD in the framework of each model for comparison with that in diffusion and Brownian motion. This comparison is of particular interest for small t since the asymptotics of the above solutions for large t is diffusive.

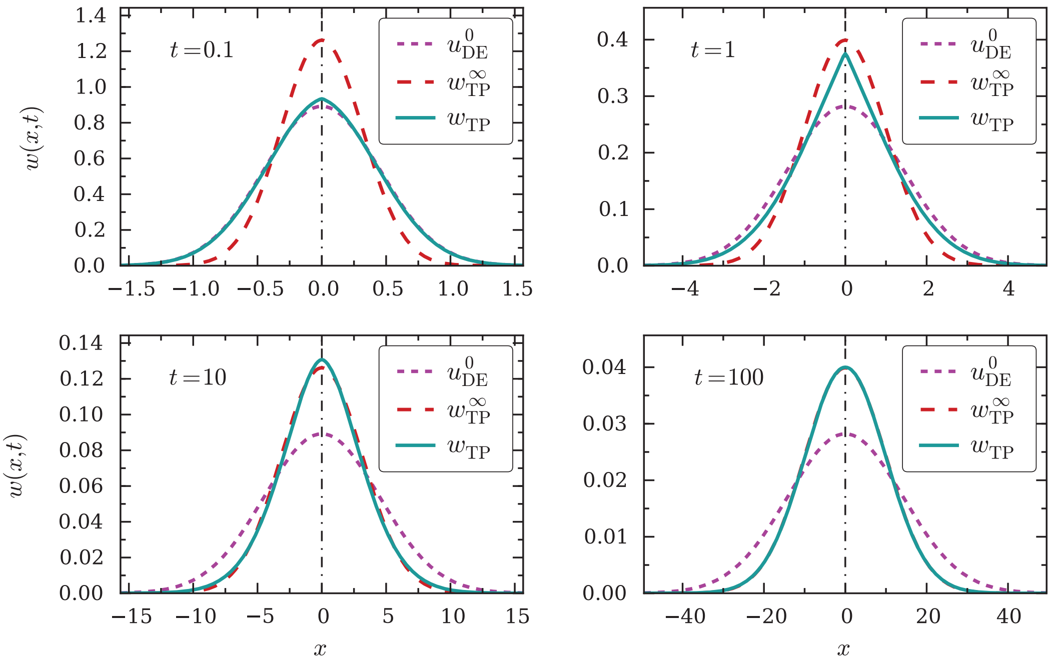

FIG. 4. (Color online) Solution $w_{\rm TP}$ to the problem (5.14)–(5.16) with $D_1 = 1$, $k_1 = 0.5$, $k_2 = 0.5$, $\gamma = 0$, and $\alpha = 1$ in comparison with that of the diffusion equation and the diffusion asymptotics $w^\infty_{\rm TP}$ (5.23) with $\gamma = 0$ (see the text).

In this section we calculate the MSD, defined by $\langle x^2(t)\rangle \equiv \int_{-\infty}^{\infty} x^2 u(x,t)dx$, for the solutions of the problems, considered in the previous section, with the initial condition $u|_{t=0} = \delta(x)$. The solution $u(\cdot,t)$ is to be a probability distribution function for any $t \geqslant 0$, i.e., the necessary condition is $\int_{-\infty}^{\infty} u(x,t)dx = 1$. Therefore, absorption is necessarily absent, i.e., $\gamma = 0$.

Concerning the diffusion equation, it is well known that the MSD for the solution to the problem

$$\frac{\partial u_{\mathrm{DE}}}{\partial t} - D\frac{\partial^2 u_{\mathrm{DE}}}{\partial^2 x} = 0, \quad x \in \mathbb{R}, \quad t > 0,$$
$$u_{\mathrm{DE}}|_{t=0} = \delta(x)$$

linearly depends on time and is equal to

$$\langle x^2_{\mathrm{DE}}(t)\rangle = 2Dt, \quad t \geqslant 0.$$

However, this temporal behavior of the MSD is wrong at short times, where it must be ballistic.

The MSD in the framework of the Jeffreys-type model is defined through the solution u_{Je} to the problem (5.1)–(5.3) with $\gamma = 0$. Therefore, the MSD is the solution to the problem

$$\tau\frac{d^2}{dt^2}\langle x^2_{\mathrm{Je}}\rangle + \frac{d}{dt}\langle x^2_{\mathrm{Je}}\rangle = 2(D_1 + D_2), \quad t > 0,$$
$$\langle x^2_{\mathrm{Je}}\rangle\big|_{t=0} = 0, \quad \frac{d}{dt}\langle x^2_{\mathrm{Je}}\rangle\big|_{t=0} = 0.$$

Hence, the MSD is equal to

$$\langle x^2_{\mathrm{Je}}(t)\rangle = 2(D_1 + D_2)[t - \tau(1 - e^{-t/\tau})]$$
$$\sim \begin{cases} \dfrac{D_1 + D_2}{\tau}t^2 & \text{as} \quad t \to 0 \\ 2(D_1 + D_2)t & \text{as} \quad t \to \infty. \end{cases} \tag{6.1}$$

The MSD in the framework of the $D_{N=1}$ approximation to the linear Boltzmann equation with $\gamma = 0$ is the same.

The temporal behavior of the MSD given by Eq. (6.1) is the same as that in the Brownian motion described by the standard Langevin equation with initial velocities having Maxwellian distribution [3–5]: It is ballistic as $t \to 0$ and diffusive as $t \to \infty$. Therefore, the behavior of the MSD in the two models is consistent with that in the normal diffusion and Brownian motion.

The MSD in the framework of the two-phase model is defined through the solution w_{TP} to the problem (5.14)–(5.16) with $\gamma = 0$. Therefore, the MSD is the solution to the problem

$$\tau\frac{d^2}{dt^2}\langle x^2_{\mathrm{TP}}\rangle + \frac{d}{dt}\langle x^2_{\mathrm{TP}}\rangle = 2(D_1 + D_2), \quad t > 0,$$
$$\langle x^2_{\mathrm{TP}}\rangle\big|_{t=0} = 0, \quad \frac{d}{dt}\langle x^2_{\mathrm{TP}}\rangle\big|_{t=0} = 2\alpha D_1.$$

Hence the MSD is equal to

$$\langle x^2_{\mathrm{TP}}(t)\rangle = 2\{(D_1 + D_2)[t - \tau(1 - e^{-t/\tau})]$$
$$+ \alpha D_1\tau(1 - e^{-t/\tau})\}, \quad t \geqslant 0,$$

where D_2 and τ are given by the relations (4.12a). This differs from the behavior (6.1) if $\alpha > 0$.

VII. INITIAL-VALUE PROBLEMS FOR THE JEFFREYS-TYPE EQUATION WITH ABSORPTION AND A STATIONARY POINT SOURCE

In this section we study the classic problem of the diffusion of a substance from a stationary point source. We suppose that the substance is absorbed (degraded), therefore, we set $f = -\gamma u + \delta(x)$. We suppose also that the initial concentrations and flux are equal to zero.

The study reveals that in the model described by the $D_{N=1}$ approximation to the linear Boltzmann equation a finite portion of the substance does not move and this portion increases with time, approaching a limit. Alternatively, in the Jeffreys-type and two-phase models the substance always moves.

A. Jeffreys-type model

In the one-dimensional case the problem (3.4) and (4.4) with $f = -\gamma u + \delta(x)$, $u_0 = 0$, and $J_0 = 0$ takes the form

$$\tau\frac{\partial^2 u_{\mathrm{Je}}}{\partial t^2} + (1 + \tau\gamma)\frac{\partial u_{\mathrm{Je}}}{\partial t} - \tau D_1\frac{\partial^3 u_{\mathrm{Je}}}{\partial x^2\partial t}$$
$$-(D_1 + D_2)\frac{\partial^2 u_{\mathrm{Je}}}{\partial x^2} + \gamma u_{\mathrm{Je}} = \delta(x), \quad x \in \mathbb{R}, \quad t > 0, \tag{7.1}$$

$$u_{\mathrm{Je}}|_{t=0} = 0, \quad \frac{\partial u_{\mathrm{Je}}}{\partial t}\bigg|_{t=0} = \delta(x). \tag{7.2}$$

The Fourier transform of this problem yields

$$\tau\frac{\partial^2 \mathcal{F}u_{\mathrm{Je}}}{\partial t^2} + [1 + \tau(D_1\xi^2 + \gamma)]\frac{\partial \mathcal{F}u_{\mathrm{Je}}}{\partial t}$$
$$+ [(D_1 + D_2)\xi^2 + \gamma]\mathcal{F}u_{\mathrm{Je}} = 1, \quad \xi \in \mathbb{R}, \quad t > 0,$$

$$\mathcal{F}u_{\mathrm{Je}}(\xi,t) = \frac{1}{\lambda_1(\xi) - \lambda_2(\xi)}\left\{\frac{1}{\tau}\left[\frac{e^{\lambda_1(\xi)t} - 1}{\lambda_1(\xi)} - \frac{e^{\lambda_2(\xi)t} - 1}{\lambda_2(\xi)}\right]\right.$$
$$\left. + [e^{\lambda_1(\xi)t} - e^{\lambda_2(\xi)t}]\right\},$$

where $\lambda_{1,2}$ are the characteristic values, given by Eq. (5.6). The asymptotic behavior (5.8) of the characteristic values leads to the asymptotic behavior

$$\mathcal{F}u_{\mathrm{Je}}(\xi,t) = O\left(\frac{1}{\xi^2}\right) \quad \text{as} \quad \xi \to \pm\infty.$$

Hence the solution u_{Je} is a continuous function of x [48].

The mass of the substance is equal at any time to that in similar problems for the diffusion and telegraph equations

$$\int_{-\infty}^{\infty} u_{\mathrm{DE}}(x,t)dx = \int_{-\infty}^{\infty} u_{\mathrm{TE}}(x,t)dx = \int_{-\infty}^{\infty} u_{\mathrm{Je}}(x,t)dx$$
$$= \frac{1 - e^{-\gamma t}}{\gamma}, \quad t \geqslant 0, \tag{7.3}$$

where u_{DE} is the solution of the diffusion equation

$$\frac{\partial u_{\mathrm{DE}}}{\partial t} - (D_1 + D_2)\frac{\partial^2 u_{\mathrm{DE}}}{\partial^2 x}$$
$$+ \gamma u_{\mathrm{DE}} = \delta(x), \; x \in \mathbb{R}, \quad t > 0,$$

with the initial condition

$$u_{\mathrm{DE}}|_{t=0} = 0,$$

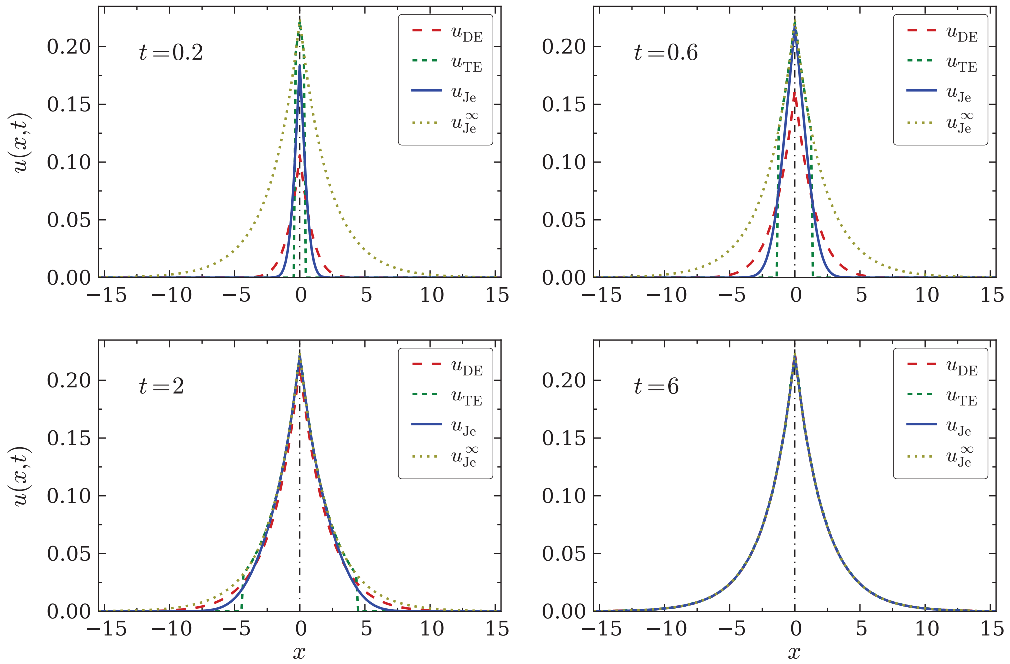

FIG. 5. (Color online) Solution u_{Je} to the problem (7.1) and (7.2) with $\tau = 1$, $D_1 = 1$, $D_2 = 4$, and $\gamma = 1$ in comparison with those of the diffusion and telegraph equations (see the text).

and u_{TE} is the solution of the telegraph equation

$$\tau\frac{\partial^2 u_{\mathrm{TE}}}{\partial t^2} + (1+\tau\gamma)\frac{\partial u_{\mathrm{TE}}}{\partial t} - (D_1 + D_2)\frac{\partial^2 u_{\mathrm{TE}}}{\partial^2 x} + \gamma u_{\mathrm{TE}} = \delta(x), \quad x \in \mathbb{R}, \quad t > 0,$$

with the initial conditions

$$u_{\mathrm{TE}}|_{t=0} = 0, \quad \left.\frac{\partial u_{\mathrm{TE}}}{\partial t}\right|_{t=0} = \delta(x).$$

Note that the mass does not depend on τ.

Fig. 5 shows the solution u_{Je}, obtained with the parameters $\tau = 1$, $D_1 = 1$, $D_2 = 4$ and $\gamma = 1$. The figure shows also the steady state solution u_{Je}^{∞} of the equation (7.1).

For comparison the figure shows also the solutions u_{DE} and u_{TE}. One can see the vertical front of the solution u_{TE}. The solution u_{Je} is intermediate between the solutions of the diffusion and telegraph equations.

B. Two-phase model

Here we study the behavior of the net concentration $w_{\mathrm{TP}} = u_{\mathrm{TP}} + v_{\mathrm{TP}}$, where u_{TP} and v_{TP} are the concentrations of the free and bound phases, respectively. In the one-dimensional case the problem (4.8) and (4.9) and the problem (4.10) and (4.11) with $f = -\gamma u + \delta(x)$, $u_0 = 0$, and $v_0 = 0$ lead to the problem

$$\frac{\partial^2 w_{\mathrm{TP}}}{\partial t^2} + (k_1 + k_2 + \gamma)\frac{\partial w_{\mathrm{TP}}}{\partial t} - D_1\frac{\partial^3 w_{\mathrm{TP}}}{\partial x^2 \partial t} - k_2 D_1 \frac{\partial^2 w_{\mathrm{TP}}}{\partial x^2} + k_2\gamma w_{\mathrm{TP}} = (k_1 + k_2)\delta(x), \quad x \in \mathbb{R}, \quad t > 0, \tag{7.4}$$

$$w_{\mathrm{TP}}|_{t=0} = 0, \quad \left.\frac{\partial w_{\mathrm{TP}}}{\partial t}\right|_{t=0} = \delta(x). \tag{7.5}$$

Note that Eq. (7.4), expressed through the parameters τ, D_1, and D_2, takes the form

$$\tau\frac{\partial^2 w_{\mathrm{TP}}}{\partial t^2} + (1+\tau\gamma)\frac{\partial w_{\mathrm{TP}}}{\partial t} - \tau D_1 \frac{\partial^3 w_{\mathrm{TP}}}{\partial x^2 \partial t} - (D_1 + D_2)\frac{\partial^2 w_{\mathrm{TP}}}{\partial x^2} + \left(1 + \frac{D_2}{D_1}\right)\gamma w_{\mathrm{TP}} = \delta(x)$$

[cf. with Eq. (7.1); the difference is in the last term on the left-hand side].

The Fourier transform of the problem (7.4) and (7.5) yields

$$\frac{\partial^2 \mathcal{F}w_{\mathrm{TP}}}{\partial t^2} + (k_1 + k_2 + \gamma + D_1\xi^2)\frac{\partial \mathcal{F}w_{\mathrm{TP}}}{\partial t} + k_2(D_1\xi^2 + \gamma)\mathcal{F}w_{\mathrm{TP}} = k_1 + k_2, \quad \xi \in \mathbb{R}, \quad t > 0,$$

$$\mathcal{F}w_{\mathrm{TP}}|_{t=0} = 0, \quad \left.\frac{\partial \mathcal{F}w_{\mathrm{TP}}}{\partial t}\right|_{t=0} = 1.$$

The solution to this problem is

$$\mathcal{F}w_{\mathrm{TP}}(\xi,t) = \frac{1}{\lambda_1(\xi) - \lambda_2(\xi)}\left\{(k_1 + k_2)\left[\frac{e^{\lambda_1(\xi)t} - 1}{\lambda_1(\xi)} - \frac{e^{\lambda_2(\xi)t} - 1}{\lambda_2(\xi)}\right] + [e^{\lambda_1(\xi)t} - e^{\lambda_2(\xi)t}]\right\},$$

where $\lambda_{1,2}$ are the characteristic values, given by Eq. (5.19).

The asymptotic behavior (5.8) of the characteristic values leads to the asymptotic behavior

$$\mathcal{F}w_{\mathrm{TP}}(\xi,t) = O\left(\frac{1}{\xi^2}\right) \quad \text{as} \quad \xi \to \pm\infty.$$

This means that the solution w_{TP} is a continuous function of x [48].

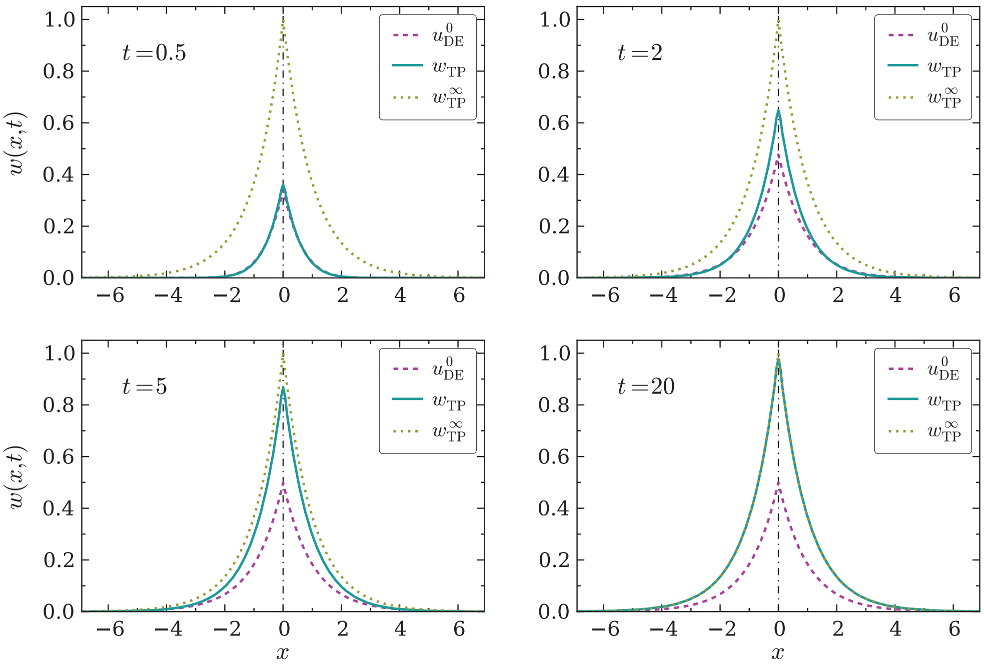

FIG. 6. (Color online) Solution $w_{\rm TP}$ to the problem (7.4) and (7.5) with $D_1 = 1$, $k_1 = 0.5$, $k_2 = 0.5$, and $\gamma = 1$ in comparison with that of the diffusion equation (see the text).

Figure 6 shows the solution $w_{\rm TP}$, obtained with the parameters $D_1 = 1$, $k_1 = 0.5$, $k_2 = 0.5$ (which corresponds to $\tau = 1$ and $D_2 = -0.5$), and $\gamma = 1$. The figure shows also the steady state solution $w^\infty_{\rm TP}$ of Eq. (7.4). For comparison the figure shows the solution $u^0_{\rm DE}$ to the problem for Eq. (4.6a) with $k_1 = k_2 = 0$, $f = -\gamma u + \delta(x)$, and the homogeneous initial condition, i.e., this would be the concentration of the free substance if the interphase mass transfer were absent.

C. The $D_{N=1}$ approximation to the linear Boltzmann equation

In the one-dimensional case the problem (4.18) and (4.19) with $F = \delta(x)$, $u_0 = 0$, and $J_0 = 0$ takes the form

$$\begin{aligned}\tau\frac{\partial^2 u_{\rm Bo}}{\partial t^2}+(1+\tau\gamma)\frac{\partial u_{\rm Bo}}{\partial t}-\tau D_1\frac{\partial^3 u_{\rm Bo}}{\partial x^2\partial t}&\\ -(D_1+D_2')\frac{\partial^2 u_{\rm Bo}}{\partial x^2}+\gamma u_{\rm Bo}&\\ =\delta(x)-\tau D_1\frac{\partial^2\delta(x)}{\partial x^2},\quad x\in\mathbb{R},\quad t>0,&\end{aligned} \tag{7.6}$$

$$u_{\rm Bo}|_{t=0}=0,\qquad \left.\frac{\partial u_{\rm Bo}}{\partial t}\right|_{t=0}=\delta(x), \tag{7.7}$$

with $D_2' = D_2 + \tau\gamma D_1$. The Fourier transform of this problem yields

$$\begin{aligned}\tau\frac{\partial^2\mathcal{F}u_{\rm Bo}}{\partial t^2}+[1+\tau(D_1\xi^2+\gamma)]\frac{\partial\mathcal{F}u_{\rm Bo}}{\partial t}&\\ +[(D_1+D_2')\xi^2+\gamma]\mathcal{F}u_{\rm Bo}&\\ =1+\tau D_1\xi^2,\quad \xi\in\mathbb{R},\quad t>0,&\\ \mathcal{F}u_{\rm Bo}|_{t=0}=0,\qquad \left.\frac{\partial\mathcal{F}u_{\rm Bo}}{\partial t}\right|_{t=0}=1&\end{aligned}$$

and leads to the following solution:

$$\begin{aligned}&\mathcal{F}u_{\rm Bo}(\xi,t)\\ &\quad=\frac{1}{\lambda_1(\xi)-\lambda_2(\xi)}\left\{\left(\frac{1}{\tau}+D_1\xi^2\right)\left[\frac{e^{\lambda_1(\xi)t}-1}{\lambda_1(\xi)}-\frac{e^{\lambda_2(\xi)t}-1}{\lambda_2(\xi)}\right]\right.\\ &\qquad\left.+[e^{\lambda_1(\xi)t}-e^{\lambda_2(\xi)t}]\right\},\end{aligned}$$

where $\lambda_{1,2}$ are the characteristic values, given by Eq. (5.6) with D_2' instead of D_2.

The asymptotic behavior (5.8) of the characteristic values leads to the asymptotic behavior

$$\mathcal{F}u_{\rm Bo}(\xi,t)=\frac{1-e^{-k_2' t}}{k_2'}+O\left(\frac{1}{\xi^2}\right)\quad\text{as}\quad \xi\to\pm\infty,$$

where k_2' is given by the relation (4.12b) for k_2 with D_2' instead of D_2, i.e.,

$$k_2'=\frac{1}{\tau}\left(1+\frac{D_2'}{D_1}\right).$$

Therefore, the solution $u_{\rm Bo}$ has the form

$$u_{\rm Bo}(x,t)=u^s_{\rm Bo}(x,t)+u^r_{\rm Bo}(x,t),$$

where

$$u^s_{\rm Bo}(x,t)=\frac{1-e^{-k_2' t}}{k_2'}\delta(x)$$

is the singular term, while the regular term $u^r_{\rm Bo}$ is a continuous function. The presence of the singular term means that in this model a finite portion of the substance does not move and this portion increases with time up to the value $1/k_2'$ as $t\to\infty$.

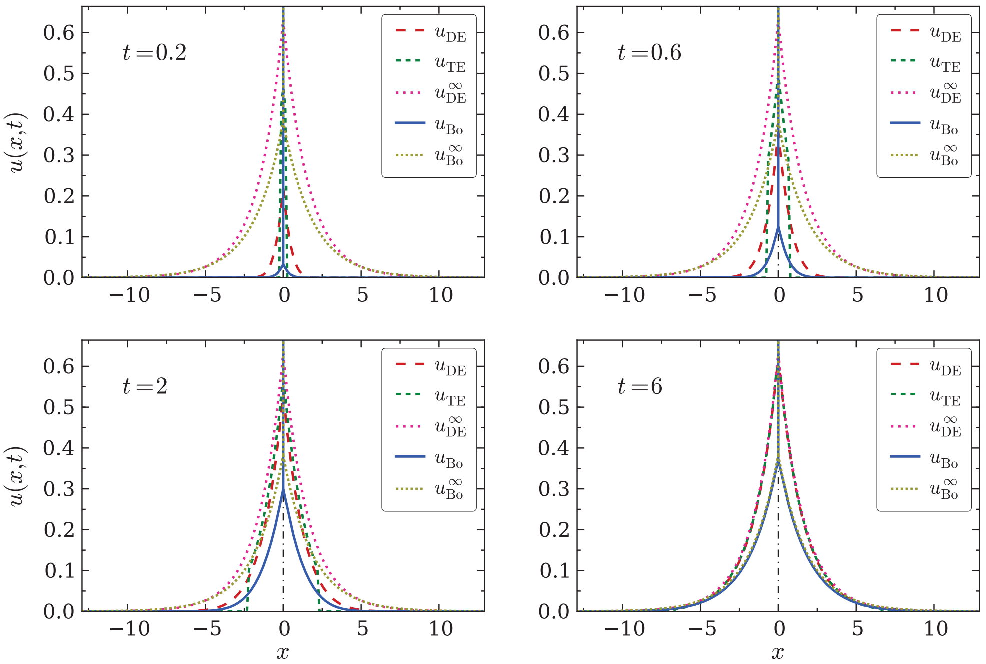

FIG. 7. (Color online) Solution $u_{\rm Bo}$ to the problem (7.6) and (7.7) with $\tau = 1$, $D_1 = 1$, $D_2 = 0.25$, and $\gamma = 0.5$ in comparison with those of the diffusion and telegraph equations (see the text). The vertical lines stand for the singular term $u_{\rm Bo}^s$.

The steady state solution of Eq. (7.6) satisfies the equation

$$-(D_1 + D_2')\frac{\partial^2 u_{\rm Bo}^\infty}{\partial x^2} + \gamma u_{\rm Bo}^\infty = \delta(x) - \tau D_1 \frac{\partial^2 \delta(x)}{\partial x^2},$$

$x \in \mathbb{R}$. The Fourier transform of the steady state solution is

$$\mathcal{F}u_{\rm Bo}^\infty(\xi) = \frac{1 + \tau D_1 \xi^2}{(D_1 + D_2')\xi^2 + \gamma} \equiv \frac{1}{D_1 + D_2'}\left[\tau D_1 + \frac{D_1 + D_2}{(D_1 + D_2')\xi^2 + \gamma}\right].$$

Therefore, the steady state solution is

$$u_{\rm Bo}^\infty(x) = u_{\rm Bo}^s(x) + u_{\rm Bo}^r(x), \qquad (7.8)$$

where

$$u_{\rm Bo}^s(x) = \frac{\tau D_1}{D_1 + D_2'}\delta(x) \equiv \frac{1}{k_2'}\delta(x) \qquad (7.9)$$

is the singular term and

$$u_{\rm Bo}^r(x) = \frac{D_1 + D_2}{2\sqrt{(D_1 + D_2')^3\gamma}}\exp\left(-\sqrt{\frac{\gamma}{D_1 + D_2'}}|x|\right) \qquad (7.10)$$

is the regular (continuous) term.

Figure 7 shows the solution $u_{\rm Bo}$, obtained with the parameters $c = \sqrt{15/4}$, $\kappa = 0.5$, $\sigma = 0.5$, isotropic scattering, i.e., $K \equiv (4\pi)^{-1}$ (therefore, $\sigma_1 = \sigma$ and $\sigma_2 = \sigma$), and $F = \delta(x)$ (which corresponds to $\tau = 1$, $D_1 = 1$, $D_2 = 0.25$, $D_2' = 0.75$, and $\gamma = 0.5$). All the figures show also the steady state solution $u_{\rm Bo}^\infty$, given by Eqs. (7.8)–(7.10).

For comparison the figure shows also the diffusion approximation $u_{\rm DE}$ to the Boltzmann equation, given by Eq. (A4) with the first of the initial conditions (7.7), and the telegraph approximation $u_{\rm TE}$, given by Eq. (A6) with the initial conditions (7.7). The figure shows also the steady state diffusion approximation $u_{\rm DE}^\infty$.

There are two qualitative peculiarities that distinguish the $D_{N=1}$ approximation from the diffusion and the telegraph ones. First, a finite portion of the substance in the $D_{N=1}$ approximation does not move. Second, the steady state distribution for the $D_{N=1}$ approximation is different from that for the diffusion and telegraph approximations. Nevertheless, the mass of the substance in all these approximations is the same at any time:

$$\int_{-\infty}^{\infty} u_{\rm DE}(x,t)dx = \int_{-\infty}^{\infty} u_{\rm TE}(x,t)dx = \int_{-\infty}^{\infty} u_{\rm Bo}(x,t)dx = \frac{1 - e^{-\gamma t}}{\gamma}, \quad t \geqslant 0$$

[cf. with the same relation (7.3) in the Jeffreys-type model].

VIII. CONCLUSION

We have considered three models of nonanomalous mass transfer, leading to the Jeffreys-type equation. In the framework of the Jeffreys-type model this equation combines the diffusion and telegraph ones through the Jeffreys-type law, which combines in turn Fick's law and Cattaneo's equation. In the framework of the two-phase model the Jeffreys-type equation describes the concentrations of the free (mobile) and bound (immobile) phases of a substance as well as the net concentration. The Jeffreys-type equation in the form of the $D_{N=1}$ approximation ranks after the diffusion and telegraph equations in the hierarchy of the spherical harmonics approximations to the linear Boltzmann equation.

Solutions of the Jeffreys-type equation show qualitatively different behavior in all these models. The two-phase model shows nothing unusual, while the Jeffreys-type model and the $D_{N=1}$ approximation to the linear Boltzmann equation exhibit distinctive features.

The first problem we studied is the transfer of a substance initially confined at a point. In this case the Jeffreys-type model and $D_{N=1}$ approximation coincide. The study has revealed that in these models a finite portion of the substance does not move, though this portion diminishes exponentially with time. In addition, we have calculated the mean-square displacement for the solutions of the first problem. The temporal behavior of the MSD in the Jeffreys-type model and in the $D_{N=1}$ approximation is found to be the same as that in the Brownian motion described by the standard Langevin equation, i.e., it is ballistic as $t \to 0$ and diffusive as $t \to \infty$.

The second problem we have studied is the transfer of a substance from a stationary point source. The study has revealed that in the $D_{N=1}$ approximation a finite portion of the substance does not move and this portion increases with time up to a value as $t \to \infty$.

A tentative interpretation of the local immobilization phenomena is that in a dense crowd inner particles have no space to move, but when the crowd is scattered the particles become mobile.

The two problems we have studied are one dimensional. An important question requires further consideration: Are the solutions of the three-dimensional problems for the Jeffreys-type equation left non-negative?

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APPENDIX A: APPROXIMATIONS TO THE LINEAR BOLTZMANN EQUATION IN THE FRAMEWORK OF THE SPHERICAL HARMONICS METHOD

One of the methods to obtain approximate solutions of the linear Boltzmann equation (4.13) is the spherical harmonics method [34,47]. In this method the particle phase space density is expanded into the generalized Fourier series

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},t) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \psi_n^m(\boldsymbol{x},t) Y_n^m(\boldsymbol{\Omega}), \tag{A1}$$

where Y_n^m are the spherical harmonics [49] and the coefficients are expressed by

$$\psi_n^m(\boldsymbol{x},t) = \int_{\mathbb{S}^2} \psi(\boldsymbol{x},\boldsymbol{\Omega},t)\overline{Y_n^m(\boldsymbol{\Omega})}d\boldsymbol{\Omega},$$

where the overline means the complex conjugate. Note that the expansion (A1) can be expressed through the particle density u (4.15) and flux $\boldsymbol{J}$ (4.16). Indeed, note that

$$\psi_0^0(\boldsymbol{x},t)Y_0^0 \equiv \frac{1}{4\pi}u(\boldsymbol{x},t)$$

and

$$\sum_{m=-1}^{1} \psi_1^m(\boldsymbol{x},t)Y_1^m(\boldsymbol{\Omega}) \equiv \frac{3}{4\pi c^2}\boldsymbol{J}(\boldsymbol{x},t)\cdot\boldsymbol{\Omega}.$$

Therefore, the expansion (A1) takes the form

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},t) = \frac{1}{4\pi}u(\boldsymbol{x},t) + \frac{3}{4\pi c^2}\boldsymbol{J}(\boldsymbol{x},t)\cdot\boldsymbol{\Omega} + \sum_{n=2}^{\infty}\sum_{m=-n}^{n}\psi_n^m(\boldsymbol{x},t)Y_n^m(\boldsymbol{\Omega}).$$

The collision kernel is also expanded into the spherical harmonics:

$$K(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = \sum_{n=0}^{\infty} K_n \sum_{m=-n}^{n} Y_n^m(\boldsymbol{\Omega})\overline{Y_n^m(\boldsymbol{\Omega}')}, \tag{A2}$$

where

$$K_n = 2\pi\int_{-1}^{1} K(\mu)P_n(\mu)d\mu,$$

P_n are the Legendre polynomials, with $K_0 = 1$ due to the normalization $\int_{\mathbb{S}^2} K(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')d\boldsymbol{\Omega} = 1$, which is equivalent to $\int_{-1}^{1} K(\mu)d\mu = (2\pi)^{-1}$. The expansions (A1) and (A2) are substituted into the linear Boltzmann equation. Due to orthogonality of the spherical harmonics this leads to an infinite system of coupled partial differential equations for the functions ψ_n^m.

The first equation of the infinite system is the continuity equation (4.14). The second (vector) equation can be obtained with the help of integrating the linear Boltzmann equation, multiplied by $\boldsymbol{\Omega}$, over the unit sphere. The second equation relates the gradient of the particle density ∇u, flux $\boldsymbol{J}$, its time derivative $\partial\boldsymbol{J}/\partial t$, and coefficients ψ_2^m.

1. Diffusion approximation

The classic diffusion approximation is obtained if the coefficients ψ_n^m, $n > 1$, in the expansion (A1) are negligible and the coefficients ψ_1^m are quasistationary. The latter condition is equivalent to quasistationarity of flux $\boldsymbol{J}$, i.e., $\partial\boldsymbol{J}/\partial t \approx 0$. In this case the particle density and flux are related by the (truncated second) equation

$$(\kappa + \sigma_1)\,\boldsymbol{J} + \frac{c^2}{3}\nabla u = 0, \tag{A3}$$

where

$$\sigma_n = \sigma(1 - K_n), \quad n = 1,2,\ldots;$$

clearly, $\sigma_n > 0$. Note that Eq. (A3) is identical to Fick's law (2.2). The continuity equation (4.14) and Eq. (A3) imply that the particle density satisfies the diffusion equation

$$\frac{\partial u}{\partial t} - \frac{c^2}{3\,(\kappa+\sigma_1)}\Delta u + \kappa u = F. \tag{A4}$$

2. The P_N approximations

The classic P_N approximations are obtained if the coefficients ψ_n^m, $n > N \geqslant 1$, in the expansion (A1) are negligible.

Particularly in the P_1 approximation the particle density and flux are related by the (truncated second) equation

$$\frac{\partial \boldsymbol{J}}{\partial t} + (\kappa + \sigma_1)\boldsymbol{J} + \frac{c^2}{3}\nabla u = 0, \tag{A5}$$

which is an extension of Eq. (A3). Note that Eq. (A5) is similar to Cattaneo's equation (3.1). The continuity equation (4.14) and Eq. (A5) imply that the particle density satisfies the telegraph equation

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2} + (2\kappa + \sigma_1)\frac{\partial u}{\partial t} - \frac{c^2}{3}\Delta u + \kappa(\kappa + \sigma_1)u \\ = (\kappa + \sigma_1)\,F + \frac{\partial F}{\partial t}.\end{aligned} \tag{A6}$$

3. The D_N approximations

Recently, D_N approximations were proposed [35]. They generalize the diffusion approximation, which can be considered as the D_0 approximation. The D_N approximations are obtained if the coefficients $\psi_n^m, n > N+1$, in the expansion (A1) are negligible and the coefficients ψ_{N+1}^m are quasistationary. The coefficients ψ_{N+1}^m can be expressed through ψ_N^m and the D_N approximation is described by ψ_n^m, $n = 0,\ldots,N$. In the case $N = 1$ the coefficients ψ_2^m can be expressed through flux $\boldsymbol{J}$. As a result, in the $D_{N=1}$ approximation the particle density and flux are related by the equation

$$\begin{aligned}\frac{\partial \boldsymbol{J}}{\partial t} + (\kappa + \sigma_1)\boldsymbol{J} + \frac{c^2}{3}\nabla u \\ = \frac{c^2}{15(\kappa + \sigma_2)}(3\Delta \boldsymbol{J} + \nabla \operatorname{div} \boldsymbol{J}),\end{aligned} \tag{A7}$$

which is a generalization of Eq. (A5). (We used the notation $D_{N=1}$ instead of D_1 since the latter stands for the coefficient.) The continuity equation (4.14) and (A7) imply that the particle density satisfies the Jeffreys-type equation

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2} + (2\kappa + \sigma_1)\frac{\partial u}{\partial t} - \frac{4c^2}{15(\kappa + \sigma_2)}\frac{\partial \Delta u}{\partial t} \\ - \left[\frac{c^2}{3} + \frac{4c^2}{15(\kappa + \sigma_2)}\kappa\right]\Delta u + \kappa(\kappa + \sigma_1)u \\ = (\kappa + \sigma_1)F + \frac{\partial F}{\partial t} - \frac{4c^2}{15(\kappa + \sigma_2)}\Delta F.\end{aligned} \tag{A8}$$

APPENDIX B: GUYER-KRUMHANSL MODEL

In this section we consider heat transfer. The energy equation without sources and sinks has the form

$$C\frac{\partial T}{\partial t} + \operatorname{div} \boldsymbol{q} = 0, \tag{B1}$$

where $T \equiv T(\boldsymbol{x},t)$ is temperature, $\boldsymbol{q} \equiv \boldsymbol{q}(\boldsymbol{x},t)$ is heat flux, and C is the volumetric heat capacity. The equation of Guyer and Krumhansl relating heat flux and temperature is [8,10,36]

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{1}{\tau_R}\boldsymbol{q} = -\frac{c^2 C}{3}\nabla T + \frac{\tau_N c^2}{5}(\Delta \boldsymbol{q} + 2\nabla \operatorname{div} \boldsymbol{q}), \tag{B2}$$

where c is the average speed of phonons, τ_N is a relaxation time for momentum-conserving collisions (normal process), and τ_R is a relaxation time for momentum-nonconserving collisions (umklapp process) in the phonon gas. An equivalent equation was obtained in the framework of extended irreversible thermodynamics [14].

The energy equation (B1) and the equation of Guyer and Krumhansl imply that temperature satisfies the homogeneous Jeffreys-type equation

$$\frac{\partial^2 T}{\partial t^2} + \frac{1}{\tau_R}\frac{\partial T}{\partial t} - \frac{3\tau_N c^2}{5}\frac{\partial \Delta T}{\partial t} - \frac{c^2}{3}\Delta T = 0. \tag{B3}$$

This equation is related to Eq. (4.20) by $\tau = \tau_R$, $D_1 = 3\tau_N c^2/5$, and $D_2 = (\tau_R/3 - 3\tau_N/5)c^2$; in addition, the inequalities $D_2 \gtreqless 0$ are equivalent to $5\tau_R \gtreqless 9\tau_N$. The initial conditions for Eq. (B3) are

$$T|_{t=0} = T_0, \qquad \left.\frac{\partial T}{\partial t}\right|_{t=0} = -\frac{1}{C}\operatorname{div} \boldsymbol{q}_0,$$

where $T_0 \equiv T_0(\boldsymbol{x})$ and $\boldsymbol{q}_0 \equiv \boldsymbol{q}_0(\boldsymbol{x})$ are the initial temperature and heat flux, respectively. These are the same as the initial conditions (4.19) with $F = 0$ and $\gamma = 0$.

The equation of Guyer and Krumhansl (B2), written through τ, D_1, and D_2, has the form

$$\tau\frac{\partial \boldsymbol{q}}{\partial t} + \boldsymbol{q} = -(D_1 + D_2)C\nabla T + \frac{\tau D_1}{3}(\Delta \boldsymbol{q} + 2\nabla \operatorname{div} \boldsymbol{q}), \tag{B4}$$

which differs from the similar equation (4.17) in the framework of the $D_{N=1}$ approximation to the linear Boltzmann equation. In a steady state Eq. (B4) takes the form

$$\boldsymbol{q} = -(D_1 + D_2)C\nabla T + \frac{\tau D_1}{3}(\Delta \boldsymbol{q} + 2\nabla \operatorname{div} \boldsymbol{q}),$$

which differs qualitatively from Fourier's law.

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