Space-fractional advection-diffusion and reflective boundary condition

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Anomalous diffusive transport arises in a large diversity of disordered media. Stochastic formulations in terms of continuous time random walks (CTRWs) with transition probability densities showing space- and/or time-diverging moments were developed to account for anomalous behaviors. A broad class of CTRWs was shown to correspond, on the macroscopic scale, to advection-diffusion equations involving derivatives of noninteger order. In particular, CTRWs with Lévy distribution of jumps and finite mean waiting time lead to a space-fractional equation that accounts for superdiffusion and involves a nonlocal integral-differential operator. Within this framework, we analyze the evolution of particles performing symmetric Lévy flights with respect to a fluid moving at uniform speed v. The particles are restricted to a semi-infinite domain limited by a reflective barrier. We show that the introduction of the boundary condition induces a modification in the kernel of the nonlocal operator. Thus, the macroscopic space-fractional advection-diffusion equation obtained is different from that in an infinite medium.

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I. INTRODUCTION

Diffusion processes not following Gaussian statistics are observed in various complex systems [1–8]. Subdiffusive and superdiffusive phenomena imply rates of spreading, respectively smaller or greater than the Fickian rate. One of the most efficient models for diffusive transport is based on the continuous time random walk (CTRW) approach [7]. Depending on the underlying stochastic kinetics considered, subdiffusive, normal, superdiffusive, or mixed effects occur.

When no boundary condition is imposed, a wide class of uncoupled and unbiased CTRW models yields fractional diffusion equations in the coarse-grained limit [9,10].

Time-fractional diffusion [11] accounts for subdiffusive effects and comes from broad waiting time distributions, whereas space-fractional diffusion arises from wide jump distributions [12,13]. Allowing both long rests and long jumps yields space-time-fractional diffusion equations [7,14,15]. Space-fractional diffusion with advection in an infinite medium was addressed in [16,17] for Lévy flights.

CTRWs are point processes with reward [9,10,18]. The point process is a sequence of independent identically distributed (i.i.d.) positive random variables T_i, representing waiting or survival times between successive events. Starting at time $t=0$, the nth event occurs at time $t_n=\Sigma_{i=1}^{n}T_i$. The rewards in turn are random variables X_i representing successive one-dimensional jumps. Considering the spreading of particles within a fluid moving at constant speed v in an infinite medium, a particle initially at position x_0 at time $t=0$ is located in

$$x(t) = x_0 + \sum_{i=1}^{N(t)} X_i + vt \tag{1}$$

at time t. Here $N(t)\equiv\max\{n/t_n\leqslant t\}$ is the number of jumps a tagged particle performs during time interval $[0,t]$. Then, $\Sigma_{i=1}^{N(t)}X_i$ is the position with respect to the moving frame whose origin travels distance vt during $[0,t]$.

For uncoupled CTRWs, the X_i are independent of the T_j. In an infinite medium, and in the absence of nonuniform force fields, it is reasonable to assume that the X_i also are i.i.d. as in [9,10,18].

Letting l and τ_0, respectively, be characteristic space and time scales for X_i and T_i, the coarse-grained evolution equation for the concentration of particles is obtained in the limit $(l,\tau_0)\to 0$.

In the absence of advection, and when the jump lengths X_i are distributed according to an α-stable symmetric Lévy law [19], with moreover the survival probability being of Mittag-Leffler type with index β, the macroscopic evolution obeys the following space-time-fractional variant of the standard diffusion equation [9,10]:

$$\partial_t^{\beta} c(x,t) = K\nabla_x^{\alpha} c(x,t) \tag{2}$$

with $l^{\alpha}/\tau_0^{\beta}=K$, $\beta\in(0,1]$, and $\alpha\in(0,2]$. If, moreover $\alpha\in(1,2]$, Eq. (2) can be interpreted as a generalization of Fick's diffusion law [20]. In the fractional variant, the local rate of the concentration is replaced by a time derivative of fractional order $\beta\in(0,1)$, and the divergence of the concentration gradient by a Riesz-Feller derivative of order. In Fourier coordinates, the symmetric Riesz-Feller derivative of order $\alpha\in(0,2)$ is defined by $\nabla_x^{\alpha}\equiv-|k|^{\alpha}$ [13]. In real space, and for $\alpha\in(1,2)$, it satisfies

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$$\nabla_x^\alpha f(x) = \frac{-1}{2\cos(\alpha\pi/2)\Gamma(2-\alpha)}\partial_x^2\int_R (|x-y|^{1-\alpha}f(y)dy. \tag{3}$$

When $\alpha=2$, the right-hand side of Eq. (3) is the usual Laplacian.

The only survival probability distribution leading to a local time derivative ($\beta=1$) is the exponential distribution with finite mean waiting time τ_0. In the latter case, and if we further constrain α to the interval (0,2), particles perform Lévy flights. Brownian motions in turn are limiting cases of Lévy flights. They correspond to $\alpha=2$, and are the only Lévy flights with finite variance. Lévy flights with $\alpha \in (0,1]$ have, in addition, an infinite mean.

For $v \neq 0$, the macroscopic limit of symmetric Lévy flights is a space-fractional advection-diffusion equation, with the advection term unchanged with respect to the classical advection-diffusion equation [16,17]. Space-fractional advection-diffusion equations have been successfully applied to model the evolution of tracers in heterogeneous porous media [21,22].

When considering experimental devices and attempting to check models for mass transport in a given finite medium, we need to consider boundary conditions. Lévy statistics for the jump length account for long-range interactions on the small scale and correspond to nonlocal (in space) operators on the large scale. The presence of a boundary may modify the nonlocal spatial operator [23]. Boundary conditions cannot be uncoupled from the fractional partial differential equation as when the order of the space derivative is an integer [24]. The case of diffusion in the presence of an absorbing boundary was considered in [25], where an expression was obtained for the propagator of Lévy flights.

Here, we model the influence of a semipermeable wall within the framework of space-fractional partial differential equations, with and without advection. The wall is permeable to the fluid and impermeable to the tracer.

We first develop a CTRW model for particles performing symmetric Lévy flights in a semi-infinite medium limited by a reflective boundary, with and without advection. We assume that the particles arriving at the boundary are bounced back as in elastic collisions.

Then, we derive the evolution equations in the coarse-grained limit. We obtain space-fractional models involving a nonlocal operator, very similar to a Riesz-Feller derivative with respect to space, except that the kernel takes account of the boundary condition.

Finally, a finite difference method, inspired by [13–15], allows us to numerically solve the macroscopic model. Numerical and analytical solutions when available are checked against direct Monte Carlo simulations.

II. INFLUENCE OF A WALL ON THE MICROSCOPIC LEVEL

The concentration of particles performing a CTRW satisfies a generalized master equation [4], which is an integral equation resuming the CTRW itself. We will see that it is sensitive to the presence of a boundary.

A. The underlying random walk in free space

Brownian motion is a CTRW with a Gaussian probability distribution function (PDF) for the jump length. Instead, we consider a symmetric α-stable Lévy law, which is more general and allows for long-range correlations. In porous media, spatial correlations may arise from heterogeneous free paths for moving particles due to unequal clustering of solid matter with coherence lengths varying over many length scales (see for instance [26]). Then, highly disordered and unsteady local fluid flows carry particles of tracer whose motion is represented by a succession of jumps. We further assume that jumps may be performed with respect to a frame moving at speed v (e.g., within a fluid moving with mean velocity v). Since we aim at describing the transport of matter in situations bridging between diffusion and propagation, we pay special attention to values of $\alpha \in (1,2)$ focusing on the influence of a boundary condition.

1. With $v=0$

In an infinite domain, consider particles being at x_0 at the instant $t=0$, and performing an uncoupled CTRW, which may be influenced by the environment so that the length of the nth jump does depend on the place it starts from. The spatial dependence of jumps with the location may be due to a nonuniform force field as in [27].

Assuming that the process is Markovian, the probability distribution functions of waiting times T_i between successive jumps are exponential of the form $\psi_{\tau_0}(t)=e^{-t/\tau_0}/\tau_0$. Then, the probability $P(x,t)dx$ of finding a particle in $[x,x+dx]$ at instant t satisfies the generalized master equation

$$P(x,t) = \delta_{x_0}(x)\int_t^{+\infty}\psi_{\tau_0}(t')dt' + \int_{-\infty}^{+\infty}\int_{t'=0}^{t} P(x',t')\Lambda_l(x,x')\psi_{\tau_0}(t-t')dt'dx'. \tag{4}$$

In Eq. (4), $\Lambda_l(x,x')dx$ is the probability that a particle jumping from x' arrives in $[x,x+dx]$.

In the absence of nonuniform force fields, there exists a random variable X such that the X_i are distributed as lX. The parameter l can be thought of as being the length scale of the microscopic motion. Assuming that the PDF $\varphi_1(\cdot)$ of the random variable X is a symmetric α-stable Lévy law $p_\alpha(\cdot,0)$ of order $\alpha \in (0,2]$, the resulting transition PDF between locations x' and x is $\Lambda_l(x,x')=\varphi_l(x-x')$ with $\varphi_l(X)=\varphi_1(X/l)/l$ and $\varphi_1(X)=p_\alpha(X,0)$.

Assuming that a force field constrains particles to lie in the half space $[0,+\infty)$, the generalized master equation involves now an integral over $[0,+\infty)$ instead of $(-\infty,+\infty)$. Hence, it takes the form

$$P(x,t) = \delta_{x_0}(x)\int_t^{+\infty}\psi_{\tau_0}(t')dt' + \int_{0}^{+\infty}\int_{t'=0}^{t} P(x',t')\Lambda_l(x,x')\psi_{\tau_0}(t-t')dt'dx'. \tag{5}$$

2. With $v \neq 0$

Advection modifies the transition probability density, which in general is assumed to remain translation invariant in a free space. It then issues in a not too complicated coupling between time and space [17]. The PDF for a particle to travel from x' to x between instants t' and t becomes

$$T_{v(t-t')}\varphi_l(x-x')\psi_{\tau_0}(t-t') \tag{6}$$

with T_a denoting the translation defined by $T_a f(x)=f(x-a)$.

B. Boundary condition at $x=0$

Incorporating the boundary condition into the random walk modifies the transition PDF $\Lambda_l(x,x')$, which summarizes the interplay between the boundary condition and the supposed kinetics of particles. Indeed, for walkers constrained on the right-hand side $(x>0)$ of an elastic barrier $(x=0)$, the transition probability density cannot be translation invariant. The wall is viewed as a nonuniform (in space) force field applied to the particles. In a porous medium, such a boundary may represent a wall permeable to the fluid, but impermeable to the tracer.

1. With $v=0$

We focus on particles whose motion is exactly as if they were performing a CTRW of characteristic length scale l in a free space with no nonuniform force field, except when they hit the wall. To be more precise, we still bear in mind a point process with rewards X_i as above, but the length of the nth jump, when starting from x', is X_n only if $x'+X_n$ is positive. If this expression is negative, we assume that there is no energy exchange with the wall (located in $x=0$), hence that the jump ends at $-(x'+X_n)$.

Since a jump from x' to x (with positively valued x and x') either is direct or bounces on the wall, we have

$$\Lambda_l(x,x') = \varphi_l(x-x') + \varphi_l(-x-x'). \tag{7}$$

Hence, inserting a reflective boundary condition that constrains particles to the domain $[0,+\infty)$ modifies the transition PDF $\Lambda_l(x,x')$. The analysis can be worked out from a dynamical point of view in particular cases, such as the one detailed in Appendix A, where small scale motions starting and ending on a horizontal plane, are due to a uniform vertical force field and to initial impulses whose horizontal component is distributed according to an α-stable Lévy law.

2. With $v \neq 0$

A particle that hits the wall flies from x' to $x-v(t-t')$, if and only if it would yield a jump from x' to $-x+v(t-t')$ in a free space.

Let us consider a particle performing a quasi-instantaneous jump, starting from x' between instants t' and $t'+dt'$, then being advected until instant t. It will, at that time, have abscissa x if the jump moved it to $x-v(t-t')$, which is impossible for $x<v(t-t')$. Hence, the probability density to travel from x' to x during $[t',t]$ with the last jump having occurred at instant t' is $H(x-v(t-t'))\Lambda_l(x-v(t-t'),x')\psi_{\tau_0}(t-t')$, with Λ_l satisfying Eq. (7). In the latter expression, H represents the Heaviside step function.

Methods developed for infinite media following the lines of [2,3] adapt here to the semi-infinite medium bounded by the reflective boundary condition at $x=0$. Basic tools for that are Fourier and Laplace transforms $\hat{f}(k)$ and $\tilde{g}(u)$ of functions f and g of $x\in R$, and $t\in R^+$. For $\hat{f}(k)$ we take the definition $\hat{f}(k)=\int_{-\infty}^{+\infty}e^{ikx}f(x)dx$, as in [28].

III. ON THE MACROSCOPIC LEVEL IN AN INFINITE MEDIUM

For particles performing CTRWs of the above-described type in an infinite medium, free of any force field, the evolution of the macroscopic concentration $P(x,t)$ was studied in [9–12,16,17]. Even if different points of view were adopted, the above-cited authors obtained similar equations.

We consider here the influence of a reflective boundary when particles perform Lévy flights for small values of l and τ_0 satisfying $l^\alpha/\tau_0=K$. This framework will hereafter be referenced to as the coarse-grained limit.

The probability $P(x,t)$ for particles to be in (x,t) with respect to a frame moving at speed v, satisfies [16,17] the generalized master equation

$$P(x,t) = \int_R \int_{t'=0}^{t} P(x',t')T_{v(t-t')}\Lambda_l(x,x')\psi_{\tau_0}(t-t')dt'dx' + \delta_{x_0+vt}(x)\int_t^{+\infty}\psi_{\tau_0}(t')dt'$$

with $\Lambda_l=\varphi_l$. In Fourier-Laplace coordinates [17] we obtain

$$\hat{\tilde{P}}(k,u) = e^{ikx_0}\frac{1-\hat{\varphi}_l(0)\tilde{\psi}_{\tau_0}(u-ivk)}{(u-ivk)[1-\hat{\varphi}_l(k)\tilde{\psi}_{\tau_0}(u-ivk)]},$$

and hence, in physical variables, we obtain

$$\partial_t P(x,t) + v\,\nabla\, P(x,t) = K\nabla_x^\alpha P(x,t) \tag{8}$$

with the symmetric Riesz-Feller derivative ∇_x^α on the right-hand side. The latter result was obtained by [16,17] for $\alpha \in (1,2]$. For $\alpha\in(0,1]$, Eq. (3) is no longer applicable, but Eq. (8) is still valid with ∇_x^α in physical variables involving a derivative of order 1 and a convolution with a different kernel (see Ref. [13]).

The method, developed in [16,17] following the results of [2,3], can be applied to the semi-infinite medium bounded by the reflective boundary condition at $x=0$. It relies heavily on the Fourier-Laplace transform of a function h of x and t, here denoted by $\hat{\tilde{h}}(k,u)$.

IV. INFLUENCE OF A REFLECTIVE BARRIER ON THE MACROSCOPIC LEVEL

That the case with $v=0$ is simpler and helps in preparing tools, hereafter used for more general situations, is not a surprise.

A. With $v=0$

The method pioneered in [2,3,12] consists in transforming the generalized master equation into compact form in Fourier-Laplace variables, in order to see the Fourier-Laplace transform of the time derivative of $P(x,t)$, and also a Fourier convolution involving P. Since here P is defined on a half space, we need some appropriate extension in order to obtain Fourier convolutions. We focus on initial conditions in the form of a Dirac distribution located at x_0 (with $x_0>0$), from which we can deduce all the other (initial) possibilities. Particles that are at x at instant t either came from elsewhere, or stayed there right from the start. Since the probability of performing no jump before t is $1-\int_0^t\psi_{\tau_0}(t')dt'$, the probability $P(x,t)$ of finding a particle in $x>0$ at instant t satisfies the following generalized master equation [2,3,12]:

$$P(x,t)=\delta_{x_0}(x)\left(1-\int_0^t\psi_{\tau_0}(t')dt'\right)+\int_{x'=0}^{+\infty}\int_{t'=0}^{t}P(x',t')[\varphi_l(x-x')+\varphi_l(-x-x')]\psi_{\tau_0}(t-t')dt'dx'.$$

Since φ_l is even, the integral with respect to x' is a convolution if we consider the even (with respect to x) extension P^* of P, defined by $P^*(x,t)=P(x,t)$ for $x>0$ and $P^*(x,t)=P(-x,t)$ for $x<0$. With this notation, the generalized master equation is equivalent to

$$P^*(x,t)=\int_R\int_{t'=0}^{t}P^*(x',t')\varphi_l(x-x')\psi_{\tau_0}(t-t')dt'dx'+[\delta_{x_0}(x)+\delta_{-x_0}(x)]\int_t^{+\infty}\psi_{\tau_0}(t')dt'$$

for x in R. Then, following [12] the Fourier-Laplace transform $\hat{\tilde{P}}^*$ satisfies

$$\hat{\tilde{P}}^*(k,u)=\hat{\tilde{P}}^*(k,u)\hat{\varphi}_l(k)\tilde{\psi}_{\tau_0}(u)+\frac{1-\hat{\varphi}_l(0)\tilde{\psi}_{\tau_0}(u)}{u}(e^{ikx_0}+e^{-ikx_0});$$

hence $u\hat{\tilde{P}}^*-2\cos kx_0=(e^{-|lk|^\alpha}-1)\tau_0^{-1}\hat{\tilde{P}}^*(k,u)$. For fixed k and u, when l and τ_0 tend to zero while $l^\alpha/\tau_0=K$ [9,10], we obtain that $\hat{\tilde{P}}^*(k,u)$ tends to a limit which satisfies

$$u\hat{\tilde{P}}^*(k,u)-2\cos kx_0=-K|k|^\alpha\hat{\tilde{P}}^*(k,u) \tag{9}$$

for $\alpha\in(0,2]$. Since $P^*/2$ can be thought of as being a PDF, in physical space P^* satisfies Eq. (8), with $v=0$.

For $\alpha=2$, Eq. (9) yields the classical diffusion equation $\partial_tP(x,t)=K\nabla^2P(x,t)$. However, for $\alpha\in(0,2)$, the concentration P evolves, in the diffusive limit, according to

$$\partial_tP(x,t)=K\nabla^\alpha_{x,refl}P(x,t), \tag{10}$$

with $\nabla^\alpha_{x,refl}$ being defined by

$$\nabla^\alpha_{x,refl}P(x,t)=K\frac{-1}{2\cos\alpha\pi/2\Gamma(2-\alpha)}\partial_x^2\int_{y=0}^{+\infty}[|x-y|^{1-\alpha}+(x+y)^{1-\alpha}]P(y,t)dy \tag{11}$$

for $\alpha\in(1,2)$. As in free space, a different expression holds for $\alpha\in(0,1]$.

In Eq. (10), the Riesz-Feller derivative of order $\alpha\in(1,2)$, has been replaced by the slightly different nonlocal operator $\nabla^\alpha_{x,refl}$, which takes account of the reflective boundary condition. The definitions of ∇^α_x and $\nabla^\alpha_{x,refl}$ differ in the kernels that are, respectively, proportional to $|x-y|^{1-\alpha}$ and $|x-y|^{1-\alpha}+(x+y)^{1-\alpha}$. Both kernels are not very different when $x+y$ is large. Nevertheless, omitting $(x+y)^{1-\alpha}$ would yield a nonconservative model. Indeed, solutions obtained without this term would have a decreasing integral over x, whereas the total amount of matter over the accessible domain should be constant. For solutions to Eq. (10), the integral $\int_0^{+\infty}P(x,t)dx$ is constant, since it is $\frac{1}{2}\int_{-\infty}^{+\infty}P^*(x,t)dx$, with P^* solving Eq. (8).

The method can still be adapted when the advection speed v is different from zero.

B. With $v\neq 0$

When $v\neq 0$, being at x at time t without having performed any jump between instants t' and t now means having been advected from $x-v(t-t')$ to x.

Moreover, in a semi-infinite medium limited by a reflective barrier in $x=0$, it is impossible to be in $x>0$ at time t after having a jump at t', if $x-v(t-t')$ is negative. Therefore, the generalized master equation for $x>0$ is

$$P(x,t)=\delta_{x_0+vt}(x)\int_t^{+\infty}\psi_{\tau_0}(t')dt'+\int_{x'>0}\int_{t'=0}^{t}P(x',t')H(x-v(t-t'))T_{v(t-t')}\Lambda_l(x,x')\psi_{\tau_0}(t-t')dt'dx' \tag{12}$$

with Λ_l satisfying Eq. (7). In Appendix B, Eq. (12) is shown to be equivalent to

$$P^*(x,t)=[\delta_{x_0+vt}(x)+\delta_{-x_0-vt}(x)]\int_t^{+\infty}\psi_{\tau_0}(t')dt'+\int_{t'=0}^{t}\psi_{\tau_0}(t-t')(T_{v(t-t')}(H[P^* *_F\varphi_l])+T_{-v(t-t')}\{(1-H)[P^* *_F\varphi_l]\})(x,t')dt', \tag{13}$$

which involves convolutions. We show hereafter that Eq. (13) is equivalent to a nonlocal partial differential equation for $P^*(x,t)$, which is, in the coarse-grained limit, identical to Eq. (8).

Since the Laplace transform of $\int_t^{+\infty}\psi_{\tau_0}(t')dt'$ is $u^{-1}[1-\tilde{\psi}_{\tau_0}(u)]$, we set

$$2A(k,u) \equiv \frac{1-\tilde{\psi}_{\tau_0}(u-ivk)}{u-ivk} + \frac{1-\tilde{\psi}_{\tau_0}(u+ivk)}{u+ivk} = \frac{2\tau_0(1+\tau_0 u)}{(1+\tau_0 u)^2+\tau_0^2k^2v^2}$$

and

$$2iB(k,u) \equiv \frac{1-\tilde{\psi}_{\tau_0}(u-ivk)}{u-ivk} - \frac{1-\tilde{\psi}_{\tau_0}(u+ivk)}{u+ivk} = \frac{2i\tau_0^2kv}{(1+\tau_0 u)^2+\tau_0^2k^2v^2}.$$

Then, the Laplace-Fourier transform of $[\delta_{x_0+vt}(x) + \delta_{-x_0-vt}(x)]\int_t^{+\infty}\psi_{\tau_0}(t')dt'$ is $2A\cos kx_0 - 2B\sin kx_0$. In Appendix B, the Laplace-Fourier transform of the second summand in the right-hand side of Eq. (13) is shown to be

$$\tilde{\psi}_{\tau_0}(u+ivk)\times \hat{H}*_F(\hat{\tilde{P}}^*\times\hat{\varphi}_l)(k,u) + \tilde{\psi}_{\tau_0}(u-ivk) \times(\widehat{1-H})*_F(\hat{\tilde{P}}^*\times\hat{\varphi}_l)(k,u).$$

Hence we set

$$C(k,u) \equiv \tilde{\psi}_{\tau_0}(u+ivk) - \tilde{\psi}_{\tau_0}(u-ivk) = \frac{-2ik\tau_0 v}{(1+\tau_0 u)^2+\tau_0^2k^2v^2}$$

and

$$D(k,u) \equiv 1-D'(k,u) \equiv 1-\frac{\hat{\varphi}_l(k)[\tilde{\psi}_{\tau_0}(u+ivk)+\tilde{\psi}_{\tau_0}(u-ivk)]}{2} = \frac{(1+\tau_0 u)(1+\tau_0 u-e^{-|lk|^\alpha}-\tau_0^2k^2v^2)}{(1+\tau_0 u)^2+\tau_0^2k^2v^2}.$$

Since the Fourier transform of H is $\delta/2-1/(ik)$, the Fourier-Laplace transform of the right-hand side of Eq. (13) is

$$2A\cos kx_0 - 2B\sin kx_0 + D'\hat{\tilde{P}}^*(k,u) + C\left[(\hat{\varphi}_l\hat{\tilde{P}}^*)*_F\frac{1}{ik}\right](k,u).$$

Hence, in Fourier-Laplace variables, Eq. (13) is equivalent to

$$D\hat{\tilde{P}}^*(k,u) = 2A\cos kx_0 - 2B\sin kx_0 + C\left[(\hat{\varphi}_l\hat{\tilde{P}}^*)*_F\frac{1}{ik}\right](k,u).$$

Recalling that the Fourier-Laplace transform of $\partial_t P^*$ is $u\hat{\tilde{P}}^*(k,u)-2\cos kx_0$, we see that Eq. (13) is equivalent to

$$\widehat{\partial_t P^*}(k,u) = \left(\frac{Au-D}{A}\right)\hat{\tilde{P}}^*(k,u) - \frac{2B}{A}\sin kx_0 + \frac{C}{A}\left[(\hat{\varphi}_l\hat{\tilde{P}}^*)*_F\frac{1}{ik}\right]. \quad (14)$$

With $*_L$ denoting Laplace convolution, the right-hand side of Eq. (14) is a sum of three terms. For $\alpha\in(1,2)$, and under the condition $l^\alpha/\tau_0=K$, they are, respectively, equivalent to $K\nabla_x^\alpha P^*(x,t)$ (see Appendix C), the Fourier-Laplace transforms of

$$-v\ \mathrm{sgn}(x)[\varphi_l*_F\partial_x P^*]*_L\psi_{\tau_0} - 2v[\varphi_l*_F\partial_x P^*]\delta(x)*_L\psi_{\tau_0}, \quad (15)$$

and of a vanishing small quantity (when l and τ_0 are small). In this limit, the expression in Eq. (15) tends to

$$-v\ \mathrm{sgn}(x)[\partial_x P^*(x,t)] - 2v\ \partial_x P^*(x,t)\delta(x) = -v\ \partial_x[\mathrm{sgn}(x)P^*(x,t)].$$

Hence, for every fixed value of (x,t) in $R\times R^+ - \{(0,0)\}$ the Fourier-Laplace transform of

$$\partial_t P^*(x,t) + v\ \partial_x[\mathrm{sgn}(x)P^*(x,t)] - K\nabla_x^\alpha P^*(y,t)$$

tends to zero with l and τ_0 under the condition $l^\alpha/\tau_0=K$, so that P^* satisfies Eq. (8). For $\alpha=2$, the derivative ∇_x^α is $\partial_{x^2}^2$ and we readily obtain the classical advection-diffusion equation. When α is strictly between 1 and 2, $P(x,t)$ evolves according to

$$\partial_t P(x,t) + v\ \partial_x P(x,t) = K\nabla_{x,refl}^\alpha P(x,t) \quad (16)$$

for $x>0$, with $\nabla_{x,refl}^\alpha$ being defined by Eq. (11). In the right-hand side of Eq. (16), the nonlocal operator is as in Eq. (10). The latter equation finally is only a particular case. The local advection term $v\partial_x$ is not affected by the boundary condition.

Hence, in the diffusive limit, Eq. (16) rules the evolution of the probability density of finding a particle at position x at time t performing a Lévy flight. The result also can be obtained, and illustrated numerically, by comparing solutions to Eq. (16) and direct Monte Carlo simulations.

V. NUMERICAL DISCUSSION OF EQUATION (16)

After necessary details concerning a numerical scheme allowing us to discretize Eq. (16), we compare the numerical solutions with direct Monte Carlo simulations.

A. Numerical scheme

In Sec. IV we proved that, when $P(x,t)$ solves Eq. (16) in the half space $x>0$, the even extension P^* solves Eq. (8) in the real line. Therefore, numerical schemes available for Eq. (8) can be adapted to Eq. (16).

For $\alpha\in(1,2)$, according to [14,15] an efficient discretization of the Riesz-Feller derivative $\nabla_x^\alpha P^*$, with space mesh h, is

$$(\nabla_x^\alpha P^*)_j^n = \frac{1}{2\,h^\alpha|\cos(\alpha\pi/2)|}\sum_{k=0}^{\infty}(-1)^k\binom{\alpha}{k}(P_{j-1+k}^{*n}+P_{j+1-k}^{*n}). \quad (17)$$

Here, f_n^j denotes the discretized value at point jh at instant $n\Delta t$ of function f. For $v=0$, the explicit scheme based upon Eq. (17) was shown in [14,15] to converge to solutions to Eq. (8) for time steps $\Delta t\leqslant h^\alpha|\cos\pi\alpha/2|/(K\alpha)$. For $\alpha\in(0,1]$, Eq. (17) has to be modified.

An accurate discretization for $\nabla_{x,refl}^\alpha$ is

$$(\nabla^{\alpha}_{x,refl}P)^n_j = \frac{1}{2\ h^{\alpha}|\cos(\alpha\pi/2)|}\sum_{k=0}^{\infty}(-1)^k\binom{\alpha}{k}(P^n_{|j-1+k|} + P^n_{|j+1-k|}), \quad (18)$$

with $\delta_{j,j'}$ denoting Kronecker's symbol. In order to match accuracy requirements and to avoid instabilities, the three-point scheme of order 2

$$(v\partial_x P)^n_j = \frac{v}{2h}(-3P^n_j + 4P^n_{j+1} - P^n_{j+2})$$

is a good compromise for the advection term $v\ \partial_x P$.

Using the above discretizations, we finally obtain for the space derivatives involved in Eq. (16) the following explicit scheme:

$$P^{n+1}_j = P^n_j + K\ \Delta t(\nabla^{\alpha}_{x,refl}P)^n_j + \Delta t(v\ \partial_x P)^n_j.$$

A stability analysis based on von Neumann's method indicates that the convergence condition $\Delta t < h^{\alpha}|\cos \pi\alpha/2|/(K\alpha)$ is not enough when $v \neq 0$ in a half space. It must be complemented by $h^{\alpha-1} < v\ S(\alpha)$, as in [29]. Here, for $K=1$, S is defined by $S(\alpha)=[6+3\alpha(\alpha-1)-\alpha(\alpha-1)(2-\alpha)]/30|\cos(\alpha\pi/2)|$.

The numerical tool previously described allows us to measure the importance of the correction proposed for the kernel of the Riez-Feller derivative in the presence of a reflective barrier. We compare solutions to Eq. (16) and Eq. (8) for $K=1$, $\alpha=1.5$, $v=0$, for $t=3$ [Fig. 1(a)] and for $t=10$ [Fig. 1(b)]. As observed, not taking into account the influence of the wall yields inexact values. The effect of the boundary is mainly visible between the wall and the support of the initial condition. Advection decreases the difference between solutions to Eq. (16) and Eq. (8). This is not a surprise, since when advection is present there are fewer particles near the wall as time increases.

Since the proof [14,15] that the scheme converges only holds for $v=0$, and also in order to obtain a numerical proof of Eq. (16), we carried out comparisons with Monte Carlo simulations.

B. Direct simulations of Lévy flights with a reflective wall

We proved in Sec. IV that when $l^{\alpha}/\tau_0=K$ and in the coarse-grained limit, the density $P(x,t)$ of particles performing Lévy flights satisfies Eq. (16). Hence, the normalized frequency distribution of Q particles initially at x_0 and performing Lévy flights tends to the continuous solution for large Q.

A theorem due to Zolotarev and detailed in [30,31] states that for $\alpha \in (1,2)$, the random variable $Z = (\sin\alpha\ \theta/\cos\theta^{\alpha})[\cos(\alpha-1)\theta/W]^{(1-\alpha)/\alpha}$ follows a symmetric stable Lévy law. The independent random variables θ and W are distributed, respectively, uniformly in $[-\pi/2,\pi/2]$, and exponentially with expectation 1. The trajectories of Q particles performing Lévy flights are obtained from this result, combined with facilities offered by MATHEMATICA software for uniform and exponential distributions.

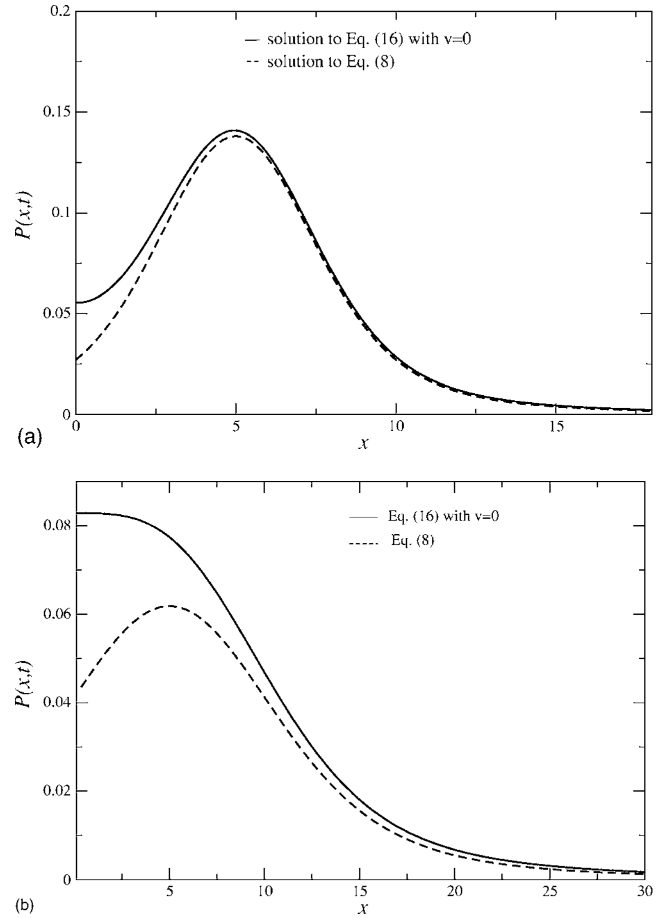

FIG. 1. Concentration profiles with (full line) and without (dashed line) a reflective barrier at $x=0$, for $v=0$, $\alpha=1.5$, and $K=1$, at times $t=3$ (a) at the left, and 10 (b) at the right. The initial condition satisfies $P(x,0)=\delta_{x_0}$ at $x_0=5$. For $x>0$, the solution to Eq. (16) is above the solution to Eq. (8) especially between the barrier and x_0. Indeed, particles jumping to the right of x_0 escape this region equally often with or without the boundary condition. In constrast, escapes due to jumps to the left are more difficult with than without the wall.

C. Comparisons in the diffusive limit

Checks against exact solutions for $v=0$, give us confidence in the choice of steps h and Δt. Figure 2 shows a comparison between the frequency distribution obtained (for $v=0$) from Monte Carlo simulations with $Q=10\,000$ and $\tau_0=0.02$ (with $l^{\alpha}=\tau_0$), and the exact solution to Eq. (16) for $K=1$ and $\alpha=1.5$. In this case, exact solutions are available for Eq. (16), and they coincide with the issues of the previously described discretization. The good fit observed illustrates that, in the diffusive limit, the concentration evolves according to Eq. (16). In the case $v \neq 0$, the comparison with numerical solutions leads to the same conclusion (see Fig. 3).

VI. CONCLUSIONS

In media where the transport of matter on the small scale is dominated by symmetric Lévy flights, the macroscopic evolution equation is a space-fractional advection-diffusion

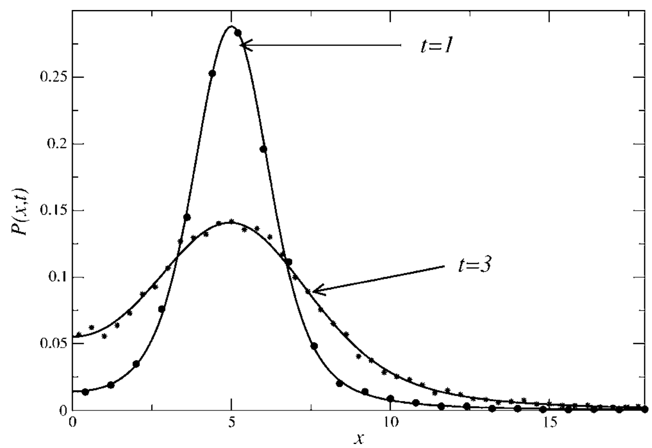

FIG. 2. The solutions to Eq. (16) (full line), compared with direct Monte Carlo simulations of $Q=10\,000$ particles performing Lévy flights (symbols) with a reflective barrier at $x=0$, for $v=0$, $\alpha=1.5$, and $K=1$. The initial condition satisfies $P(x,0)=\delta_{x_0}$ at $x_0=5$.

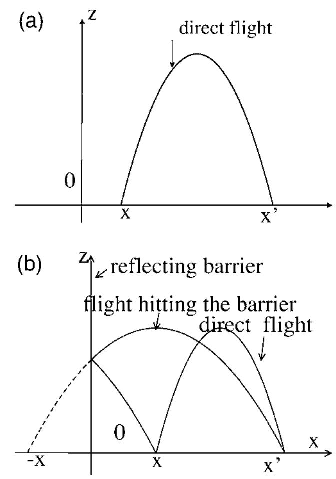

FIG. 4. Trajectories of ballistic motions in a uniform force field, with and without a reflecting barrier at $x=0$, with respect to the laboratory frame. At the left: a direct flight from x' to x. At the right: a direct flight from x' to x, and a flight hitting the reflective barrier before ending at abscissa x, without any global drift.

equation. We showed that, due to its nonlocal character, the kernel of the space-fractional derivative has to be modified when a boundary condition is imposed. The advection term is as in free space. We focused here on a reflective barrier. Small scale dynamics due to conservative forces, superimposed on randomly distributed impulsions (e.g., Appendix A), results in a modified transition probability density of the random walk "with the wall" and given by Eq. (7). The latter equation served as a small scale definition of the barrier. It was chosen by analogy with the above-mentioned dynamical illustration. Furthermore, for Lévy flights with $\alpha=2$ (Brownian motions), it corresponds to Neumann boundary condition $\partial_x P(0,t)=0$. Nevertheless, other models can be imagined for the effect of a barrier at the small scale, which may imply different kernels for the space-fractional diffusion equation.

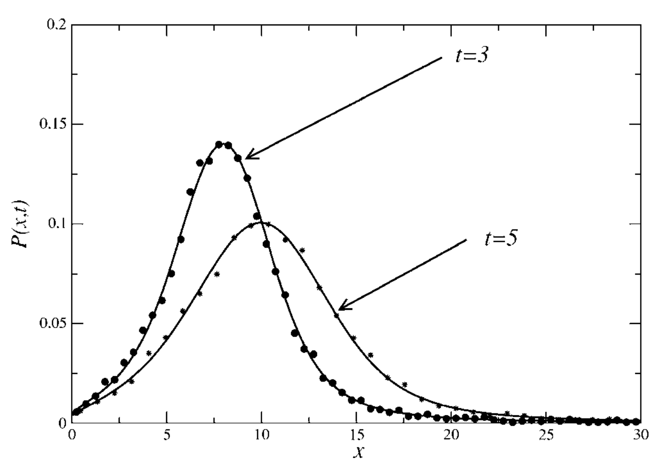

FIG. 3. The solutions to Eq. (16) (full line), compared with direct Monte Carlo simulations of $Q=10\,000$ particles performing Lévy flights (symbols) with a reflective barrier at $x=0$, for $v=1$, $\alpha=1.5$, and $K=1$. The initial condition satisfies $P(x,0)=\delta_{x_0}$ at $x_0=5$.

APPENDIX A: AN ILLUSTRATION OF THE INTERPLAY BETWEEN LÉVY FLIGHTS AND A REFLECTIVE WALL

As an example of a microscopic dynamics described by Lévy flights, imagine that in a uniform force field with direction z (orthogonal to x) and acceleration g, identical particles undergo jumps due to impulsions with uniform component V_z along z, while the x component V_x is randomly distributed. Then, in free space, the trajectories are drawn on parabolas in (x,z) coordinates. The duration of each flight is $\tau_f=2V_z/g$. We assume that τ_f is small. Far away from the wall, ballistic motions start and end with $z=0$, as on the left of Fig. 4. Assuming that the random variable V_x is distributed according to an α-stable Lévy law implies that the PDF of the jump length $L=V_x\tau_f$ is of the form $\varphi_l(L)$.

Particles hitting the reflective barrier at $x=0$ exchange no energy: elastic shocks only change the sign of the x component of the momentum, in the laboratory frame. Hence, each particle following a parabolic trajectory follows, after being bounced back by the wall, the mirror image of the portion of parabola situated on the left side of the wall.

In a medium at rest, for a particle that is at x' at instant t', the probability to jump to x during time interval $(t',t'+dt')$ and to stay there until time t has density

$$[\varphi_l(x-x')+\varphi_l(-x-x')]\psi_{\tau_0}(t-t').$$

The above description can still be applied when impulsions V_x are computed with respect to a frame moving along x with uniform speed v. In the laboratory frame, the x component of the speed is V_x+v, and flight durations still are τ_f. Particles starting from x' at instant t' may hit the wall at an intermediate instant $\tau_i<\tau_f$ such that $x'+(V_x+v)\tau_i=0$. In the latter case, $v+V_x$ is negative. Then each particle follows a parabolic trajectory symmetric to the free trajectory with respect to $x=0$, and the velocity has x component $-V_x-v$. Hence, the flight ends at time $t'+\tau_f$ at $(-v-V_x)(\tau_f-\tau_i)=-x'-(v+V_x)\tau_f$, which is symmetrical to $x'+(v+V_x)\tau_f$. A particle jumping from x' at instant t', and that hits the wall without jumping again until time t, is at $-x'-(v+V_x)\tau_f+v(t-t'-\tau_f)$ at instant t. The latter expression is equal to x if and only if $-(x+x')+v(t-t')=L+2v\tau_f$. Negative values of $x-v(t-t')$ are forbidden by the presence of the wall. Hence, in the very small τ_f limit, the transition PDF from (x',t') to (x,t) is $H(x-v(t-t'))[\varphi_l(x-x'-v(t-t'))+\varphi_l(-x-x'+v(t-t'))]+\psi_{\tau_0}(t-t')$.

APPENDIX B: FROM EQUATION (12) TO EQUATION (13)

From Eq. (7) we have $\Lambda_l(x,x')=\varphi_l(x-x')+\varphi_l(-x-x')$, with φ_l even. Setting $X=x'+v(t-t')$ yields

$$\int_{x'>0} P(x',t')T_{v(t-t')}\varphi_l(x-x')dx'$$

$$=\int_{X>v(t-t')} P(X-v(t-t'),t')\varphi_l(x-X)dX$$

$$=\int_{-\infty}^{+\infty} H(X-v(t-t'))P^*(X-v(t-t'),t')\varphi_l(x-X)dX$$

$$=\int_{-\infty}^{+\infty} T_{v(t-t')}[HP^*](X,t')\varphi_l(x-X)dX,$$

since P^* is even.

Similarly, with $X'=-x'+v(t-t')$ we have

$$\int_{x'>0} P(x',t')T_{v(t-t')}\varphi_l(-x-x')dx'$$

$$=\int_{X'<v(t-t')} P(-X'+v(t-t'),t')\varphi_l(x-X')dX'.$$

The latter expression is equal to $\int_{X'<v(t-t')}P^*(X'-v(t-t'),t')\varphi_l(x-X')dX'$, in turn equal to

$$\int_{-\infty}^{+\infty} [(1-H)P^*](X'-v(t-t'),t')\varphi_l(x-X')dX'$$

$$=\int_{-\infty}^{+\infty} T_{v(t-t')}[(1-H)P^*](X',t')\varphi_l(x-X')dX'.$$

Hence, Eq. (12) is equivalent to

$$P(x,t)=\delta_{x_0+vt}(x)\left(1-\int_0^t \psi_{\tau_0}(t')dt'\right)$$

$$+\int_{t'=0}^{t} H(x-v(t-t'))\int_{y\in R}[T_{v(t-t')}P^*$$

$$+T_{v(t-t')}(1-H)P^*](y,t')\varphi_l(x-y)\psi_{\tau_0}(t-t')dy\,dt'$$

for $x>0$. In the right-hand side of the above expression, the integral with respect to y is $[T_{v(t-t')}P^* *_F\varphi_l](x,t)$, and the double integral is equal to

$$\int_{t'=0}^{t} \psi_{\tau_0}(t-t')T_{v(t-t')}(H[P^* *_F\varphi_l])dt'.$$

Noticing that $T_{v(t-t')}[H(P^* *_F\varphi)]$ has support $[v(t-t'),+\infty[$ and that its mirror image is $T_{-v(t-t')}[(1-H)(P^* *_F\varphi_l)]$ proves that Eq. (12) is equivalent to Eq. (13).

The Fourier transforms of $T_{v(t-t')}(H[P^* *_F\varphi_l])$ and of $T_{-v(t-t')}\{(1-H)[P^* *_F\varphi_l]\}$ are, respectively, $e^{ikv(t-t')}\times[\hat{H} *_F(\hat{P}^*\hat{\varphi}_l)](k,t')$, and $e^{-ikv(t-t')}[(\widehat{1-H}) *_F(\hat{P}^*\hat{\varphi}_l)](k,t')$.

Moreover, the Laplace transform of $e^{ikt}\psi_{\tau_0}(t)$ is $\tilde{\psi}_{\tau_0}(u-ikv)$, and $\int_{t'=0}^{t}e^{ik(t-t')}\psi_{\tau_0}(t-t')[\hat{H} *_F(\hat{P}^*\hat{\varphi}_l)](k,t')dt'$ is the Laplace convolution of $e^{ikt}\psi_{\tau_0}(t)$ and $[\hat{H} *_F(\hat{P}^*\hat{\varphi}_l)](k,t')$. Hence the Laplace-Fourier transform of

$$\int_{t'=0}^{t} \psi_{\tau_0}(t-t')H(x-v(t-t'))T_{v(t-t')}(H[P^* *_F\varphi_l])dt'$$

is

$$\tilde{\psi}_{\tau_0}(u-ikv)[\hat{H} *_F(\widehat{\tilde{P}^*}\hat{\varphi}_l)](k,u).$$

Similarly, the Laplace-Fourier transform of

$$\int_{t'=0}^{t} H(x-v(t-t'))\psi_{\tau_0}(t-t')T_{-v(t-t')}(1-H)[P^* *_F\varphi_l]dt'$$

is

$$\tilde{\psi}_{\tau_0}(u+ikv)[(\widehat{1-H})(\widehat{\tilde{P}^*}\hat{\varphi}_l)](k,u).$$

APPENDIX C: LIMITING BEHAVIOR OF THE RIGHT-HAND SIDE OF (14)

The right-hand side of Eq. (14) contains three terms. The first one is $[(Au-D)/A]\hat{\tilde{P}}^*(k,u)$ with

$$\frac{Au-D}{A}=(e^{-|lk|^\alpha}-1)\tau_0^{-1}-\frac{\tau_0(kv)^2}{1+\tau_0 u}.$$

Let us first consider $(e^{-|lk|^\alpha}-1)\tau_0^{-1}$. For β in $[1,2]$, the function h_β defined by $h_\beta(X)=(e^{-X}-1+X)X^{-\beta}$ is continuous, positively valued, and bounded by, say, M_β on $[0,+\infty[$. It behaves as $X^{2-\beta}$ near 0, as $X^{1-\beta}$ in a neighborhood of $+\infty$. For $\alpha\in(1,2]$, set $\beta=1+\alpha^{-1}+\varepsilon$, with ε being positive but small. Then $\hat{w}_{\alpha,\beta}(k)\equiv h_\beta(|k|^\alpha)$ is an even continuous and bounded function of k which belongs to $L_1(R)\cap L_2(R)$. Hence it is the Fourier transform of some bounded function $w_{\alpha,\beta}$, and we have

$$e^{-|lk|^\alpha}-1=-|lk|^\alpha+|lk|^{\alpha\beta}\hat{w}_{\alpha,\beta}(lk).$$

This implies that $[(Au-D)/A]\hat{\tilde{P}}^*(k,u)-K\widehat{\nabla^\alpha\tilde{P}^*}(k,u)$ is the Fourier transform of $l^{1+\alpha\varepsilon}$ times the Fourier convolution of $-K\nabla_x^{\alpha+1+\alpha\varepsilon}P^*$ by $w_{\alpha,\beta}(x/l)$. The latter tends to zero with l. A similar result holds for $\alpha\in(0,1]$, except that then $\hat{w}_{\alpha,\beta}$ only belongs to $L_2(R)$.

Now $[\tau_0(kv)^2/(1+\tau_0 u)]\hat{\tilde{P}}^*(k,u)$ is the Fourier-Laplace transform of $v^2 e^{-t/\tau_0}\partial_x^2 P^*$, which tends to zero with τ_0. Hence the term with $\hat{\tilde{P}}^*(k,u)$ in the right-hand side of Eq. (14) is $-K|k|^\alpha \hat{\tilde{P}}^*(k,u)$, plus a vanishingly small quantity when (l,τ_0) tends to zero under the condition $l^\alpha \tau_0^{-1}=K$.

For the second term we have

$$\frac{B}{A}\sin kx_0 = \frac{\tau_0 kv}{1+\tau_0 u}\sin kx_0 = \frac{v e^{-t/\tau_0}}{2}[\partial_x(\widehat{\delta_{x_0}-\delta_{-x_0}})].$$

Hence $(B/A)\sin kx_0$ is the Fourier-Laplace transform of a vanishingly small quantity. The third summand in the right-hand side of Eq. (14) is

$$\frac{C}{A}[\hat{\varphi}_l\hat{\tilde{P}}^*]*_F\frac{1}{ik} = \frac{-2i\,k\,v e^{-|lk|^\alpha}}{1+\tau_0 u}[\hat{\varphi}_l\hat{\tilde{P}}^*]*_F\frac{1}{ik},$$

where we can see π times the Hilbert transform of $[\hat{\varphi}_l\hat{\tilde{P}}^*]$, multiplied by $-2ik$. Then we have (see [32])

$$-2ik\left([\hat{\varphi}_l\hat{\tilde{P}}^*]_F\frac{1}{ik}\right)[\hat{\varphi}_l\hat{\tilde{P}}^*] = \frac{2}{ik}*_F(-ik\widehat{\varphi_l\tilde{P}^*}) - 2(\varphi_l\tilde{P}^*)(0,u),$$

itself equal to the Fourier transform of

$$-\operatorname{sgn}(x)[(\partial_x\tilde{P}^*)*_F\varphi_l) - 2(\varphi_l\tilde{P}^*)\delta.$$

Hence $(C/A)[\hat{\varphi}_l\hat{\tilde{P}}^*]*_F 1/ik$ is the Fourier-Laplace transform of

$$-v\,\operatorname{sgn}(x)[(\partial_x P)*_F\varphi_l]*_L\psi_{\tau_0} - 2v(\varphi_l\tilde{P}^*)\delta*_L\psi_{\tau_0}.$$

When l and τ_0 tend to zero, the above expression tends to $-v\,\partial_x P(x,t)$.

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