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Integral propagator solvers for Vlasov–Fokker–Planck equations

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Abstract

We briefly discuss the use of short-time integral propagators on solving the so-called Vlasov–Fokker–Planck equation for the dynamics of a distribution function. For this equation, the diffusion tensor is singular and the usual Gaussian representation of the short-time propagator is no longer valid. However, we prove that the path-integral approach on solving the equation is, in fact, reliable by means of our generalized propagator, which is obtained through the construction of an auxiliary solvable Fokker–Planck equation. The new representation of the grid-free advancing scheme describes the inherent cross- and self-diffusion processes, in both velocity and configuration spaces, in a natural manner, although these processes are not explicitly depicted in the differential equation. We also show that some splitting methods, as well as some finite-difference schemes, could fail in describing the aforementioned diffusion processes, governed in the whole phase space only by the velocity diffusion tensor. The short-time transition probability offers a stable and robust numerical algorithm that preserves the distribution positiveness and its norm, ensuring the smoothness of the evolving solution at any time step.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Many physical systems are described by advection–diffusion equations, having the form of the so-called Vlasov–Fokker–Planck equation (VFPE) which governs the time evolution of a distribution or probability density function in a phase space. The scope and the importance of this equation in many branches of physics and mathematics are beyond any doubt [1–3]. For decades, an extensive literature dealing with solution methods for this equation

has been developed, specially in the frame of kinetic theory, to study local and nonlocal transport processes [4], which are of capital importance in cold and fusion plasmas. This kind of equations also appears with different names as, for instance, the so-called nonlinear Haïssinski equation, drawing bunch processes in electron ring storages [5]. Moreover, it is usual to find the VFPE coupled to Poisson or Maxwell equations to self-consistently describe the nonlinear dynamics of the distribution function f [6–8]. Typically, the VFPE is written as

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}} + \mathbf{a}\cdot\frac{\partial f}{\partial \mathbf{v}} = -\frac{\partial}{\partial \mathbf{v}}\cdot\left[\mathbf{D}_v - \frac{\partial}{\partial \mathbf{v}}\cdot\mathbb{D}_{vv}\right] f(\mathbf{v},\mathbf{x},t), \tag{1}$$

where $\mathbf{a}$ is the deterministic acceleration term, while $\mathbf{D_v}$ and $\mathbb{D}_{vv}$ are the drift vector and the diffusion tensor respectively, arising from the effects of collective interactions. These coefficients may also be functions of all the variables involved in the derivatives. Spatial inhomogeneities are accounted for by the Vlasov term $\mathbf{v}\cdot\partial/\partial\mathbf{x}$. This equation is nothing but a special case of a generalized Fokker–Planck equation (FPE), which may have a non-homogeneous source term ρ, in the $(N+N)$-dimensional space, given by

$$\frac{\partial f}{\partial t} = \mathbf{L}_{\mathrm{FP}}(\mathbf{q},t)f(\mathbf{q},t) + \rho(\mathbf{q},t) = -\frac{\partial}{\partial \mathbf{q}}\cdot\left[\mathcal{A}(\mathbf{q},t) - \frac{\partial}{\partial \mathbf{q}}\cdot\mathbb{D}(\mathbf{q},t)\right] f + \rho(\mathbf{q},t). \tag{2}$$

Here $\mathbf{q}\in\mathbb{R}^{\mathbf{N}}\times\mathbb{R}^{\mathbf{N}}$ which coincides with the six components vector $(\mathbf{v},\mathbf{x})$ for a point in the $2N$-fold phase space $(\mathbf{v},\mathbf{x})$. The drift vector $\mathcal{A}$ and the symmetric diffusion tensor $\mathbb{D}$ components, as well as ρ, may also depend on f through a nonlinear integro-differential relation [5]. Thus, (1) can be cast into (2) by taking the components $\mathbb{D}_{\mathbf{xv}}$ and $\mathbb{D}_{\mathbf{xx}}$ of the symmetrical diffusion tensor as zero, being $\mathcal{A} = (\mathcal{A}_v,\mathcal{A}_x) = (\mathbf{a}+\mathbf{D}_v,\mathbf{v})$. Among a great variety of solution methods [7, 9], for the last two decades, those semi-analytical approaches aided by numerical computation have roused great interest. In this group, the path-sum, path-integral or propagator methods describe the evolution of a distribution function by means of an approximate propagator or Green's function (see, for instance, [10–13] and references therein). An interesting discussion about the physical sense of this path-integral approach and its relation to continuous Markovian processes can also be found in the early works [14, 15]. This propagator is usually obtained by analytical methods under the restrictive condition of being valid for a very short-time range of the evolution. In this sense, this method strictly combines computational and analytical efforts due to the fact that many almost useless theoretical approximated solutions could not be directly applied without numerical calculations. On the other hand, this integral method provides a comprehensible and suitable approach to solve a VFPE because of its probabilistic interpretation. This makes the method truly meaningful, robust and stable under a computational point of view. More precisely, this approach is based upon the fact that (2) could be solved through the integral evolution equation

$$f(\mathbf{q},t) = \int f(\mathbf{q}',t')\Pi(\mathbf{q},t\mid\mathbf{q}',t')\,\mathrm{d}\mathbf{q}' + \int \mathrm{d}\mathbf{q}'\int_{t'}^{t}\mathrm{d}T\,\rho(\mathbf{q}',T)\Pi(\mathbf{q},t|\mathbf{q}',T), \tag{3}$$

if a propagator $\Pi(\mathbf{q},t\mid\mathbf{q}',t')$ were known [11]. In this integral form of (2), Π plays the role of a Green's function, under a purely analytical point of view, but it may have a probabilistic meaning, since it could be understood as a conditional transition probability from point $\mathbf{q}'$ at time t' to point $\mathbf{q}$ at time $t > t'$ [16]. Obviously, an exact propagator Π cannot be found if the equation for f is not solvable. In these cases, only approximate non-unique propagators $P_\tau \approx \Pi$ can be obtained for small values of $\tau = t - t'$. A well-known short-time propagator $P_\tau = P_\tau(\mathbf{q},\mathbf{q}'|t)$ as a transition probability from time $t' = t$ to time $t+\tau$ is the multi-variate Gaussian distribution [1], which in N-dimensional space reads

$$\Pi(\mathbf{q},t+\tau;\mathbf{q}',t) \approx P_\tau = \mathrm{e}^{-\mathbf{Q}\cdot\mathbb{D}^{-1}\cdot\mathbf{Q}/4\tau}/\|4\pi\tau\mathbb{D}'\|^{1/2}, \qquad \mathbf{Q} = \mathbf{q}-\mathbf{q}'-\tau\mathcal{A}', \tag{4}$$

where the primed functions are computed in the source (or pre-point) variables $\mathbf{q}'$, instead of being evaluated at the field (or post-point) ones $\mathbf{q}$. By $\|\cdot\|$ we denote in this paper the determinant of a matrix. Observe that (4) demands the diffusion tensor to be invertible ($\|\mathbb{D}\| \neq 0$) which fails for the Vlasov–Fokker–Planck equation (1), since the diffusion tensor has no **xx** and **xv** components that would explicitly describe xx self-spreading in configuration or position space and xv cross-diffusion processes. However, the possibility of applying the integral solution method (3) to a VPFE cannot be rejected; in fact, we shall show in this paper that an alternative propagator can be determined by constructing an auxiliary solvable VFPE following the method given in [17]. This procedure establishes a suitable representation of the Dirac's delta function, as the transition probability for $\tau = 0$, in terms of an orthogonal functional basis, that also leads to a representation of P_τ for a finite and small time step τ.

We will show here that such a short-time propagator exists but it has to contain powers of τ higher than 1 to properly describe xv cross-diffusion and xx self-diffusion processes, although neither of them is explicitly displayed in the differential form of the VFPE.

2. A simple propagator for the VFPE

As a first approach to our discussion, let us consider (1) for the $(1+1)$-dimensional case. This is a Klein–Kramers equation [1] describing the evolution of a probability density function $f(v, x, t)$ for a common Brownian motion

$$\frac{\partial f}{\partial t} = -v\frac{\partial f}{\partial x} - \frac{\partial}{\partial v}\left[A - \frac{\partial}{\partial v}D_{vv}\right] f = \mathbf{L}f, \qquad A(v, x) = D_v + a(x) \tag{5}$$

where $D_v = -\nu v$, the acceleration $a(x)$ comes from a force field, while ν and $D_{vv} = D$ are two given constants. As is well known, this equation describes the evolution of the probability density f of a system whose microdynamics is governed by a second-order Markovian process through the Langevin equations

$$\frac{\mathrm{d}}{\mathrm{d}t}(x, v) = (v, -\nu v + a(x) + \Gamma(t)) = (v, A(v, x) + \Gamma(t)) \tag{6}$$

for the stochastic variables $(x(t), v(t))$. As usual [1, 18, 19], the zero-mean delta-correlated white Gaussian noise Γ has intensity $D = D_{vv}$. The term $A = a(x) - \nu v$ plays the role of the effective deterministic acceleration.

Focusing now our attention on the transition probability density Π, also satisfying (5) for $\tau = t - t' > 0$, we observe that, for small values of τ, the first-order moments $\overline{x}$ and $\overline{v}$, with respect to the transition probability Π, are

$$\overline{v} = v' + A(v', x')\tau \qquad \text{and} \qquad \overline{x} = x' + v'\tau + \tfrac{1}{2}A(v', x')\tau^2, \tag{7}$$

as it can be directly derived from the previous Langevin equations, being also valid for any D_v and D. We have used $\overline{h} = h'$ for $\tau = 0$ provided that $\overline{h} = \int h\Pi\,\mathrm{d}x\,\mathrm{d}v$ with $\int \Pi\,\mathrm{d}x\,\mathrm{d}v = 1$. The second-order moments $\overline{x^2}$, $\overline{xv}$ and $\overline{v^2}$ can also be computed as functions of powers in τ, giving the non-vanishing elements σ_{ij}^2 of the covariance matrix $(\boldsymbol{\sigma}^2)$:

$$\sigma_{vv}^2 = 2D\tau \qquad \sigma_{xv}^2 = D\tau^2 \qquad \text{and} \qquad \sigma_{xx}^2 = \tfrac{2}{3}D\tau^3. \tag{8}$$

Observe that the noise term D takes part in all diffusion processes in the whole phase space. For a non-constant diffusion coefficient D should be replaced by $D' = D_{vv}(v', x', t)$. A simple analysis of these relations shows that an effective spreading in configuration space takes place as governed by a diffusion coefficient proportional to τ^2. The xv cross-diffusion processes appear as depending on τ; meanwhile drift effects are governed by the net acceleration A

computed at time t. These properties strongly suggest the possibility of extending the short-time transition probability (4)–(5) by an appropriate definition of an effective diffusion tensor, involving components depending on τ^2 and τ^3. Note that the drift processes, related to (7), also involve second-order powers in τ.

Therefore, the short-time transition probability density associated with (5) would have the Gaussian form of (4) with the formal diffusion coefficients D_{xv} and D_{xx} replaced by $\sigma_{xv}^2/2\tau$ and $\sigma_{xx}^2/2\tau$ with appropriate mean values. This fact can be easily tested by solving (5) for the exact propagator Π for $t > t'$ with constants A and D. The same results hold for non-constant coefficients if one deals with an approximate short-time propagator P_τ derived by constructing an auxiliary VFPE, as proposed in [17]. In essence, such an auxiliary problem is obtained by means of the Dirac delta-operator property $g(\mathbf{q})\delta(\mathbf{q}-\mathbf{q}') = g_1(\mathbf{q}')g_2(\mathbf{q})\delta(\mathbf{q}-\mathbf{q}')$, with $\delta(\mathbf{q}-\mathbf{q}') = \delta(\mathbf{v}-\mathbf{v}')\delta(\mathbf{x}-\mathbf{x}')$. The decomposition $g = g_1 g_2$ has to be applied to $g = \mathcal{A}_i$ ($g = D_{ij}$) after a simple inspection that allows us to formally replace $\mathbf{L}\delta$ by $\mathbf{L}^*\delta$. This procedure will give rise to a solvable VFPE in the form $\partial P_\tau/\partial\tau = \mathbf{L}^* P_\tau$. The most elementary operator $\mathbf{L}^*$ is similar to $\mathbf{L}$ in (5) after having taken A and D as constant functions ($g_2 = 1$ for both coefficients) since they are computed in the source variables at time t. The auxiliary equation can be solved by Fourier transforming of P_τ as $\tilde{P}(\omega, k; \tau) = \iint \exp(-\mathrm{i}\omega v - \mathrm{i}kx) P_\tau \mathrm{d}v\mathrm{d}x$ with natural boundary conditions for f in unbounded space. Dealing now t and all primed variables as constant parameters, the elementary Cauchy problem

$$\frac{\partial \tilde{P}}{\partial \tau} = \left[k\frac{\partial}{\partial \omega} - \mathrm{i}\omega A' - \omega^2 D' \right] \tilde{P}; \qquad \tilde{P}(\tau = 0) = \mathrm{e}^{-\mathrm{i}\omega v' - \mathrm{i}kx'} \tag{9}$$

is solvable by the method of characteristics, giving

$$\tilde{P} = \exp\left[-\frac{\tau D'}{3}(k^2\tau^2 + 3\omega k\tau + 3\omega^2) - \mathrm{i}\omega(v' + A'\tau) - \mathrm{i}k\left(x' + v'\tau + \frac{1}{2}A'\tau^2 \right) \right] \tag{10}$$

and finally, after Fourier inversion, we have

$$P_\tau = \frac{\sqrt{3}}{2\pi\tau^2 D'} \exp\left[-\frac{1}{D'\tau}\left(3\frac{X^2}{\tau^2} - 3\frac{XV}{\tau} + V^2 \right) \right]. \tag{11}$$

This simple expression for P_τ can be recast as a product of two one-dimensional probability transition functions as

$$P_\tau = \frac{\mathrm{e}^{-\frac{1}{D\tau}(V - \frac{3}{2\tau}X)^2}}{\sqrt{\pi D\tau}} \frac{\mathrm{e}^{-\frac{3}{4D\tau^3}X^2}}{\sqrt{4\pi D\tau^3/3}} = \frac{\mathrm{e}^{-\frac{1}{4D\tau}V^2}}{\sqrt{4\pi D\tau}} \frac{\mathrm{e}^{-\frac{3}{D\tau^3}(X - \tau V/2)^2}}{\sqrt{\pi D\tau^3/3}}. \tag{12}$$

Here, we have defined $V = v - \overline{v}$ and $X = x - \overline{x}$, in view of (7) and (10). This solution clearly illustrates the above discussion about xv cross-diffusion and xx self-diffusion as two processes intrinsically governed by the velocity diffusion tensor. At the same time, we recall that the drift in phase space is described by $\overline{v}$ and $\overline{x}$ for small τ. These two terms have a clear unambiguous physical meaning because both of them are intrinsically related to the phase-space deterministic trajectories in the short-time regime. The advection and diffusion processes in configuration space are clearly described by the reduced distribution $P_\tau(x, x')$,

$$P_\tau(x, x') = \sqrt{\frac{3}{4\pi D'\tau^3}} \exp\left[-\frac{3}{4D'\tau^3}\left(x - x' - v'\tau - \frac{1}{2}A'\tau^2 \right)^2 \right], \tag{13}$$

found after integrating P_τ over v. This marginal probability transition has the form of the usual Gaussian distribution with an effective diffusion coefficient $D_{xx} = D'_{vv}\tau^2/3$. However, because of the non-unique nature of P_τ [1, 15] one can explore the possibility of finding another propagator for which xx self-diffusion in the reduced x space does not appear explicitly.

In truth, if $v\partial/\partial x\delta(v-v')$ in $\mathbf{L}^*\delta$ is rewritten as $v'\partial/\partial x\delta(v-v')$, an alternative propagator is obtained as

$$P_\tau^{II} = \frac{1}{\sqrt{4\pi D'\tau}} \exp\left[-\frac{V^2}{4D'\tau}\right]\delta(x-x'-v'\tau). \tag{14}$$

This new Green's function can be understood as a degenerated Guassian distribution coming from (11) after computing the limit $\tau^3 \to 0$ keeping τ finite. With (14) the integral advancing scheme can be seen as a splitting procedure. Here, the integral over x' can be performed analytically yielding to a simple drift in x space. This splitting operator depending on a Dirac delta function is not unique but, in any case, the apparent suppression of the diffusive effects in real space may cause the numerical advancing scheme to destroy the distribution smoothness.

The previous results can be extrapolated to the general case of a Vlasov–Fokker–Planck equation in $(N+N)$-dimensional phase space. Although $N \leqslant 3$ in most cases, of physical interest, it is useful to give a suitable expression for P_τ in this $2N$-fold space that could be simplified if geometrical or physical properties can be invoked to reduce the dimensionality of the general problem. In such a case, f becomes homogenous with respect to one or several variables and the form of P_τ is simplified by integrating over the set of variables not appearing in f. In this sense, we stress that for space homogenous problems $\mathbf{v}\cdot\partial f/\partial\mathbf{x}$ disappears and the aforementioned integration can be carried out over $\mathbf{x}$ in P_τ, to get a propagator depending on velocity variables.

Hence, let us now consider the $(N+N)$-fold case of (1) for $\mathbf{v}\in\mathbb{R}^N$ and $\mathbf{x}\in\mathbb{R}^N$ rewritten as

$$\frac{\partial f}{\partial t} = -\left[\frac{\partial}{\partial\mathbf{x}}\cdot\mathbf{v} + \frac{\partial}{\partial\mathbf{v}}\cdot(\mathbf{D}_v+\mathbf{a}) - \frac{\partial}{\partial\mathbf{v}}\cdot\mathbb{D}_{vv}\right] f = \mathbf{L}f(\mathbf{v},\mathbf{x},t), \tag{15}$$

where we have assumed that the acceleration $\mathbf{a} = \mathbf{a}(\mathbf{x},\mathbf{v},\mathbf{t})$ satisfies $\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{a} = 0$. In the notation of (2) $\mathbf{q} = (\mathbf{v},\mathbf{x})$ is, more explicitly, the vector $(q_1,\ldots,q_N,q_{N+1},\ldots,q_{2N}) = (v_1,\ldots,v_N,x_1,\ldots,x_N)$, with $\mathcal{A}_{v_i} = A_i = D_{v_i} + a_i$, $\mathcal{A}_{x_i} = v_i$ and $\mathbb{D}_{x_iv_j} = \mathbb{D}_{x_ix_j} = 0$. We can now define

$$\mathbf{L}^* = -\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}} - \frac{\partial}{\partial\mathbf{v}}\cdot\left[\mathbf{A}' - \frac{\partial}{\partial\mathbf{v}}\cdot\mathbb{D}'\right] \tag{16}$$

as the simplest auxiliary operator $\mathbf{L}^*$ to obtain a short-time propagator similar to (11). Note that the vector $\mathbf{A}'$ coincides with $\mathbf{D}_v+\mathbf{a}$ computed on primed variables. The elements of the $N\times N$ tensor $\mathbb{D}'$, with $\mathbb{D}_{ij} = D_{vivj}$, are also evaluated in the source variables. After Fourier transforming the equation $\partial P_\tau/\partial\tau = \mathbf{L}^*P_\tau$, we find for P_τ the non-degenerated Gaussian distribution

$$P_\tau(\mathbf{v},\ \mathbf{x};\ \mathbf{v}',\ \mathbf{x}'|t) = \frac{1}{(2\pi)^N\sqrt{\|(\boldsymbol{\sigma}^2)\|}} \exp\left[-\frac{1}{2}(\mathbf{q}-\overline{\mathbf{q}})\cdot(\boldsymbol{\sigma}^2)^{-1}\cdot(\mathbf{q}-\overline{\mathbf{q}})\right] \tag{17}$$

where the mean $\overline{\mathbf{q}}$ is

$$(\overline{\mathbf{v}},\overline{\mathbf{x}}) = (\mathbf{v}'+\mathbf{A}'\tau, \mathbf{x}'+\mathbf{v}'\tau+\tfrac{1}{2}\mathbf{A}'\tau^2) \tag{18}$$

and the $2N\times 2N$ non-singular covariance tensor has the 2×2 block matrix structure

$$(\boldsymbol{\sigma}^2) = \begin{pmatrix}(\boldsymbol{\sigma}^2)_{\mathbf{vv}} & (\boldsymbol{\sigma}^2)_{\mathbf{vx}}\\ (\boldsymbol{\sigma}^2)_{\mathbf{xv}} & (\boldsymbol{\sigma}^2)_{\mathbf{xx}}\end{pmatrix} = \begin{pmatrix}2\tau\mathbb{D}' & \tau^2\mathbb{D}'\\ \tau^2\mathbb{D}' & \frac{2}{3}\tau^3\mathbb{D}'\end{pmatrix} \tag{19}$$

with determinant $\|(\boldsymbol{\sigma}^2)\| = \tau^{4N}D_t^2/3^N$, where $D_t = \|\mathbb{D}'\|$. As expected, P_τ clearly expresses how cross- and self-diffusion processes are driven by the velocity diffusion coefficients, whereas drifting obeys a simple deterministic motion of a particle in phase space for a finite

time interval τ. The approximate probability transition can be decomposed as the product of two distributions $P_{\mathbf{v}}$ and $P_{\mathbf{x}}$, each one acting in a N-dimensional space, as

$$P_\tau = P_{\mathbf{v}}(\mathbf{v}, \mathbf{v}'|\mathbf{x}')P_{\mathbf{x}}(\mathbf{x}, \mathbf{x}'|\mathbf{v}_m), \tag{20}$$

where we have defined $\mathbf{v}_m = (\mathbf{v} + \mathbf{v}')/2$ and

$$P_{\mathbf{v}} = \sqrt{\frac{1}{(4\pi\tau)^N D_t}} \exp\left[-\frac{\mathbf{V}\cdot\mathbb{D}'^{-1}\cdot\mathbf{V}}{4\tau}\right], \qquad P_{\mathbf{x}} = \sqrt{\left(\frac{3}{\pi\tau^3}\right)^N \frac{1}{D_t}} \exp\left[-3\frac{\mathbf{Z}\cdot\mathbb{D}'^{-1}\cdot\mathbf{Z}}{\tau^3}\right] \tag{21}$$

with $\mathbf{V} = \mathbf{v} - \mathbf{v}' - \mathbf{A}'\tau$ and $\mathbf{Z} = \mathbf{x} - \mathbf{x}' - \mathbf{v}_m\tau$.

It must be underlined that $P_{\mathbf{v}}$ depends on $\mathbf{x}'$ through $\mathbf{A}'$. If this short-time propagator, only working on the reduced velocity space, can be obtained for the Fokker–Planck equation without the Vlasov term, the full P_τ can be generated by a simple product expressed above, where the part $P_{\mathbf{x}}$ is constructed with the effective diffusion tensor $\tau^2\mathbb{D}'/12$ as a first approximation. Moreover, $P_{\mathbf{x}}$ contains the drag effects in the configuration x space through the deterministic part $\mathbf{x} - \bar{\mathbf{x}}$ in the Z variables. This also suggests that the method in constructing this part of the integral operator can be combined with Montecarlo or deterministic methods [6, 7] by simply replacing $x'_k + v_{Mk}\tau$ and $v'_k + A'_k\tau$ by the deterministic solution of the classical motion equations in terms of τ instead of t. It has to be emphasized that the form of the auxiliary operator $\mathbf{L}^*$ and, consequently P_τ, is not unique. This allows us to choose another one, leading to a more suitable integral operator consistent with the properties of the real VFPE operator.

On the other hand, the treatment of prescribed boundary conditions can be performed as proposed in [11]. In this work, the boundary conditions are incorporated in a surface integral involving only P_τ for unbounded space and its derivatives. To end with this section let us note that the procedure to get a meaningful P_τ is also applicable to any Fokker–Planck equation having a singular diffusion tensor, by an appropriate construction of $\mathbf{L}^*$ leading to a solvable auxiliary VFPE.

3. Application to a Brownian motion

As a simple application to solve a VFPE let us consider the study of the probability density evolution associated with a well-known Brownian motion equation for an ensemble of interacting particles, as in a collisional plasma, in the presence of a harmonic force field. The equation has the form of (5) for $f(v, x, t)$. The external deterministic acceleration is $a(x) = -\omega^2 x$ and the friction force coming from the collective interaction is $D_v = -\nu v$. In this case, the problem is analytically solvable for both transient and steady states [3, 8] having the stationary solution

$$f_s(v, x) = \mathcal{N}\exp\left[-\frac{\nu}{2D}(v^2 + \omega^2 x^2)\right], \qquad (v, x) \in \mathbb{R}\times\mathbb{R}, \tag{22}$$

where $\mathcal{N}$ is a normalization constant. We examine the evolution of f by numerically computing the grid-free path-integral scheme (3) using and comparing both split propagators (14) and (12). From the theoretical point of view, these propagators should be equivalent to finding an analytical expression, from which f could be extracted by evaluating the limits $n \to \infty$ and $\tau \to 0$ for a fixed $t = n\tau$. However, our purpose is to describe f at any time step when P_τ is used replacing the unknown exact propagator Π. Therefore, it is presumable that such an equivalence among all short-time Green's functions does not hold in describing numerical solutions. By a simple integration with a short-time propagator, f can be advanced in time from any initial condition, here a histogram-type distribution, preserving the norm and the

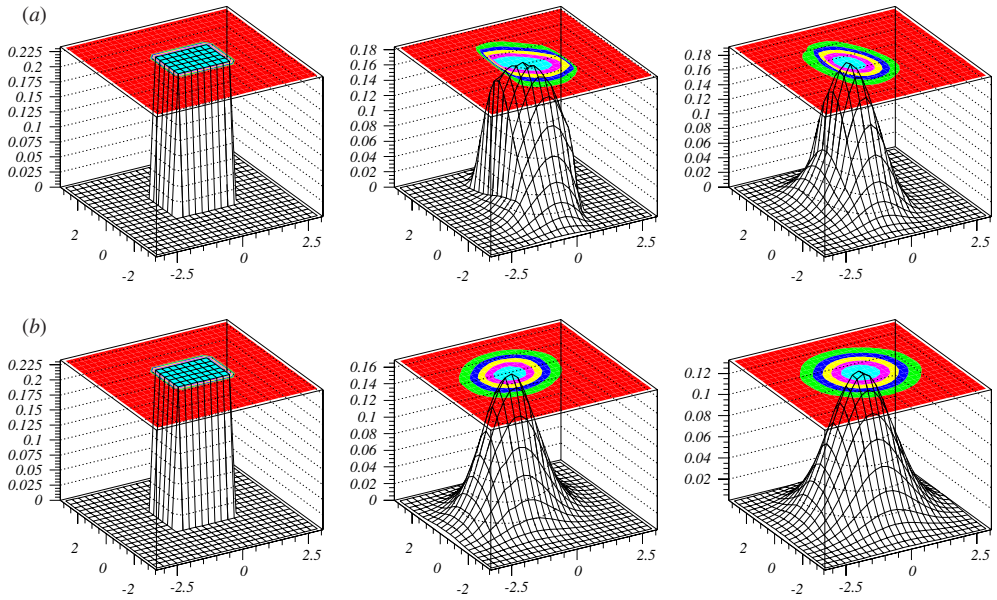

Figure 1. Contour levels and distribution function f profiles for a Brownian motion. (*A*) the convective propagator without explicit xv and xx diffusive terms is used. Here, a misleading non-smooth steady-state distribution is obtained. (*B*) The same problem is solved when f is advanced in time with the full short-time propagator (12). In this case, the expected numerical Gaussian distribution is obtained for any initial condition $f(v, x, 0)$.

non-negative nature of f. First, apply the split operator (14) that has no explicit description of both cross- and self-diffusion processes. This short-time probability transition function gives the advancing scheme

$$f(v, x, t + \tau) = \int P_v(v, v'|x - v'\tau) f(v', x - v'\tau, t)\, \mathrm{d}v', \tag{23}$$

which can be understood as a simple explicit finite-difference scheme with respect to x, related to $v\partial f/\partial x$, because its action is a drifting of the information contained in $f(v, x, t)$ by translation from the cell $x = x_i$ to a new cell x_j associated with $x - v'\tau$. A similar integral operator, which only attends to the drift processes in real configuration space, can be found in [20] for convection-dominated transport. The reduction of the propagator techniques to a finite-difference method for small time steps is briefly commented in [12]. Hence, all the values of f in every position $x - v'\tau$ should be computed before performing the integration over v' with P_v. However, for $\tau v'$ larger than the grid length Δx, the loss of information is unavoidable in a finite computational domain, because f could not be defined for certain positions. This fact enforces us to take a very small time step to prevent this loss of information throughout the iterative process. Any way, this method only describes advective effects in x, driving the solution to nonphysical behaviour, as shown in the figure. Surprisingly, the transient and steady-state solutions strongly depend on the initial distribution $f(v, x, 0)$. Since the main advantage of the path-sum solution is the possibility of taking large time steps, it is indispensable to use the full expression (11) or its split form (12). When this operator is used, the smoothness of f is preserved from the first iteration for any τ. A physically acceptable evolution is found. Now, the convective and diffusive processes are properly described until

the expected steady state is reached, as shown in the last three frames in the figure. In all the cases, the time step is about $1/10$ of the relaxation time $1/\nu$. The integrals are performed by a simple midpoint rule over a uniform 40×80 grid in a $(-5, 5) \times (-5, 5)$ finite domain. The computation takes about 5 s in a 2.8 GHz PC.

As a conclusion, we can assert that the application of (14) leads to misleading results in the description of f, because cross-diffusion and self-diffusion in xv and xx spaces are explicitly dropped as a consequence of having neglected τ^3 which is also finite in a numerical integration scheme. In contrast, when the Gaussian short-time transition probability (12) is used, there is no appreciable difference with the analytical results. Although both approaches deal with split operators, the splitting method has to contain all diffusion processes in each operator to avoid the loss of information to preserve a physically meaningful evolution of f. In this sense, any splitting method on solving the Vlasov–Fokker–Planck equation, based on advancing in time the diffusive part in velocity space and drifting the resulting function in configuration space, could cause an improper description of transient and steady states.

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