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Short-time propagators for nonlinear Fokker–Planck equations

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Abstract. Path-integral solutions to time-evolution equations in statistical physics have recently aroused great interest. The main problem in applying these methods is to find a valid propagator in the short-time regime of evolution. A new method is proposed to obtain a set of accurate short-time propagators by the construction of a simple auxiliary Fokker–Planck equation. This equation takes into account the full relevant functional dependence of the original drift and diffusion terms. By using a suitable decomposition of the drift and diffusion coefficients it is possible to derive a new representation of the Dirac δ-function. From this representation the short-time behaviour of the solutions is given not only for the infinitesimal time interval, but also for a discrete finite one which has a more practical numerical sense. This picture leads to accurate short-time propagators which include the prescribed boundary conditions.

1. Introduction

One of the mathematical models for nonlinear dynamical systems is provided by the Fokker–Planck equation [1] which arises in many branches of physics. This equation has been the main tool in dealing with problems in kinetic theory in gases [2,3], lasers, diffusion, deposition and nucleation processes under Markovian approximations [4,5]. However, the problem of finding analytical solutions far from the equilibrium remains unsolved in most physical systems of interest. Numerical methods have attracted great attention and a large number of techniques have been developed [6–10]. Computational approaches do not always take into account the essential requirements of time-dependent solutions such as conservation laws and entropy increase, as well as a suitable representation of some specific boundary conditions [11–13]. Thus, to find proper numerical treatments for solving Fokker–Planck equations an alternative method based on Green's function P has been developed. In this way, the time-evolution picture of density $f(\boldsymbol{q}, t)$ reads in a N-dimensional space with definition domain $\mathcal{D}$

$$f(\boldsymbol{q}, t+\tau) = \int_{\mathcal{D}} P(\boldsymbol{q}, t+\tau|\boldsymbol{q}', t) f(\boldsymbol{q}', t) \mathrm{d}^N q'. \tag{1.1}$$

This procedure, also called the path-integral method, assumes the system to be described with path sums for small time steps [14–25] using an approximate Green function [26] or a short-time propagator $P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t)$ whose functional dependence only needs to be known for a small evolution time τ with initial Dirac δ condition for $\tau = 0$.

The short-time propagator is usually reduced to a simple Gaussian probability density [27–29] providing the conditional probability of finding a particle in position $\boldsymbol{q}$ in time $t + \tau$

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starting in position $\boldsymbol{q}'$ in time t. Nevertheless, this Gaussian short-time propagator fails in describing the higher moments of the distribution function $f(\boldsymbol{q}, t)$ and in accounting for non-natural boundary conditions, even for linear processes. Therefore, the aim of this paper is to provide a general method to obtain short-time propagators for a given Fokker–Planck equation. The construction of an auxiliary solvable Fokker–Planck equation in the short-time regime gives a suitable representation of the Dirac δ-function fitted to the original problem. Because of the non-unique form of such a short-time propagator, it is possible to find a function $P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t)$ which approximates the unknown exact $P(\boldsymbol{q}, t+\tau|\boldsymbol{q}, t)$ in the short-time regime by an accurate functional dependence in $\boldsymbol{q}$. Further, second-order corrections in time step τ for P_τ may be achieved by an iterative self-adjusting process to ensure the correct evolution for higher moments of the distribution f.

2. Analytical grounds

The time-evolution equation for distribution functions of any physical system takes the general form

$$\frac{\partial f}{\partial t} = \mathcal{L} f(\boldsymbol{q}, t) \tag{2.1}$$

where $\mathcal{L}$ is an integro-differential operator acting on $f(\boldsymbol{q}, t)$ defined in a N-dimensional space $\Re^N$ over the domain $\mathcal{D}$ for the set of macroscopic variables $\{q_i\}$. The relation between the initial condition $f(\boldsymbol{q}, 0)$ and the transient $f(\boldsymbol{q}, t)$ defines the existence of an integral time-evolution operator $\mathcal{U}_{t,t'}$ such that, for $t > 0$ one has

$$f(\boldsymbol{q}, t) = \mathcal{U}_{t,0} f_0(\boldsymbol{q}) \tag{2.2}$$

$\mathcal{U}_{t,t'}$ is generally an integral operator that satisfies

$$f = \mathcal{U}_{t,t'} f(\boldsymbol{q}, t') = \int_{\mathcal{D}} f(\boldsymbol{q}', t') \Pi(\boldsymbol{q}, t|\boldsymbol{q}', t') \mathrm{d}^N q'. \tag{2.3}$$

The essential properties of the integral kernel Π are determined by the following set of integral equations [30], also satisfied by the conditional probability in Markovian processes [1]:

$$\lim_{t \to t'} \mathcal{U}_{t,t'} = \mathcal{I} \qquad \lim_{t \to t'} \mathcal{U}_{\tau,t} = \mathcal{U}_{\tau,t'} \tag{2.4}$$

$$\mathcal{U}_{t,t'} = \mathcal{U}_{t,t''} \mathcal{U}_{t'',t'} \qquad t' \leqslant t'' \leqslant t \tag{2.5}$$

where $\mathcal{I}$ symbolizes the identity integral operator, i.e. the integral kernel Π is reduced to the Dirac δ-function. Thus for $t \geqslant t'' \geqslant t'$ the family of time-dependent propagators $\{\mathcal{U}_{t,t'}\}$ associated to the operator $\mathcal{L}$ fulfils the relations

$$\lim_{t \to t'} \Pi(\boldsymbol{q}, t|\boldsymbol{q}', t') = \delta(\boldsymbol{q} - \boldsymbol{q}') \tag{2.6}$$

and

$$\Pi(\boldsymbol{q}, t|\boldsymbol{q}', t') = \int_{\mathcal{D}} \Pi(\boldsymbol{q}, t|\boldsymbol{q}'', t'') \Pi(\boldsymbol{q}'', t''|\boldsymbol{q}', t') \mathrm{d}^N q''. \tag{2.7}$$

The general $\mathcal{L}$ treated in this work refers to the Fokker–Planck operator $\boldsymbol{L}_{FP}$

$$\mathcal{L} = \boldsymbol{L}_{FP}(\boldsymbol{q}, t) = -\frac{\partial}{\partial q_i}\left[A_i(\boldsymbol{q}, t) - \frac{\partial}{\partial q_j} D_{ij}(\boldsymbol{q}, t)\right] \tag{2.8}$$

where the drift and diffusion coefficients A_i and D_{ij} may depend on time t and position $\boldsymbol{q}$ even through some functional relation on the function $f(\boldsymbol{q}, t)$. For a great number of physical problems, the Fokker–Planck equation arises from the analysis of microscopic dynamical

systems and random processes driven by white or coloured noise. In such a context, the propagator Π is the conditional transition probability $P(\boldsymbol{q}, t+\tau|\boldsymbol{q}, t)$ and the integral time solution (2.7) is called the consistency or Chapman–Kolmogorov equation [1,4]. The problem of finding P is as difficult as solving the original equation. Nevertheless, the short-time behaviour of this Green function can be found from first-order time expansion in $\tau = t - t'$ of the formal solution

$$P(\boldsymbol{q}, t|\boldsymbol{q}', t') = \delta(\boldsymbol{q}-\boldsymbol{q}') + \sum_{n=1}^{\infty} \int_{t'}^{t} \mathrm{d}t_1 \ldots \times \int_{t'}^{t_{n-1}} \mathrm{d}t_n \, \boldsymbol{L}_{FP}(\boldsymbol{q}, t_1) \ldots \boldsymbol{L}_{FP}(\boldsymbol{q}, t_{n-1}) \boldsymbol{L}_{FP}(\boldsymbol{q}, t_n) \delta(\boldsymbol{q}-\boldsymbol{q}') \tag{2.9}$$

usually named *the Dyson series* [1, 31], which reduces to the simple form

$$P(\boldsymbol{q}, t|\boldsymbol{q}', t') = \mathrm{e}^{\tau \boldsymbol{L}_{FP}(q)} \delta(\boldsymbol{q}-\boldsymbol{q}') \tag{2.10}$$

for time-independent drift and diffusion coefficients. Both formal solutions yield a new approximate one given by

$$P(\boldsymbol{q}, t+\tau|\boldsymbol{q}', t) = \{1 + \tau \boldsymbol{L}_{FP} + \mathrm{O}(\tau^2)\} \delta(\boldsymbol{q}-\boldsymbol{q}'). \tag{2.11}$$

Up to second order in τ this asymptotic relation can be rewritten as

$$P(\boldsymbol{q}, t+\tau|\boldsymbol{q}', t) \simeq P_\tau = \mathrm{e}^{\tau \boldsymbol{L}_{FP}(q,t)} \delta(\boldsymbol{q}-\boldsymbol{q}') \tag{2.12}$$

because the addition of terms in τ^2 does not lead off this limit, i.e. $\lim_{\tau\to 0}[1+\alpha\tau+\mathrm{O}(\tau^2)]^{1/\tau} = \mathrm{e}^{\alpha}$. The approximate propagator $P_\tau = P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t)$ has been defined to distinguish it from the true one, P. Note that in the limit of small time ($\tau \to 0$) both P and P_τ fall into the function $\delta(\boldsymbol{q}-\boldsymbol{q}')$. Thus, to solve (2.12) in the short-time regime a suitable representation of the δ-function is needed. In unbounded N-dimensional spaces this representation is usually provided through the complex Fourier transform

$$\delta(\boldsymbol{q}-\boldsymbol{q}') = \frac{1}{(2\pi)^N} \int \exp(\mathrm{i}\boldsymbol{K}\cdot(\boldsymbol{q}-\boldsymbol{q}'))\mathrm{d}^N K. \tag{2.13}$$

The insertion of this relation in (2.12) leads to the well known short-time propagator for a Fokker–Planck equation for $\tau > 0$:

$$P_\tau = \frac{1}{||D'||^{1/2}(4\pi\tau)^{N/2}} \times \exp\left[-\frac{D'^{-1}_{ij}(q_i - q_i' - A_i'\tau)(q_j - q_j' - A_j'\tau)}{4\tau}\right] \tag{2.14}$$

$$D'_{ij} = D_{ij}(\boldsymbol{q}', t) \qquad A_i' = A_i(\boldsymbol{q}', t)$$

which firstly holds for non-singular symmetrical diffusion tensor $\{D_{ij}\}$ whose determinant $\|D\|$ does not vanish. Primes indicate that the coefficients depend on the source—prepoint—variables $\boldsymbol{q}'$ instead of the field—postpoint—variables $\boldsymbol{q}$ to compute the integration involved in (1.1). This short time propagator has been derived by direct evaluation of the coefficients in primed variables and performing all the explicit differentiations in L_{FP} over the integral kernel in (2.13). This can be made using the δ-function property

$$G(\boldsymbol{q})\delta(\boldsymbol{q}-\boldsymbol{q}') = G(\boldsymbol{q}')\delta(\boldsymbol{q}-\boldsymbol{q}') \tag{2.15}$$

which is valid bearing in mind the consequent integration. These substitutions mean that system forces extracted from those A_i and D_{ij} coefficients do not experience a great change of magnitude during the small evolution time τ. It is worth saying here that if the derivatives involved in L_{FP} over A_i and D_{ij} are performed before their action on the Fourier integral kernel, the resulting P_τ is somewhat different

$$P_\tau = \frac{\mathrm{e}^{-\tau\Omega(q,t)}}{||D||^{1/2}(4\pi\tau)^{N/2}} \times \exp\left[-\frac{D^{-1}_{ij}(q_i - q_i' - \tau Q_i)(q_j - q_j' - \tau Q_j)}{4\tau}\right] \tag{2.16}$$

where the functions $Q_k(\boldsymbol{q}, t)$ and $\Omega(\boldsymbol{q}, t)$ are

$$Q_k = A_k - 2\frac{\partial D_{km}}{\partial q_m} \qquad \Omega = \frac{\partial}{\partial q_k}\left[A_k - \frac{\partial D_{km}}{\partial q_m}\right]. \tag{2.17}$$

This essentially means that the form of P_τ is not unique. Here all the derivatives of the coefficients are explicitly included in the propagator itself, whereas (2.14) all these differentiations are included in the representation of the δ-function, as shown in [28]. Between both propagators there is a wide class of valid ones, all of them being equivalent in the limit $\tau \to 0$. For instance, see the early works [27, 28, 32–37] and the interesting reports [38, 39].

It is worth noting at this stage that the function in (2.16) is not generally normalized to unity in $\Re^N$ for a finite time step τ. Then, the basic property of number conservation is violated in a numerical treatment of integral evolution solution by means of (1.1) if a non-normalized P_τ is used. For this reason, one does not expect to preserve the correct evolution of the other higher moments in an integral numerical scheme. Furthermore, both previous propagators would not normalize for any bounded space $\mathcal{D} \subset \Re^N$. The reason for this property is easily understood by paying attention to the Fourier representation of the δ-function which is only valid in unbounded spaces. A numerically efficient approximant P_τ should behave as the exact $P(\boldsymbol{q}, t+\tau|\boldsymbol{q}', t)$ for small but finite time step τ. This implies that the essential properties of the true transition probability have to be included in the short-time approximation. These properties for P_τ are summarized in three respects:

(i) P_τ has to be normalized to unity in the defining region $\mathcal{D}$ i.e.

$$\int_{\mathcal{D}} P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t)\mathrm{d}^N q = 1. \tag{2.18}$$

(ii) In the limit $\tau \to 0$ it has to produce the exact first- and second-order moments, A_i and D_{ij}, of the Kramers–Moyal expansion, being all higher order ones identically null [1, 40, 41] i.e. $A_i(\boldsymbol{q}', t) = \lim_{\tau\to 0}\frac{1}{\tau}\int_{\mathcal{D}}(q_i - q_i')P_\tau\,\mathrm{d}^N q$, $2D_{ij}(\boldsymbol{q}', t) = \lim_{\tau\to 0}\frac{1}{\tau}\int_{\mathcal{D}}(q_i - q_i')(q_j - q_j')P_\tau\,\mathrm{d}^N q$.

(iii) It has to satisfy the initial condition

$$P_{\tau=0}(\boldsymbol{q}, \boldsymbol{q}'|t) = \delta(\boldsymbol{q} - \boldsymbol{q}'). \tag{2.19}$$

At the same time, a further important condition should be added to the above ones. The Fokker–Planck equation generally leads to smooth variation of the distribution moments in a relatively large timescale.

This property means that the exact propagator P as well as the approximant P_τ do not lead to a non-zero transition density per unit of time $W(\boldsymbol{q}|\boldsymbol{q}', t)$. Then, following [4], for all real $\epsilon > 0$ the limit

$$\lim_{\tau\to 0}\frac{P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t)}{\tau} = W(\boldsymbol{q}|\boldsymbol{q}', t) = 0 \tag{2.20}$$

has to converge uniformly in $\boldsymbol{q}$ and $\boldsymbol{q}'$ with $|\boldsymbol{q} - \boldsymbol{q}'| \geqslant \epsilon$.

3. Short-time propagators

Taking into account the previous discussions on the non-uniqueness of P_τ, the problem to obtain integral transient and stationary solutions for f consists in finding appropriate short-time propagators. These possible P_τ may be understood as local in time and globally valid in space coordinates if the essential properties in section 2 are preserved. Restricting our attention to the possibility of obtaining different representations of the δ-function, the main point is how to define and construct the one which is adequate for each problem.

We recall that the way to obtain (2.14) and (2.16) starts by rewriting the formal solution (2.11) in the form

$$P_\tau = \{1 + \tau \boldsymbol{L}_{FP} + \mathrm{O}(\tau^2)\}\delta(\boldsymbol{q} - \boldsymbol{q}') \simeq \mathrm{e}^{\tau \boldsymbol{L}^*_{FP}(\boldsymbol{q},t|\boldsymbol{q}')}\delta(\boldsymbol{q} - \boldsymbol{q}') \tag{3.1}$$

where $\boldsymbol{L}^*_{FP}(\boldsymbol{q}, t|\boldsymbol{q}')$ is a Fokker–Planck-type operator having its coefficients evaluated on source variables $\boldsymbol{q}'$ without their explicit derivatives in the first case. Alternatively, in the second example all explicit derivatives have been calculated and the coefficients are computed in field coordinates $\boldsymbol{q}$, as said in the previous section. More precisely, the Gaussian propagator P_τ formally corresponds to the solution of a Fokker–Planck equation for $\partial P_\tau/\partial\tau$ with constant coefficients $A_i(\boldsymbol{q}', t)$ and $D_{ij}(\boldsymbol{q}', t)$.

Thus, the starting point to develop an accurate and reliable P_τ is to construct an auxiliary operator $\boldsymbol{L}^*_{FP}$ from which one can extract the correct moments A_i and D_{ij} of the original equation by means of the properties given in the above sections. By using this operator one would build a representation of the δ-function in terms of a set of orthogonal functions $\{\phi(\boldsymbol{\lambda}, \boldsymbol{q})\}$, replacing the usual Fourier transform picture (2.13). Let us consider the formal short-time solution (3.1), whose factor $\boldsymbol{L}_{FP}(\boldsymbol{q}, t)\delta(\boldsymbol{q} - \boldsymbol{q}')$ is transformed into $\boldsymbol{L}^*_{FP}(\boldsymbol{q}, t|\boldsymbol{q}')\delta(\boldsymbol{q} - \boldsymbol{q}')$ with $A_i\delta$ and $D_{ij}\delta$ decomposed as (no summation convection here)

$$\begin{aligned} A_i(\boldsymbol{q}, t)\delta(\boldsymbol{q} - \boldsymbol{q}') &= a_i(\boldsymbol{q}, t|\boldsymbol{q}')\alpha_i(\boldsymbol{q}', t)\delta(\boldsymbol{q} - \boldsymbol{q}') \\ D_{ij}(\boldsymbol{q}, t)\delta(\boldsymbol{q} - \boldsymbol{q}') &= d_{ij}(\boldsymbol{q}, t|\boldsymbol{q}')\beta_{ij}(\boldsymbol{q}', t)\delta(\boldsymbol{q} - \boldsymbol{q}'). \end{aligned} \tag{3.2}$$

Then, relation (3.1) may be given as a functional picture of a new operator $\boldsymbol{L}^*_{FP}(\boldsymbol{q}, t|\boldsymbol{q}')$ defined as

$$\boldsymbol{L}^*_{FP}(\boldsymbol{q}, t|\boldsymbol{q}') = -\frac{\partial}{\partial q_i}\left[a_i(\boldsymbol{q}, t|\boldsymbol{q}')\alpha_i(\boldsymbol{q}', t) - \frac{\partial}{\partial q_j}d_{ij}(\boldsymbol{q}, t|\boldsymbol{q}')\beta_{ij}(\boldsymbol{q}', t)\right]. \tag{3.3}$$

The functions a_i and d_{ij} are fixed in order to contain in them the physically relevant functional dependence on $\boldsymbol{q}$ shown by the original coefficients. In this way, the equation

$$P_\tau = \mathrm{e}^{\tau \boldsymbol{L}^*_{FP}(\boldsymbol{q},t|\boldsymbol{q}')}\delta(\boldsymbol{q} - \boldsymbol{q}') \tag{3.4}$$

may be understood as the formal solution of an auxiliary Fokker–Planck equation

$$\frac{\partial P_\tau}{\partial \tau} = \boldsymbol{L}^*_{FP}P_\tau(\boldsymbol{q}, \tau|\boldsymbol{q}^*, 0) \tag{3.5}$$

where t as well as $\boldsymbol{q}'$ are treated as constant parameters. The notation $(\boldsymbol{q}, t|\boldsymbol{q}')$ means that the referred functions may depend on prepoint and postpoint variables $\boldsymbol{q}'$ and $\boldsymbol{q}$. Obviously, this set of factorizations is only a guiding way to construct an auxiliary Fokker–Planck operator. The resulting equation should be solved under the prescribed conditions of the original problem. This is to say that boundary conditions and the asymptotic characteristic functional behaviours of A_i and D_{ij} can be collected in the δ representation through the new functions α_i and β_{ij}. Thus, not only are the coefficients derivatives totally or partially included in the δ representation [28], but also their functional asymptotic behaviours may be included. The set of factors provided through (3.2) generates, at most, $N^2 + N$ new coefficients d_{ij} and a_i, in substitution to the original $A_i(\boldsymbol{q}', t)$ and $D_{ij}(\boldsymbol{q}', t)$ in (2.14) to obtain a generalized form of this common short-time propagator. Note that if the trivial definitions $\alpha_i = 1$, $\beta_{ij} = 1$ and $a_i = A_i(\boldsymbol{q}', t)$, $d_{ij} = D_{ij}(\boldsymbol{q}', t)$ are used, from (3.5) we recover the usual propagator (2.14) in unbounded spaces. In this case, under specified boundary conditions, the solution of (3.5) gives a suitable form of P_τ, valid for small and finite time step τ in bounded spaces.

A special ansatz for the auxiliary functions is provided by setting $\beta_{ij} = 1$. Each $d_{ij}(\boldsymbol{q}, t|\boldsymbol{q}')$ will then coincide with $D_{ij}(\boldsymbol{q}', t)$. Therefore, in (3.5) the diffusion tensor is evaluated at source points. Since the contribution of diffusion processes to time evolution is usually slower than

convective effects, these definitions may be chosen for many problems of physical relevance. Defining N new functions a_i such that all factors $A_i\delta$ are rewritten as

$$A_i(\boldsymbol{q},t)\delta(\boldsymbol{q}-\boldsymbol{q}')=\tilde{\alpha}_i(\boldsymbol{q}',t)a_i(\boldsymbol{q},t|\boldsymbol{q}')\delta(\boldsymbol{q}-\boldsymbol{q}') \tag{3.6}$$

the auxiliary problem is reduced to an ordinary Fokker–Planck equation for the operator

$$\boldsymbol{L}^*_{FP}=\frac{\partial}{\partial q_i}\left[\tilde{\alpha}_i(\boldsymbol{q}',t)a_i(\boldsymbol{q},t|\boldsymbol{q}')-D_{ij}(\boldsymbol{q}',t)\frac{\partial}{\partial q_j}\right]. \tag{3.7}$$

Under this choice, (3.5) may be reduced to a simple solvable Fokker–Planck equation in a new set of N properly scaled coordinates $\{\boldsymbol{v}\}$ in such a way that $v_k=q_k/\tilde{\alpha}_k$. The new drift vector coincides with $a_i=a_i(\boldsymbol{v})$ and the new constant diffusion coefficients are given by $d_{ij}=D_{ij}(\boldsymbol{q}',t)/(\tilde{\alpha}_i\tilde{\alpha}_j)$. Using the well known methods of solution one can extract from this equation a δ representation as the limit

$$\delta(\boldsymbol{q}-\boldsymbol{q}')=\lim_{\boldsymbol{q}^*\to\boldsymbol{q}'}\delta(\boldsymbol{q}-\boldsymbol{q}^*)=\lim_{\boldsymbol{q}^*\to\boldsymbol{q}'}\int\phi(\boldsymbol{q},\lambda)\phi(\boldsymbol{q}^*,\lambda)\mathrm{d}^N\lambda \tag{3.8}$$

in terms of orthogonal functions $\{\phi(\boldsymbol{q},\lambda)\}$, if this limit exits. The insertion of this representation in (3.1) will give a new form for P_τ. However, the way to obtain P_τ is just to solve (3.5) with the initial condition $\delta(\boldsymbol{q}-\boldsymbol{q}^*)$ before proceeding to the limit $\boldsymbol{q}^*\to\boldsymbol{q}'$.

This method has already been sucessfully applied in previous works related to the kinetic equation appearing in plasma physics [22, 23]. To illustrate the procedure let us consider the nonlinear Fokker–Planck equation for the dynamics of electrons in one component plasma, which is quadratic in the distribution f for isotropic velocity space. The drift and diffusion coefficients depend only on the radial spherical coordinate v. Following (3.6) they may be factorized as [22]

$$\begin{aligned}A_v(v,t)\delta(v-v')&=\left[\frac{2}{v}-v\alpha(v',t)\right]D_{vv}(v',t)\delta(v-v')\\ D_{vv}(v,t)\delta(v-v')&=D_{vv}(v',t)\delta(v-v')\end{aligned} \tag{3.9}$$

where $a_v(v,t|v')=(2/v-v\alpha(v',t))$. The terms $\alpha(v',t)=(2/v'-A_v(v',t)/D_{vv}(v',t))/v'$, as well as $D_{vv}(v',t)$, are bounded and sufficiently smooth functions. Thus, the problem is reduced to a radial Ornstein–Uhlenbeck process in spherical coordinates. (3.5) is solved under reflecting conditions at the origin $v=0$. Note that the geometrical drift factor depending on $2/v$ has been kept in field variables. This dependence is an essential feature of the Fokker–Planck equation in spherical coordinates for any A_i, D_{ij}. By direct application of (3.1) the auxiliary equation is solved in terms of Laguerre polynomials in [22] finding both transient and steady states by numerical computation for any initial condition f_0.

Note that the common propagator (2.14) containing the drift and diffusion coefficients computed at source variables fails over the region on which these functions diverge. For instance, consider the previous one-dimensional process for which the $A(q=v)$ behaves as $2/q$ in the neighbourhood of the origin. This means that the deterministic force exerted on a test particle in position $q'\simeq 0$ will strongly drive it to a position $q>0$ with a non-zero probability P. Looking at (2.14) one observes that for a particle in $q'\simeq 0$ the propagator P_τ vanishes for any finite τ because $A(q')$ diverges. This would mean that the probability of finding such a particle in position $q>0$ after time τ would be zero, in clear contradiction with the expected behaviour. This unphysical result has been solved by keeping the relevant factor $2/v$ in source variables.

On account of this example, it is worth emphasizing that under changes of variables the geometrical induced drift has to be computed in field coordinates since they directly set up the boundary conditions for the main problem. At the same time, note that if the convective

functions A_i contain explicitly the geometrical induced factor $1/|\boldsymbol{q}'|$ (2.14) would not be applicable for a finite τ because of the singularity at the origin, as said before. Therefore, if $1/|\boldsymbol{q}'|$ is preserved in source variables, the essential property of smooth behaviour in the small region for the forces is destroyed under such singularity. So it is desirable to directly place these conflictive functional asymptotic dependences on the δ representation, ensuring the smooth functions to appear in source variables.

On the other hand, it must be emphasized that one of the main advantages of this picture is the fact that after solving (3.5) all the properties (2.18)–(2.20) are fully satisfied since P_τ is also a solution of a Fokker–Planck equation.

This kind of auxiliary equation may be solved by reduction to an eigenvalue problem [1]. Since there are a great variety of analytical solutions of simple Fokker–Planck equations in the literature, it is expected that a suitable choice of $\tilde{\alpha}_j$ would provide a convenient function P_τ applicable to the original equation.

In many physical systems of interest using curvilinear coordinates the common situations depicted in previous paragraphs can be achieved by using the representation

$$\delta(q-q') = q\frac{g(q)}{g(q')} \times \int_0^\infty \left[\frac{q}{q'}\right]^\mu J_\mu(\lambda q) J_\mu(\lambda q')\lambda \, \mathrm{d}\lambda \tag{3.10}$$

for the radial contribution to $\delta(\boldsymbol{q}-\boldsymbol{q}')$ in terms of Bessel functions [42–44] J_μ of order μ. The function $g(q)$ is chosen in accordance with the factorizations (3.2) defining $\boldsymbol{L}^*_{FP}$. Particular attention deserves the reduction of (2.12) to an N-dimensional Ornstein–Uhlenbeck process [1, 45] if $\tilde{\alpha}_k = -\gamma_k(\boldsymbol{q}', t)q_k$ which solves the problem even for bounded spaces. In other words, the selection of the auxiliary equation does not imply a practical limitation on the determination of $P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t)$. Moreover, the fitness of the propagator has to be made in such a way that the resulting auxiliary problem drastically simplifies all the calculations by using well known analytical results [46–51].

At this point it must be remarked that this procedure may lead to a formal solution P_τ validated for small and finite evolution time, even in the case of singular diffusion matrix for which (2.14) fails, see the alternate method given in [38]. If the determinant $\|D\|$ vanishes it is possible to derive another expression replacing the Gaussian (2.14) by a convenient choice of factorization functions β_{ij} that would eventually provide an analytical solvable function P_τ from (3.5).

4. Numerical evaluation

The time evolution of the initial distribution $f(\boldsymbol{q}, 0) = f_0$ is provided through (1.1). For a total time of evolution $t_n = n\tau$ the function $f(\boldsymbol{q}, t_n + \tau) = f^{n+1}$ is given as the iterative evolution equation

$$f^{n+1}(\boldsymbol{q}) = \int_{\mathcal{D}} P_\tau(\boldsymbol{q}, \boldsymbol{q}'|t_n) f^n(\boldsymbol{q}') \mathrm{d}^N q'. \tag{4.1}$$

where the integration can be carried out using any of the well known numerical schemes. However, it is convenient to define a transition matrix $\mathcal{Q}^n$ which determines f^{n+1} from f^n. For time-independent A and D the matrix $\mathcal{Q}^n$ has to be computed only at the first time step. A simple rectangle rule for numerical integration scheme leads to a discrete transition matrix whose elements Q^n_{ij} are understood as a transition probability process in discrete variables. Once the N points discretized spatial grid $\{q_i\}$ with length Δq is fixed, this matrix can be constructed by a simple procedure as (in the one-dimensional case)

$$Q^n_{ij} = P_\tau(q_i, q_j|n\tau)\frac{\Delta q}{N_r(j)} \tag{4.2}$$

where $P_\tau(q, q'|t)$ is computed in $t = n\tau$, $q = q_i$ and $q' = q_j$. The numerical function $N_r(j)$ has to be chosen to ensure the numerical normalization of P_τ such that

$$\sum_i P_\tau(q_i, q_j|t)\Delta q = \sum_i Q_{ij}^n = 1 \tag{4.3}$$

which also ensures the constant norm of f^n and its positiveness at any time t_n. If P_τ is normalized to unity, one expects $N_r(j)$ not to deviate too much from this value. This numerical value may be used to check the accuracy of the numerical integration scheme. For this reason, N_r only corrects the truncation numerical errors and makes the discrete and continuous schemes equivalent. In the limit $\tau \to 0$, each Q_{ij}^n approach the δ Kronecker function δ_{ij} in agreement with (2.19) for the continuous case. By increasing the value of τ, the number of non-zero elements of the transition matrix increases. Thereby this matrix will have at least N non-zero elements $Q_{ii} = 1/\Delta q$ for $\tau = 0$ and $N(2k + 1)$ non-null coefficients for a finite time step. k is fixed after computing the number of non-vanishing elements providing a finite value of P_τ. For the transition from point q_i to q_j, the index j takes the values laying from $j_{min} = i - k$ to $j_{max} = i + k$. This reduces the computation time for the evaluation of (4.1) as

$$f_i^{n+1} = \sum_{j=j_{min}}^{j=j_{max}} Q_{ij}^n f_j^n. \tag{4.4}$$

Because all elements of $\mathcal{Q}^n$ are bounded and satisfy (4.3), any initial distribution function f_0 yields the numerical positive function f^n which also behaves as a distribution function in the same sense as f_0. For this reason, the integral method becomes numerically stable under any selection of discretization factors τ and Δq.

In relation to the convergence of the numerical solution, note that formal expression (3.1) for the auxiliary $\boldsymbol{L}_{FP}^*$ operates over $f(q, t)$ through a propagator whose dependence on τ can be essentially described as $1/\sqrt{\tau}\exp[-K^2/\tau]$. Thus, for the functional $K = K(\boldsymbol{q}; \boldsymbol{q}', t) \neq 0$ the term $[\tau \boldsymbol{L}_{FP}^*]^n P_\tau$ originates a set of factors $\exp[-K^2/\tau]/[\tau^n\sqrt{\tau}]$, identified with the rest $O(\tau^n)$. All these factors decay to zero faster than any power of τ. The numerical scheme is then expected to approach any transient solution under a more precise functional form than the one provided by finite-difference schemes. In many physical systems there is more than one conserved quantity during time evolution. In fact, there may be three collisional invariants—number n_0, momentum P and energy T—as occurs in the Fokker–Planck equation in plasma physics. To preserve conservation laws or the predicted evolution of the distribution moments, one may again use the non-uniqueness form of P_τ to improve the matrix $\mathcal{Q}^n$ by adding suitable second-order corrections in τ to its characteristic mean and variance. A way to achieve this goal is to perform the effective drift, say for example $A(q') = A(q_j)$ which appears in the mean of (2.14), using a recursive parameter $\psi_n(\tau^2)$. This parameter can be computationally adjusted by direct evaluation or by a recursion procedure such as

$$\psi_n = \psi_{n-1} + C(T - T_n) \tag{4.5}$$

which minimizes the difference between exact moment T and the numerical T_n in the nth iteration for $C \neq 0$. The initial value ψ_0 may be zero if ψ_n is added to A, or $\psi_0 = 1$ if A is moved to $A\psi_n$ as shown in [22, 23]. Note that this procedure leads to the contribution of terms of higher order than τ added to any short-time propagator, meaning that the appropriate Fokker–Planck equation can be reproduced from it ([16]). This contribution in no way destroys the consistency with the original problem if it is ensured that ψ_n is a correction of order τ^m with $m \geqslant 2$.

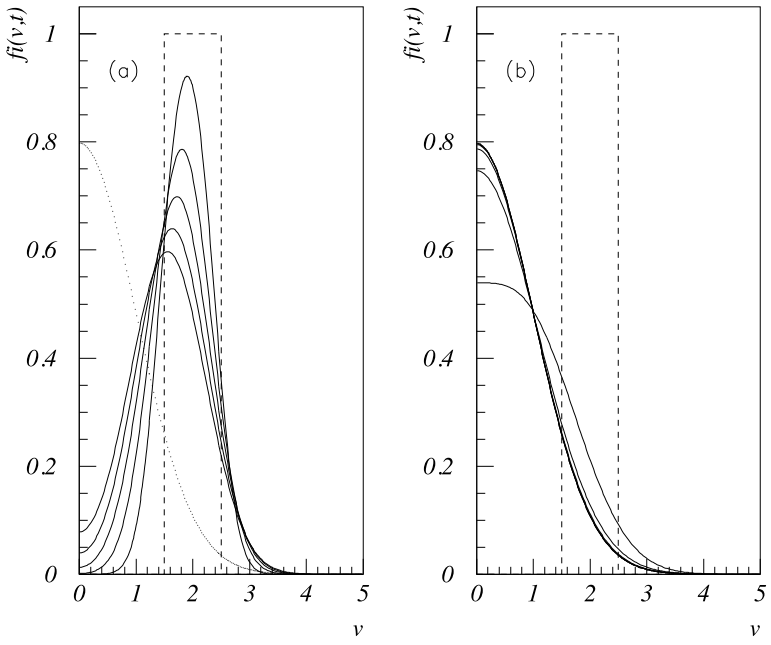

Figure 1. Ornstein–Uhlenbeck process in $(0, \infty)$. (*a*) First five iterations with time step $\tau = 0,05 = t_r/10$ and $\Delta q = \frac{6}{201}$. Dots mean steady analytical solution. (*b*) Evolution of integral solution f_i in time steps $n = 100$, 400, 800 and 1000.

5. Examples

This section illustrates the above algorithm with some representative problems (for physical applications related to plasma physics see [22, 23]).

As a first example, an Ornstein–Uhlenbeck process is treated in the interval $(0, \infty)$ under reflecting boundary conditions at $q = 0$. Secondly, a nonlinear Fokker–Planck equation which is quadratic on f is solved. Both numerical integral solutions are compared with analytical and Crank–Nicholson [52, 53] finite-difference solutions.

For the Ornstein–Uhlenbeck case, the drift and diffusion coefficients are $A = -\gamma v\,(v \geqslant 0)$ and D, where γ and D are real positive constants. Under reflecting boundary conditions, the probability current J for the exact propagator P vanishes at $v = 0$ and for $v \to \infty$, i.e.

$$J = AP - \frac{\partial}{\partial v} DP = 0 \qquad \text{if} \quad v \to 0 \qquad \text{or} \qquad v \to \infty \tag{5.1}$$

which ensures the number conservation. The analytical transition probability P is (for $\gamma = 1$, $D = 1$)

$$P(v, t|v't') = \frac{1}{\sqrt{\pi y}} \{ \mathrm{e}^{-\frac{(v - zv')^2}{y}} + \mathrm{e}^{-\frac{(v+zv')^2}{y}} \} \tag{5.2}$$

$$z = \mathrm{e}^{-(t-t')} \qquad y = 1 - z^2 \tag{5.3}$$

which provides the time evolution of any initial distribution $f_0(v)$ and the steady-state Gaussian solution $f_s = \sqrt{2/\pi}\,\exp(-v^2/2)$. To solve this problem through a numerical integral approach the short-time propagator (2.14) becomes useless since it is not normalized to unity in $(0, \infty)$. The difficulty is avoided if the auxiliary Fokker–Planck equation (3.5) is solved by setting

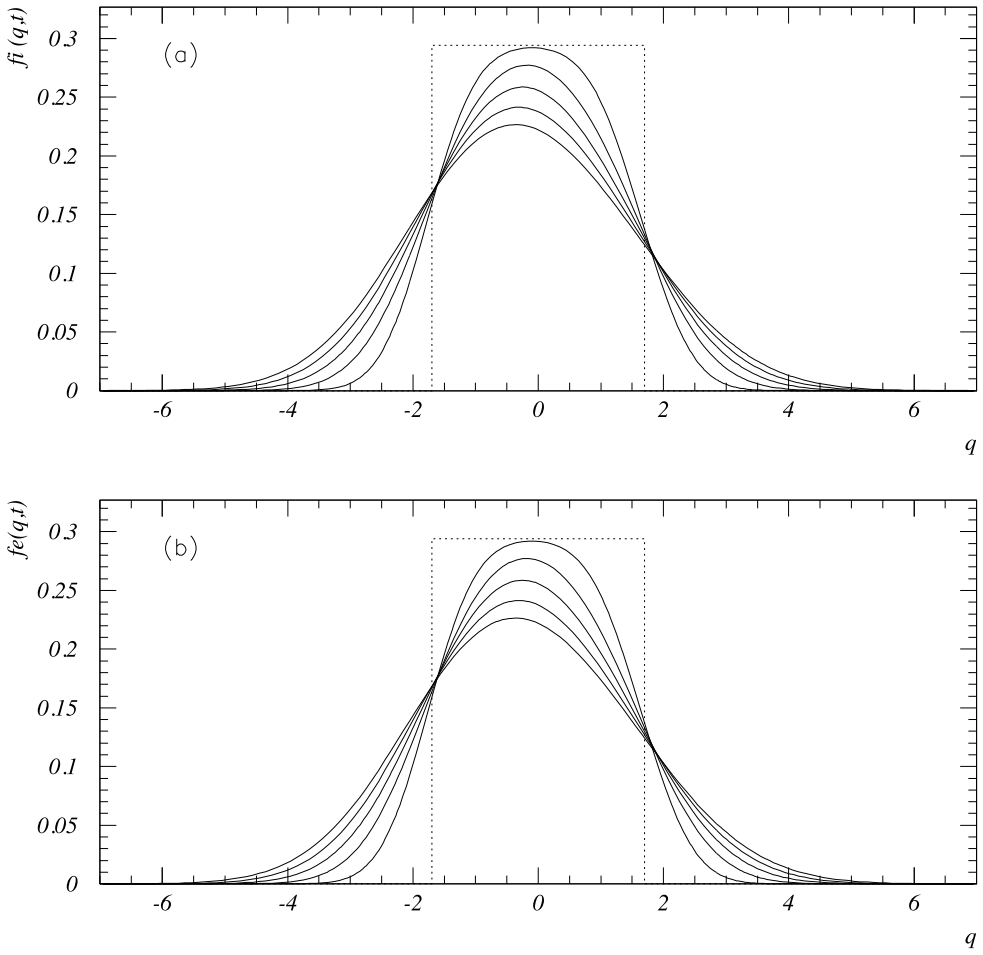

Figure 2. Numerical integral f_i (*a*) and exact f_e (*b*) solutions of non-Markovian Fokker–Planck equation (5.5) for $\gamma = 0$. The total evolution time is $t = 1$ the time step being $\tau = 0.1$. The dashed line represents the initial histogram-type distribution function. Frames (*c*) and (*d*) show the distribution tails behaviours for finite-difference f_d (circles), integral f_i (marks) and exact f_e (line) solutions. Last two frames give the moments evolutions which coincide with the exact ones within an error of order $\pm 10^{-4}$%.

$A(v)\delta(v - v') = A(v')\delta(v - v')$, preserving the reflecting boundary condition. The solution for P_τ reads [14, 48]

$$P_\tau(v, , v'|t) = \frac{\mathrm{e}^{-A(v-v'-A\tau/2)/2}}{\sqrt{4\pi\tau}} \times [\mathrm{e}^{-\frac{(v-v')^2}{4\tau}} + \mathrm{e}^{-\frac{(v+v')^2}{4\tau}}] - \frac{|A|}{2}\mathrm{e}^{Av}\ \mathrm{erfc}\left[\frac{v + v' + A\tau}{2\sqrt{\tau}}\right] \qquad (5.4)$$

where erfc[u] is the complementary error function [44] and $A = -v'$. In spite of (5.4) showing a more involved form than the real propagator for this simple problem, it can be used to solve any related Fokker–Planck equation under the same boundary conditions. The numerical solution is shown in figure 1 with an initial histogram-type distribution f_0. The behaviour of the numerical integral solution is the same as observed for the analytical f at any point of the spatial grid. The relaxation time $t_r = 1$ sets the timescale for which the first moment p of f decays a factor $1/\mathrm{e}$. In the numerical integral scheme a relatively large time step τ may

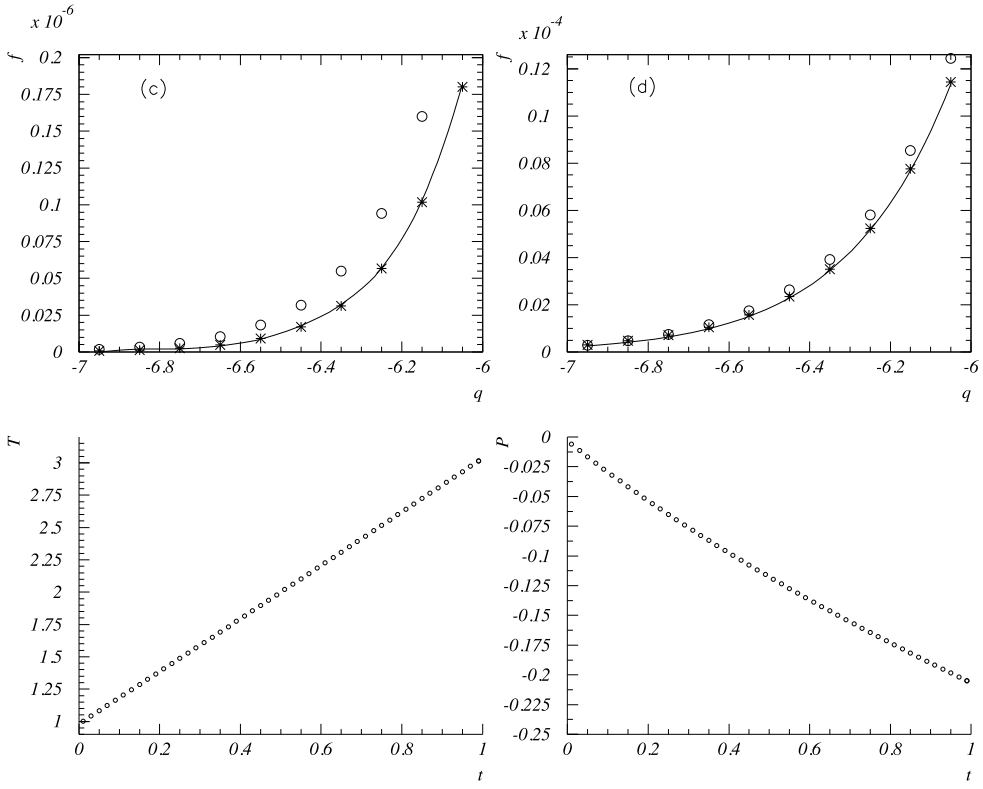

Figure 2. (Continued)

be used. In fact, the method works better for large τ not exceeding $t_r/3$. This feature means that the integral scheme provides the stationary solution in a very small number of iterations, although the number of non-zero elements in $\mathcal{Q}$ increases notably.

The second problem solved in this section refers to a kind of nonlinear Fokker–Planck equation which appears for the macroscopic description of generalized Langevin equations [54, 55]. For such stochastic representations, under the assumption of coloured noise and induced memory effects for random variables [56–58] a Fokker–Planck equation may be derived for macroscopic variables. In this equation the effective drift term A depends on the distribution f itself, providing a non-Markovian picture of such processes. In this case, the propagator P generally depends on the full history of the system through the initial f_0 and, only sometimes does a steady-state distribution exits independent of initial conditions. In this sense, the equation

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial q}\left[-\gamma q - \lambda f - \frac{\partial}{\partial q} D_0\right] f(q,t) \tag{5.5}$$

with constant diffusion $D = D_0$ represents a modified Ornstein–Uhlenbeck process including a self-consistent force $-\lambda f$. This problem can be solved analytically. Following [56], the integral expression similar to the Hopf–Cole transform (in dimensionless form with $D_0 = 1$

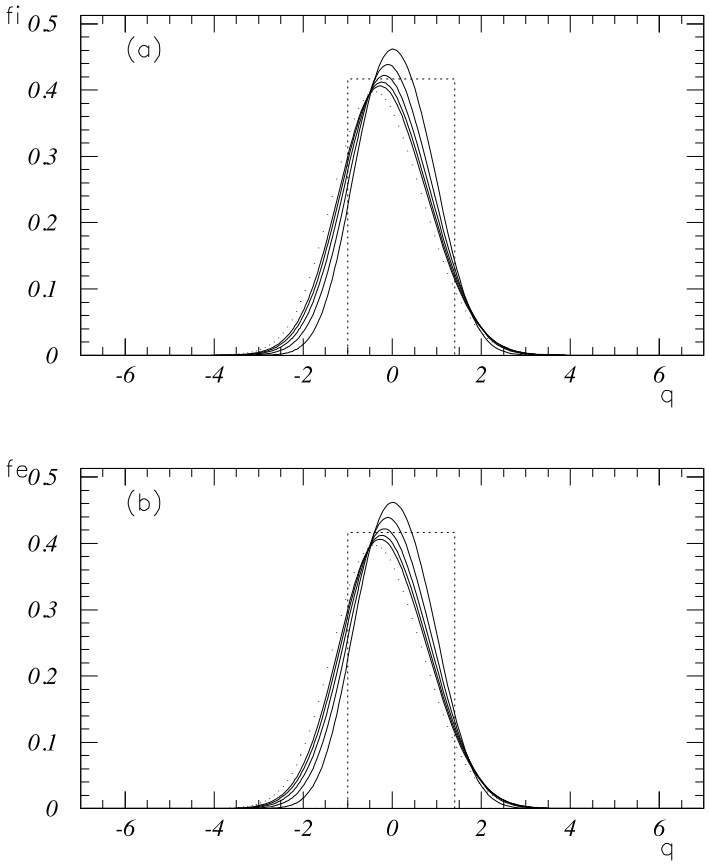

Figure 3. Integral f_i (*a*) and exact f_e (*b*) solutions for (5.5) for $\gamma = 1$, evolution time $t = 2$ and $\tau = 0.01$ in 200 time steps. For $\tau = 0.1$ the evolution is reduced to only 20 time steps providing practically the same figures. Frames (*c*) and (*d*) give the numerical moments P_n and T_n. Analytical moments differ less than 10^{-4}%.

and $\lambda = 1$)

$$Q(q,t) = \exp\left[\frac{\gamma}{2}q^2 + \int_{-\infty}^{q} f(u,t)\mathrm{d}u\right]$$
$$f(q,t) = \frac{\partial}{\partial q}\ln[Q(q,t)\mathrm{e}^{-\frac{\gamma}{2}q^2}] \tag{5.6}$$

leads to a new Fokker–Planck equation in Q associated with a non-normalizable Ornstein–Uhlenbeck process with inverted potential $A = \gamma v$ [1]

$$\frac{\partial Q}{\partial t} = -\frac{\partial}{\partial q}\left[\gamma q - \frac{\partial}{\partial q}\right]Q(q,t) \tag{5.7}$$

whose Green function $P_{ou}(q,t|q',0)$ is obtained from the the ordinary solution P relative to a simple Ornstein–Uhlenbeck process by changing γ into $-\gamma$. The function $Q(q,t)$ is then derived from $Q(q,0)$ through P_{ou}. Thus, after some algebra, the solution to (5.5) for any real γ reads

$$f(q,t) = \frac{\gamma z}{z^2-1}\frac{\int_{-\infty}^{\infty}(q'-zq)\mathrm{e}^{G(q,q')}\mathrm{d}q'}{\int_{-\infty}^{\infty}\mathrm{e}^{G(q,q')}\mathrm{d}q'} \tag{5.8}$$

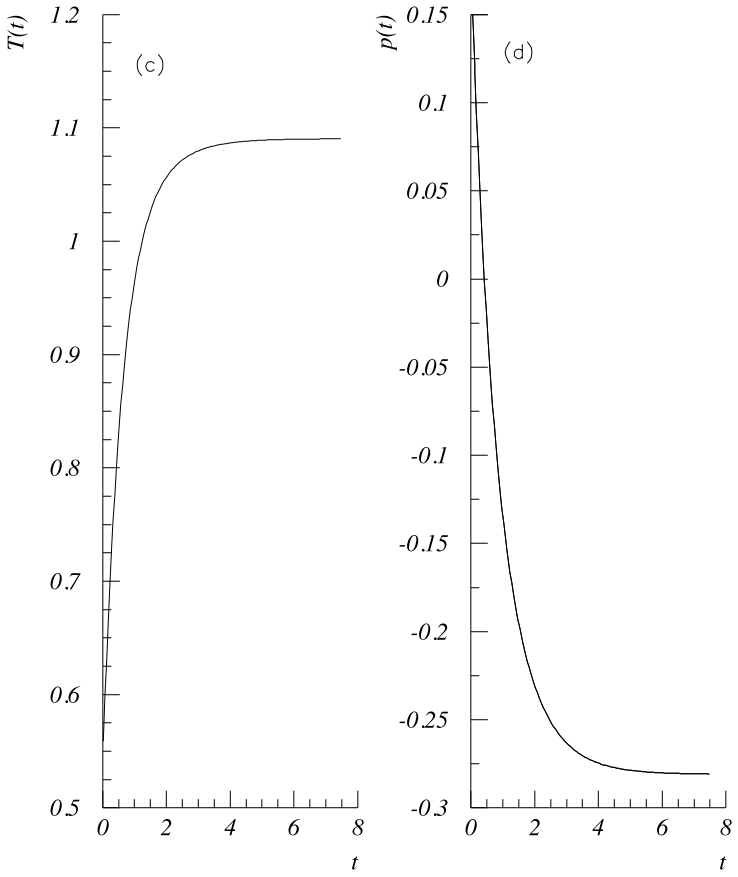

Figure 3. (Continued)

where $z = \mathrm{e}^{\gamma t}$. The integral kernel $G(q, q')$ is given by

$$G(q, q') = \int_{-\infty}^{q'} f(u, 0)\mathrm{d}u - \frac{\gamma}{2}\frac{q' - zq}{1 - z^2}. \tag{5.9}$$

For a positive γ in the limit of large values of time t (5.8) becomes independent of the initial f_0 giving the stationary solution

$$f_s(q) = \sqrt{\frac{2\gamma}{\pi}}\frac{\mathrm{e}^{-\gamma q^2/2}}{(\mathrm{e}+1)/(\mathrm{e}-1) + \mathrm{erf}(q\sqrt{\frac{\gamma}{2}})}. \tag{5.10}$$

For an initial histogram-type distribution f_0 the problem has been solved using a short-time propagator P_τ^* derived from the identification

$$A(q, t)\delta(q - q') = -[\gamma q + f(q', t)]\delta(q - q'). \tag{5.11}$$

The associated auxiliary Fokker–Planck equation (3.5) is again related to the linear Ornstein–Uhlenbeck case with convective parameter $a = -\gamma q - a_0$ for constant a_0. Thus, the short-time propagator P_τ^* is then a simple Gaussian with mean $\overline{q}$ given by

$$\overline{q} = q'\mathrm{e}^{-\gamma\tau} + f(q', t)(1 - \mathrm{e}^{-\gamma\tau})/\gamma \tag{5.12}$$

and variance σ such $\sigma^2 = 2D/\gamma(1-\exp(-2\gamma\tau))$. Note that this expression for the propagator is reduced to the usual one-dimensional (2.14) for small values of $\gamma\tau$, which is also an accurate propagator for this problem if τ is no larger than 10% of the relaxation time $t_r = 1/\gamma$. Note that if P_τ^* is used for any τ, even for $\tau \to \infty$, the nth advanced function f^n is always a well behaved function in the theory of distributions sense. The numerical stability, figure 3, of the advanced scheme is then ensured even for very large values of τ, as can be seen through the moments evolution—figure 3(*c*) and (*d*)—reaching the stationary expected behaviour.

For $\gamma = 0$ (figure 2) no stationary solution exits. However, the distribution $f(q,t)$ is advanced until $t = 1$ in only ten time steps in a very accurate approximation, as can be shown through the analysis of the distribution tails in frames (*c*) and (*d*). For large values of q the integral solution f_i behaves better than the finite-difference solution f_d. It is also shown that moments evolution in the integral scheme is quite close to the exact one.

Acknowledgment

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