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Non-linear Fokker–Planck integral propagator for plasma kinetic coefficients

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Abstract

A recent method to obtain short-time propagators for finding path-integral solutions of Fokker–Planck equations is applied here to numerically solve the non-linear kinetic Fokker–Planck equation in plasma physics. Furthermore, we extend the use of this method to solve non-homogeneous equations. Cylindrical geometry in velocity space is used and two-species plasma is considered with no linearization of the exact conservative collisional operator. Numerical singularities in the diffusion tensor determinant are avoided by the splitting of the collisional operator into two parts, each one leading to different multiplicative integral operators which describe electron–electron and electron–ion interactions separately. The accurate advancing path-integral numerical formalism preserves conservative physical properties making this procedure a promising alternative to the classical linearized collisional operators used in kinetic theory. Here, we show the feasibility of the method by giving a new calculation of Spitzer's transport coefficients.

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1. Introduction

For the last two decades, numerical evaluation of path-integral solution for the Fokker–Planck equation (FPE) [1] has attracted much interest, see for instance the early works in [2–5]. The main difficulty found in achieving a good approximate solution for a non-analytically solvable equation is to provide an accurate short-time propagator which would properly substitute the unknown exact one, also called the Green's function. Among a great variety of physical problems described by Fokker–Planck equations, special interest has been devoted to the one

[3] Deceased.

arising in plasma physics since it is an important tool to describe the collisional interaction among several species of charged particles. In recent times, computational approaches have been used to obtain the physical results in plasmas using the Fokker–Planck approximation to the full collisional Boltzmann operator, see for instance [6, 7]. Some of these computational efforts have followed similar approximations to those established in the analytical linearized method [8–11], but such a limitation is, by no means, necessary.

However, here we provide an alternative integral non-linear conservative and entropic propagator that avoids the usual recourse of using linearization of the collision operator and multipole Legendre expansions for small perturbations of the distribution function f. When using the integral method, not only no information is lost throughout the iteration process, but also, if the short-time propagator is properly derived, the distribution function tails physically behave remaining positive at any time.

We have applied the path-integral numerical computation before, when solving some simple problems related to the Fokker–Planck conservative collision operators which arise in plasma physics in spherical and cylindrical symmetries when only the electron–electron collision term is considered [12–14]. As shown in these two works, and due to the non-unique nature of the short-time propagators, second-order time corrections may be imposed in the time advance scheme to preserve, not only the positiveness and norm of the distribution function, but also the system momentum and energy for any number of iterations.

The integral method has been proved to be an efficient alternative to traditional numerical procedures, such as those based on particle simulations or finite-difference schemes. In kinetic problems, other procedures, such as Monte Carlo method or particle-in-cell, as well as the finite-difference codes, are clearly limited by the general structure of the collisional theoretical operator, which has to be simplified in order to construct an efficient algorithm. In this sense, integral operators open very interesting possibilities in kinetic calculations without the well-known limitations found in the usual methods. These procedures substitute the collisional operators by new approximated ones [15, 16], such as the so-called called Enskog–Chapman–Braginskii method. However, such approaches are burdened with the unavoidable limitation to very small deviations from thermodynamic equilibrium. In fact, when the terms driving the system away from equilibrium (as an external field) are not vanishingly small, the distribution functions develop unphysical negative tails in velocity space. Obviously, this unphysical behaviour drastically distorts the description of the system, making unfeasible many calculations of the so-called transport coefficients [17, 18], where a population of high-energy particles might be responsible for the global behaviour of the system.

In a previous paper [19], we extended a well-known procedure to calculate short-time propagators to provide a simple general method to obtain suitable Green's functions to numerically compute the path-integral solution for any homogeneous FPE. In the present paper, we tackle the problems related to the use and derivation of short-time propagators in cases of physical interest at the same time as we extend the method to solve non-homogeneous equations when source terms are present. We deal here with a two-species plasma where light charged particles interact with massive ones at rest. A short time integral collisional operator is, then, given for a generalized collisional Fokker–Planck integral–differential operator derived from interaction potentials depending on an inverse integer power of the distance.

We provide for this case a general integral operator by splitting the original collisional term into different parts, each one describing the interaction between particles of a given species with others. This procedure is thus quite general and it is demonstrated to avoid possible singularities that can appear since usual Gaussian short-time propagators for FPE are used when a singular diffusion tensor exits. This is the case found if the method is applied to the physically realistic case of interacting particles through binary Coulombian collisions.

We give two applications in order to check the validity of our integral operators. The method is, firstly, tested for the case of Maxwellian hard spheres, which can be analytically solved providing exact relaxation times for temperature isotropization. In the last section, we apply our non-linear collisional propagator to the realistic case of unmagnetized neutral plasmas to reproduce Spitzer's transport coefficients [17, 18, 20] obtained by adding a source term to the original FPE. This fact shows that the approximate Green's functions given here, can be applied to a more complicated situations in plasma physics, if the diffusion coefficients of the original FPE are properly replaced for the actual ones.

2. Fokker–Planck–Landau equation and collision operators

In this paper, we deal with a non-homogeneous Fokker–Planck equation having the general form

$$\frac{\partial f}{\partial t} = \mathbf{L}_{\mathrm{FP}}(\mathbf{q}, t) f(\mathbf{q}, t) + \rho(\mathbf{q}, t) = -\frac{\partial}{\partial q_i}\left[\mathcal{A}_i(\mathbf{q}, t) - \frac{\partial}{\partial q_j}\mathcal{D}_{ij}(\mathbf{q}, t)\right] + \rho(\mathbf{q}, t) \tag{1}$$

for the evolution of a physical distribution function $f(\mathbf{q}, t)$, where $\mathbf{q}$ represents the six components of the vector $\{\mathbf{r}, \mathbf{v}\}$ for a point in the phase space. The additional term ρ takes into account the possible existence of spatial and time dependent sources. The components $\mathcal{A}_i$ of the drift vector $\mathcal{A}$, as well as the diffusion tensor elements $\mathcal{D}_{ij}$ and ρ, may also be highly non-linear functions depending on distribution f. In this case, we shall refer to the above equation as a non-linear FPE. As usual, we mean by 'diffusion coefficients' both vector $\mathcal{A}$ and tensor $\mathcal{D}$ components. The above FPE could be solved if a propagator $\Pi(\mathbf{q}, t \mid \mathbf{q}', t')$ were known. Any distribution function $f(\mathbf{q}, t)$ could be advanced in time through the time integral evolution equation

$$f(\mathbf{q}, t) = \int f(\mathbf{q}', t')\Pi(\mathbf{q}, t \mid \mathbf{q}', t')\,\mathrm{d}\mathbf{q}' + \int \mathrm{d}\mathbf{q}' \int_{t'}^{t} \rho(\mathbf{q}', \tau)\Pi(\mathbf{q}, t \mid \mathbf{q}', \tau)\mathrm{d}\tau, \tag{2}$$

which is equivalent to the differential equation. The probabilistic meaning of this integral equation is clear, since Π could be understood as a transition probability form point $\mathbf{q}'$ at time t' to point $\mathbf{q}$ at time t. Obviously, the task of finding an exact solution for the propagator Π is, at least, as difficult as to solve the original equation. Usually, only approximate propagators can be found in the short-time regime of the evolution. A well-known short-time propagator $P_\tau = P_\tau(\mathbf{q}, \mathbf{q}'|t)$ for the transition from time $t' = t$ to time $t + \tau$ is the Gaussian distribution [1], which in an N-dimensional space reads

$$\Pi(\mathbf{q}, t + \tau; \mathbf{q}', t) \approx P_\tau = \frac{1}{\|\mathcal{D}'\|^{1/2}(4\pi\tau)^{N/2}} \times \exp\left[-\frac{\mathcal{D}'^{-1}_{ij}(q_i - q_i' - \mathcal{A}_i'\tau)(q_j - q_j' - \mathcal{A}_j'\tau)}{4\tau}\right]. \tag{3}$$

Here, primes indicate that the corresponding functions have to be evaluated in source points $\mathbf{q}'$ instead of being computed at field points $\mathbf{q}$, so that $\mathcal{B}'$ means $\mathcal{B}(\mathbf{q}', t)$. It is worth mentioning here that (3) obviously demands the diffusion tensor to satisfy $\|\mathcal{D}'\| \neq 0$. Anyway, for a given FPE it would be convenient to derive a consistent short-time propagator after a previous inspection of the relevant properties of the differential operator. This can be made in several ways, as we pointed out in [19] where we provided a simple tool to achieve this task.

The non-linear FPE arising in plasma physics to describe the motion of the single-particle distribution function $f_a(\mathbf{r}, \mathbf{v}, \mathbf{t})$ for species of kind a, reads

$$\frac{\mathrm{d}}{\mathrm{d}t} f_a - \rho_a = -\frac{\partial}{\partial v_i}\left[D_i^a - \frac{\partial}{\partial v_j} D_{ij}^a\right] f_a, \tag{4}$$

where the co-moving derivative in phase space $\mathrm{d}/\mathrm{d}t = \partial/\partial t + \mathbf{v}\cdot\partial/\partial\mathbf{r} + \mathbf{F}/m_a\cdot\partial/\partial\mathbf{v}$ is usually replaced by $\partial/\partial t$ for spatially homogeneous force-free problems, when the deterministic forces $\mathbf{F} = \mathbf{F}(\mathbf{r}, \mathbf{v}, \mathbf{t})$ vanish. The right-hand side of (4) is known as the collisional operator, because it describes the effect of collisions between charged particles of species a and particles of several species b under a given potential interaction. Though the coefficients D may be non-linear functions of f, one can observe that this equation coincides with (1), by simply identifying these diffusion coefficients with the corresponding ones in (4). Note that in the previous equation each $D^a_{i,j}$ coincides only with $\mathcal{D}_{v_i,v_j}$ for $i, j = x, y, z$, being $\mathcal{D}_{x_i,v_j} = 0$ and $\mathcal{D}_{x_i,x_j} = 0$ in the six-dimensional phase space, while, for instance, $\mathcal{A}_{r_i} = v_i$ and $\mathcal{A}_{v_i} = D^a_i + F_i/m_a$. Note as well that the second rank 6×6 tensor $\mathcal{D}_{\mathbf{r},\mathbf{v}}$ is then singular and (3) would no longer be valid as a short-time propagator.

For a better understanding of the non-linear nature of the actual problem, let us consider the Fokker–Planck equation in velocity space, with natural boundary conditions at infinity, in the Landau form [21]

$$\frac{\partial f_a}{\partial t} = \sum_b \frac{1}{8}\frac{\partial}{\partial v_i}\left\{\int \mathrm{d}\mathbf{v}' u\sigma(u)(u^2\delta_{ij} - u_i u_j)\times\left(\frac{\partial}{\partial v_j} - \frac{\partial}{\partial v'_j}\right) f_a(\mathbf{v}, t) f_b(\mathbf{v}', t)\right\}, \tag{5}$$

where $\mathbf{u} = \mathbf{v} - \mathbf{v}'$ is the relative velocity between a test particle of species a and charged particles of species b, being $u = |\mathbf{u}|$. Here, $\sigma(u)$ is a cross section related to momentum transfer, which is expressible in terms of the scattering cross section $\sigma_{\mathrm{s}}(u,\theta)$ as $\sigma(u) = \frac{1}{2}\int \mathrm{d}\phi\,\mathrm{d}(\cos\theta)(1-\cos^2\theta)\sigma_{\mathrm{s}}(u,\theta)$. For a general potential interaction $V(r) = kr^{-n}$, σ behaves as $u^{-4/n}$. The drift and diffusion coefficients D_i and D_{ij} in (4) may be easily identified from the above equation, by suitable decomposition of the integral kernel in (5) after having integrated by parts. Each one of these terms are given as a convolution integral in the form $D(\mathbf{v}, t) = \int \mathrm{d}(\mathbf{u}) f(\mathbf{v}', t)\,\mathrm{d}\mathbf{v}$, being d any of the kernels

$$d^{a/b}_i(\mathbf{u}) = -\left(1 + \frac{m_a}{m_b}\right)\frac{l^{a/b}}{4\pi}u\frac{u_i}{u^{4/n}} \qquad \text{and} \qquad d^{a/b}_{ij}(\mathbf{u}) = \frac{l^{a/b}}{8\pi}u\frac{\delta_{ij}u^2 - u_i u_j}{u^{4/n}}, \tag{6}$$

where $l^{a/b}$ is usually a constant. The resulting FPE provides the differential collisional conservative plasma operator $\mathbf{L}_{\mathrm{FP}}$. For our present aims, it is enough to consider space homogeneous situations for which the distribution function f_a for the species a depends only on velocity and time. Additional terms, such as ρ, can be treated in a straightforward manner.

From above expressions, all the diffusion coefficients are given as a sum of all contributions, due to interaction of particles of kind b with a test particle of species a as $D^a(\mathbf{v}, t) = \sum_b D^{a/b}(\mathbf{v}, t)$, where D can be any component of the vector D^a_i and the second rank tensor D^a_{ij}. Pay special attention to the fact that due to $D^{a/a}$, this sum also includes the self-interaction collisional contribution.

To analyse the transport coefficients in a plasma, when the system comes to the stationary state, it is convenient to discuss the evolution of the physically relevant distribution moments. For any FPE having the form given in (1), the time evolution of the average quantity $\langle g(\mathbf{v})\rangle = \int g f\,\mathrm{d}\mathbf{v}$ is given by

$$\langle\dot{g}\rangle = \left\langle \mathcal{A}_i\frac{\partial g}{\partial v_i} + \mathcal{D}_{ij}\frac{\partial^2 g}{\partial v_i\partial v_j}\right\rangle + \int g\rho\,\mathrm{d}\mathbf{v}. \tag{7}$$

In our problem, we are interested in three values for g, namely $g = 1$, $g = \mathbf{v}$ and $g = m_a v^2/2$ for norm, momentum and kinetic energy transfer rates for each species.

The numerical advancing method using (2) might almost be trivially applied to the case of Cartesian coordinates, if the simplest Gaussian propagator (3) were valid. Yet in practice,

the amount of numerical work happens to be so large in three dimensions as to render this possibility useless. If we consider the local plasma behaviour in the presence of an electric field E, the relevant geometry in plasma physics applications will be that of axial symmetry introduced by the field. Therefore, one should use the appropriate propagator in this cylindrical geometry. The intractable expression (3) depending on three velocity components is simplified to another one, depending only on the two relevant independent axial and radial components $v_\parallel = v_z$ and $v_\perp^2 = v_x^2 + v_y^2$. The FPE (4) is transformed into (dropping the species superscripts and sources)

$$\frac{\partial F}{\partial t} = -\frac{\partial}{\partial v_\perp}\left[D_\perp^* - \frac{\partial}{\partial v_\parallel}D_{\perp\parallel} - \frac{\partial}{\partial v_\perp}D_{\perp\perp}\right]F(v_\perp, v_\parallel; t) - \frac{\partial}{\partial v_\parallel}\left[D_\parallel - \frac{\partial}{\partial v_\perp}D_{\perp\parallel} - \frac{\partial}{\partial v_\parallel}D_{\parallel\parallel}\right]F(v_\perp, v_\parallel; t) \tag{8}$$

for the new function $F = 2\pi v_\perp f(v_\perp, v_\parallel; t)$.

The cylindrical coordinates $(v_\perp, v_\parallel, \phi)$ are defined in terms of the spherical coordinates (v, θ, ϕ) as $v_\perp = v\sin\theta$, and $v_\parallel = v\cos\theta$. In this equation, we have defined the perpendicular effective drift for F as $D_\perp^* = D_{\phi\phi}/v_\perp + D_\perp$. If an external velocity independent force $\mathbf{F}$ is present, it should be added to the drift vector $\mathbf{D}^{\mathrm{e/e}}$. As usual, if the parallel direction is taken along the field $\mathbf{F}$, $D_\parallel^{\mathrm{e/e}}$ has to be changed into $D_\parallel + F/m$.

For the special case of Coulomb collisions, we have $n = 1$ and from (6), the coefficients D are directly related to the Trubnikov's Rosenbluth-like potentials [22]

$$\psi_b(\mathbf{v}, t) = -\frac{1}{8\pi}\int |\mathbf{v} - \mathbf{v}'| f_b(\mathbf{v}'; t)\,\mathrm{d}\mathbf{v}', \qquad \varphi_b(\mathbf{v}, t) = -\frac{1}{4\pi}\int \frac{1}{|\mathbf{v} - \mathbf{v}'|} f_b(\mathbf{v}, t)\,\mathrm{d}\mathbf{v}', \tag{9}$$

as

$$D_\alpha^{\mathrm{e}/b} = -L^{\mathrm{e}/b}\left(1 + \frac{m}{m_b}\right)\frac{\partial \varphi_b}{\partial v_\alpha}, \qquad D_{\alpha\beta}^{\mathrm{e}/b} = -L^{\mathrm{e}/b}\frac{\partial}{\partial v_\alpha}\frac{\partial \psi_b}{\partial v_\beta},$$
$$D_{\phi\phi}^{\mathrm{e}/b} = -L^{\mathrm{e}/b}\frac{1}{v_\perp}\frac{\partial \psi_b}{\partial v_\perp}, \qquad \alpha, \beta = \perp, \parallel \tag{10}$$

for electron test particle ($a = \mathrm{e}$) in a medium of particles of species b named ions ($b = \mathrm{i}$). In standard notation, we have $L^{\mathrm{e/e}} = (4\pi e^2/m)^2\lambda = L^{\mathrm{e}/b}/Z^2$, where m is the electron mass, e is the electron charge, Z is the relative ion charge and λ is the Coulomb logarithm [22]. From (7), the mean rates of momentum and energy transfer [23] to the electron species e can be expressed as

$$m\frac{\mathrm{d}}{\mathrm{d}t}\langle v_\parallel\rangle = \left\langle D_\parallel^{\mathrm{e/i}} + \frac{F}{m}\right\rangle \qquad \text{and} \qquad \frac{m}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle v^2\rangle = m\left\langle v_\parallel\left[D_\parallel^{\mathrm{e/i}} + \frac{F}{m}\right]\right\rangle. \tag{11}$$

Finally, a system of physical units can be defined for any FPE in Landau form, to get dimensionless magnitudes. For the case of Coulomb binary interaction, such dimensionless form is achieved using the following set of Gaussian units for velocity and time:

$$v_0 = \sqrt{\frac{kT_0}{m}}, \qquad t_0 = \frac{v_0^3}{n_{\mathrm{e}}L^{\mathrm{e/e}}} = \frac{\sqrt{m}(kT_0)^{3/2}}{16\pi^2 e^4 \lambda n_{\mathrm{e}}}, \tag{12}$$

where k is the Boltzmann constant and T_0 is the system kinetic energy at time $t = 0$.

3. Short-time propagators for Fokker–Planck–Landau equation

We focus attention here on a FPE in the form of (4), for electrons (particles of species $a = \mathrm{e}$) in a medium of a single kind of massive ions at rest (species $b = \mathrm{i}$). The approximate

Green's function $P_\tau(\mathbf{q}, \mathbf{q}'|t)$, $P_\tau(\mathbf{q}, \mathbf{q}')$ in the following, is closely related to the unknown $\Pi(\mathbf{q}, t+\tau \mid \mathbf{q}', t)$ by means of the formal equation $P_\tau = \{1 + \tau \mathbf{L}_{\rm FP} + O(\tau^2)\}\delta(\mathbf{q} - \mathbf{q}')$, derived from the Taylor expansion of Π in powers of $\tau = t - t' > 0$ with $\Pi(\mathbf{q}, t \mid \mathbf{q}', t) = \delta(\mathbf{q} - \mathbf{q}')$ [1]. This relation, up to second order in τ, can also be expressed as

$$\Pi(\mathbf{q}, t+\tau|\mathbf{q}', t) \simeq P_\tau = \mathrm{e}^{\tau \mathbf{L}_{\rm FP}(\mathbf{q},t)}\delta(\mathbf{q} - \mathbf{q}'). \tag{13}$$

If we now use for the δ function the Fourier representation which corresponds to infinite boundaries, we arrive at the Gaussian expression (3) and then, (2) provides an integral representation of the FPE.

To derive an integral operator, we proceed following the method established in [19]. Roughly speaking, such derivation uses the already quoted symbolic property of the Dirac δ function $G(\mathbf{v})\delta(\mathbf{v} - \mathbf{v}') = G_1(\mathbf{v}')G_2(\mathbf{v})\delta(\mathbf{v} - \mathbf{v}')$ defining, among many other possibilities, the functions G_1 and G_2, such as $G(\mathbf{v}) = G_1(\mathbf{v})G_2(\mathbf{v})$. For a suitable decomposition of any function G (here D_α and/or $D_{\alpha\beta}$), one can define a new operator $= \mathbf{L}^*_{\rm FP}(\mathbf{v}, \mathbf{v}')$ and construct a solvable auxiliary homogeneous FPE for P_τ as $\partial P_\tau/\partial\tau = \mathbf{L}^*_{\rm FP} P_\tau$ [14, 19]. If we define new drift coefficients $\mathbf{A}$ for the homogeneous FPE (9) through the relations

$$\frac{D_{\phi\phi}}{v_\perp} + D_\perp = \frac{D_{\perp\perp}}{v_\perp} + A_\perp \qquad \text{and} \qquad D_\parallel = \frac{D_{\perp\parallel}}{v_\perp} + A_\parallel, \tag{14}$$

from the formal solution (13), we obtain the auxiliary problem (including a parallel force)

$$\begin{aligned}\frac{\partial P_\tau}{\partial\tau} = &-\frac{\partial}{\partial v_\perp}\left[\frac{D'_{\perp\perp}}{v_\perp} + A'_\perp - \frac{\partial}{\partial v_\parallel}D'_{\perp\parallel} - \frac{\partial}{\partial v_\perp}D'_{\perp\perp}\right]P_\tau \\ &-\frac{\partial}{\partial v_\parallel}\left[\frac{D'_{\perp\parallel}}{v_\perp} + A'_\parallel + \frac{F}{m} - \frac{\partial}{\partial v_\perp}D'_{\perp\parallel} - \frac{\partial}{\partial v_\parallel}D'_{\parallel\parallel}\right]P_\tau\end{aligned} \tag{15}$$

that also defines a new operator $\mathbf{L}^*_{\rm FP}(\mathbf{v}, \mathbf{v}')$, where the variables $\mathbf{v}'$ are now understood as constant parameters. This equation is exactly solvable when primed functions are treated as fixed parameters, giving an integral short-time propagator $P_\tau(\mathbf{v}, \mathbf{v}'|t)$, for F, as

$$P_\tau = \frac{v_\perp}{2\tau\sqrt{4\pi\, D'_{\perp\perp}\tau\, D'_t}} \exp\left(-\frac{D'_{\parallel\parallel}U^2 - 2D'_{\perp\parallel}UV + D'_{\perp\perp}V^2}{4\tau\, D'_t}\right)\mathbf{i}_0\left(\frac{2v_\perp(v'_\perp + A'_\perp\tau)}{4D'_{\perp\perp}\tau}\right), \tag{16}$$

where $U = v_\perp - v'_\perp - A'_\perp\tau$ and $V = v_\parallel - v'_\parallel - A'_\parallel\tau - F\tau/m$. Here, D_t denotes the determinant of the 2×2 non-singular cylindrical diffusion matrix. Primes indicate that the coefficients have to be computed in the source variables $\mathbf{v}'$ in time t. The function $\mathbf{i}_0$ is expressed in terms of the zero-order Bessel function I_0 as $\mathbf{i}_0(q) = I_0(q)\exp(-q)$. Observe that P_τ behaves as a Gaussian far from the origin, making the advancing scheme to be coherent with entropic increase at each time step τ.

The effective new drift coefficients A_α behave in the same way as the original ones D_α, as functions of velocity components, being both ratios A_α/D_α smooth non-vanishing bounded functions. We stress that the new functions A lead to a formally different Fokker–Planck equation which is, however, identical to the original (9) and whose solution for short τ involves only the zero-order Bessel function I_0 instead of that with variable order I_ν [24]. This can be easily shown by noting that the dependence of P_τ on $v_\perp$ comes from the solution of the auxiliary equation

$$\frac{\partial P(v_\perp)}{\partial\tau} = -\frac{\partial}{\partial v_\perp}\left[\frac{D'_{\phi\phi}}{v_\perp} - \frac{\partial}{\partial v_\perp}D'_{\perp\perp}\right]P(v_\perp), \tag{17}$$

when solved for small $v_\perp$ under reflecting boundary conditions at the origin, giving

$$P(v_\perp) = \frac{v_\perp}{2\tau\sqrt{D'_{\perp\perp}}}\left[\frac{v_\perp}{v'_\perp}\right]^\nu I_\nu\left[\frac{v_\perp v'_\perp}{2D'_{\perp\perp}\tau}\right]\exp\left[-\frac{v_\perp^2 + v_\perp^{2\prime}}{4D'_{\perp\perp}\tau}\right]. \tag{18}$$

Here, the variable order $\nu = (D'_{\phi\phi}/D'_{\perp\perp} - 1)/2$ would make the numerical evaluation of P_τ rather cumbersome, unless $D_{\phi\phi}$ coincides with $D_{\perp\perp}$ which is the case if the coefficients A are used instead of the original drift ones. The above integral propagator has already been used in [14], and its excellent computational properties have been checked when no local inhomogeneities exist and no external fields are introduced. It is worth mentioning here that, if the Gaussian (3) is used instead of (16), after rewriting it in cylindrical coordinates, an infinite series of Bessel functions appears when the integration on ϕ is performed. This fact would make the resulting propagator almost useless for numerical purposes.

To solve numerically (5), one can use (2) with (16), after having computed the diffusion coefficients for species e. Nevertheless, when we deal with massive δ-distributed ions at rest, some kind of singularities appear. By noting that the diffusion e/i tensor is a singular matrix, the usual Fokker–Planck propagator (16) might not work properly for this problem. For instance, in the plasma case for the Coulombian potential, the problem is that some of the physical functions, such as the matrix tensor determinant $\|D^{\mathrm{e/e}} + D^{\mathrm{e/i}}\|$ and drift vector $\mathbf{A}$ (or $\mathbf{D}$) are, respectively, proportional to $1/v$ and $\mathbf{v}/v^3$ for small v. These singularities, which are related to the elastic nature of the e/i collisions, make the numerical propagator values to get worse at refined grids. Therefore, it is appropriate here to deal with a more general way to find an integral solution of plasma FPE. This issue can be made by treating each contribution to the collisional term as if it were alone, before dealing with all of them as a whole.

The procedure to split the global integral operator can be easily understood if we rewrite (4) as

$$\frac{\partial f_{\mathrm{e}}}{\partial t} = \rho(\mathbf{v}, t)\left[\mathbf{L}_{\mathrm{FP}}^{\mathrm{e/e}} + \mathbf{L}_{\mathrm{FP}}^{\mathrm{e/i}}\right] f_{\mathrm{e}} + \rho(\mathbf{v}, t) = \mathbf{L}_{\mathrm{FP}} f_{\mathrm{e}}(\mathbf{v}, t) + \rho(\mathbf{v}, t), \tag{19}$$

from which (13) takes the following form:

$$\Pi \approx P_\tau = \exp\left[\tau\left(\mathbf{L}_{\mathrm{FP}}^{\mathrm{e/e}} + \mathbf{L}_{\mathrm{FP}}^{\mathrm{e/i}}\right)\right]\delta(\mathbf{v} - \mathbf{v}') \approx \mathrm{e}^{\tau\mathbf{L}_{\mathrm{FP}}^{\mathrm{e/e}}}\left[\mathrm{e}^{\tau\mathbf{L}_{\mathrm{FP}}^{\mathrm{e/i}}}\delta(\mathbf{v} - \mathbf{v}')\right], \tag{20}$$

meaning that the effect in advancing an impulsive Dirac delta distribution function in time by means of both operators L, is equivalent to consecutively superpose the action of one of them to the action of the other, as if they were independent. Here, by ρ we mean any source term leading to change particle number in any phase space volume element. This term may also be used to modelize spatial derivatives, if they are replaced by particle flux balances through each small cell wall. Recalling now that, in general, $\exp[\tau\mathbf{L}_{\mathrm{FP}}]\delta(\mathbf{v} - \mathbf{w})$ implicitly defines a short-time propagator $P_\tau(\mathbf{v}, \mathbf{w})$ with initial condition $\delta(\mathbf{v} - \mathbf{w})$, and that $\exp[\tau\mathbf{L}_{\mathrm{FP}}]H(\mathbf{v})$ means $\int P_\tau H(\mathbf{w})\,\mathrm{d}\mathbf{w}$, the definite propagator can now be written as $P_\tau = \exp\left[\tau\mathbf{L}_{\mathrm{FP}}^{\mathrm{e/e}}\right]P_\tau^{\mathrm{i}}$. The expression inside the brackets in (20) defines a short-time Green's function P_τ^{i} which takes into account the effect of electron–ion interactions, whereas $\exp\left[\tau\mathbf{L}_{\mathrm{FP}}^{\mathrm{e/e}}\right]$ describes a short time integral operator for electron–electron collisions. The integral form of P_τ can be finally given as

$$P_\tau(\mathbf{v}, \mathbf{v}') = \int P_\tau^{\mathrm{e}}(\mathbf{v}, \mathbf{w}) P_\tau^{\mathrm{i}}(\mathbf{w}, \mathbf{v}')\,\mathrm{d}\mathbf{w}. \tag{21}$$

The functions P_τ can be computed one by one, following the procedure used before in (16) to derive an auxiliary FPE with a new operator $\mathbf{L}_{\mathrm{FP}}^*$. If both functions P_τ are well behaved (as real distribution functions), the integration over $\mathbf{w}$ variables does not need to be performed if one proceeds as it follows. By multiplying both sides of this relation by $f_{\mathrm{e}}(\mathbf{v}', t)$ and carrying out the integration over primed variables, we conclude that the action of the integral operator P_τ can be finally written as

$$f_{\mathrm{e}}(\mathbf{v}, t + \tau) = \int P_\tau(\mathbf{v}, \mathbf{v}') f_{\mathrm{e}}(\mathbf{v}', t)\,\mathrm{d}\mathbf{v}' = \int P_\tau^{\mathrm{e}}(\mathbf{v}, \mathbf{w}) f_{\mathrm{e}}^{\mathrm{i}}(\mathbf{w})\,\mathrm{d}\mathbf{w}. \tag{22}$$

Here, the auxiliary function $f_{\rm e}^{\rm i}(\mathbf{w})$ is the result of advancing $f_{\rm e}$ by means of the 'ions collisional operator' $P_\tau^{\rm i}$, this is to say $f_{\rm e}^{\rm i}(\mathbf{w}) = \int P_\tau^{\rm i}(\mathbf{w},\mathbf{w}) f_{\rm e}(\mathbf{w},t)\,{\rm d}\mathbf{w}$. The second integration involving the electron propagator $P_\tau^{\rm e}$ takes account of the electron–electron interaction for which (16) can be used. This fact led us to search for short-time propagators corresponding to the differential operators $\mathbf{L}_{\rm FP}^{\rm e/e}$ and $\mathbf{L}_{\rm FP}^{\rm e/i}$ independently, when needed to avoid possible singularities. Nevertheless, for any equation in the form (5), it is always possible to use (16) for $P_\tau^{\rm e}$ with the self-interaction coefficients $D^{\rm e/e}$ since it is derived from $\mathbf{L}_{\rm FP}^{\rm e/e}$. The same can be said for P_τ^a, for any species a, to describe the action of $\mathbf{L}_{\rm FP}^{a/a}$ in a more general problem.

The function $P_\tau^{\rm i}(\mathbf{v},\mathbf{v}')$ represents the propagator associated with the plasma FPE without electron–electron contribution, which can be solved analytically in velocity space for massive ions at rest, having $f_{\rm i} = n_{\rm i}\delta(\mathbf{v})$ as a distribution function. Here, the ion density $n_{\rm i}$ equals $n_{\rm e}/Z$ for plasma neutrality. In this case, $\mathbf{L}_{\rm FP}^{\rm e/i}$ only scatters electron velocity direction, not its magnitude, and the Fokker–Planck equation for this operator is

$$\frac{\partial f}{\partial t} = n_{\rm i}\frac{L^{\rm e/i}}{8\pi v^3}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) f(v,\theta), \tag{23}$$

in terms of the angular spherical variable θ (see [22]). The corresponding equation for Green's function $P_\tau^{\rm i}$ can be solved by separation of variables with the initial δ condition in terms of Legendre polynomials, giving

$$P_\tau^{\rm i} = \Pi^{\rm e/i}(\mathbf{v}, t+\tau \mid \mathbf{v}', t) = \frac{\delta(v-v')}{2\pi v^2}\sum_{k=0}^{\infty}\left(k+\frac{1}{2}\right) P_k(\cos\theta) P_k(\cos\theta')\,{\rm e}^{-\lambda_k\tau}, \tag{24}$$

which is exact for any τ. Here, v and v' are absolute velocities and $\lambda_k = n_{\rm i}L^{\rm e/i}k(k+1)/8\pi v^3$.

The computation of the series involved in (24) may need a great number of terms for small values of the exponential argument, increasing notably the computation time. To avoid this problem, an approximate and very accurate formula can be used up to the same order in τ which holds for $P_\tau^{\rm e}$. If we define the standard series

$$P_\beta(\theta) = \frac{{\rm e}^\beta}{2}\sum_{k=0}^{\infty}(2k+1)\,{\rm e}^{-(2k+1)^2\beta} P_k(\cos\theta) P_k(\cos\theta') \tag{25}$$

for an arbitrary positive parameter β, after using integral representations for the Legendre polynomials [25], we find the approximate formula

$$P_\beta \simeq \frac{{\rm e}^{1/2\beta}}{2\beta({\rm e}^{1/\beta}-1)}\,{\rm e}^{\cos\theta\cos\theta'/2\beta} I_0\left(\frac{\sin\theta\sin\theta'}{2\beta}\right), \tag{26}$$

where I_0 stands for the Bessel function of order 0 with purely imaginary argument. Although this expression provides an approximation for small values of β, it is easy to verify that in the limit of large β it approaches the correct asymptotic limit for the series. For this reason, one expects (26) to be quite close to the exact series for all values of time step τ.

With $P_\tau^{\rm e}$ and $P_\tau^{\rm i}$, the function $f_{\rm e}$ can be advanced in time, by means of successive applications of both short-time propagators. As $P_\tau^{\rm i}$ given by (24) is exact, the order of integration can be changed, in spite of the fact that the integral operators, as well as the differential ones $\mathbf{L}_{\rm FP}$, do not commute.

To end this section, we will mention once again two facts: the propagators obtained here are only valid in the regime of short time evolution and their forms are non-unique [26, 27]. For this reason, further corrections in order τ^2 (or lower) can be introduced during the computation, resulting in a new expression for P_τ. This can be achieved having in mind that the contribution of the e/e operator should not modify the electron momentum and energy. Since P_τ is a time-dependent function, it may be changed using a fit parameter ϵ_n that minimizes the difference between numerical electron energy T_n (at time $t_n = n\tau$) and its

previous value T_{n-1}. This parameter has to be recursively calculated before applying P_τ^{i} at each time step. When the time-dependent coefficients $A_\parallel^{\mathrm{e/e}}$ are replaced by $A_\parallel^{\mathrm{e/e}}(1+\epsilon_n(\tau))$ with

$$\epsilon_n = \epsilon_{n-1} + \kappa(T_n - T_{n-1})(\kappa \neq 0, \epsilon_0 = 0), \tag{27}$$

the correct behaviour of all physical moments is observed after a series of small oscillations of T, as shown in the figures. It must be remarked that this substitution does not modify positivity, number and momentum evolution. It just restores the physically predicted behaviour for the second-order moment of the electron distribution $\langle v^2 \rangle$, which should not change at each time step when only the self-interacting collision operator acts.

4. Application to Maxwell's hard spheres' potential FPE

The validity of integral propagators obtained for the advancing scheme (22) can be checked by solving a Fokker–Planck equation, having the same conservative properties as those found in the realistic plasma physics collision operator. Now we will be concerned with the so-called Maxwell's molecule potential $V = kr^{-4}$, to compute $\sigma(u)$ in (5) that provides the coefficients

$$D_i^{\mathrm{e}/b} = -2\left(1 + \frac{m_{\mathrm{e}}}{m_b}\right)\int (v_i - v_i')\, f^b(\mathbf{v}', t)\, \mathrm{d}\mathbf{v}' \tag{28}$$

and

$$D_{ij}^{\mathrm{e}/b} = \int (\delta_{ij}u^2 - u_i u_j)\, f^b(\mathbf{v}', t)\, \mathrm{d}\mathbf{v}' \tag{29}$$

in arbitrary units. Note that the integrals appearing above can be given in terms of the distribution moments. In particular, if the mean $\langle v_\parallel \rangle = 0$ for massive ion particles $b = \mathrm{i}$ with relative charge Z and distribution $f_{\mathrm{i}} = Z\delta(\mathbf{v})$, we have, for density $n = 1$,

$$\begin{aligned}
&D_\perp = -4v_\perp(1 + Z/2), && D_\parallel = -4v_\parallel(1 + Z/2), && D_{\perp\parallel} = -(1 + Z)v_\parallel v_\perp,\\
&D_{\perp\perp} = T_\perp + T_\parallel + v_\parallel^2(1 + Z), && D_{\parallel\parallel} = 2T_\perp + v_\perp^2(1 + Z), && D_{\phi\phi} = D_{\perp\perp} + D_{\parallel\parallel} - 2T_\perp,
\end{aligned} \tag{30}$$

where $T_\perp$ and $T_\parallel$ are the anisotropic temperatures $T_\perp = 1/2\langle v_\perp^2 \rangle$ and $T_\parallel = \langle v_\parallel^2 \rangle$. The effective drift coefficients A_α are proportional to D_α. It is clear that any initial anisotropic distribution function $f_{\mathrm{e}}(\mathbf{v}, 0)$ must gradually be transformed into a Maxwellian $f_0(\mathbf{v})$ having $T_\perp = T_\parallel = T$, not only for this example but also for all the wide classes of equations depicted by (5). Here, the rate of change of the difference $\Delta = T_\perp - T_\parallel$ can be given explicitly as

$$\frac{\mathrm{d}\Delta}{\mathrm{d}t} = -\frac{\Delta}{\tau_{\mathrm{r}}} = -12\left(1 + \frac{Z}{2}\right)\Delta, \tag{31}$$

defining the relaxation time $\tau_{\mathrm{r}} = 1/(12 + 6Z)$.

Using these relations, it is possible to analyse the validity of the results contained in section 3. As no singularities are present now, the combined e/e and e/i collisional effects can be simultaneously treated with (16) computing the coefficients $D = D^{\mathrm{e/e}} + D^{\mathrm{e/i}}$. Otherwise, the split operator (22) should be equivalent to advance in time f_{e}. These features can be checked by computing in both schemes both τ_{r} values, and comparing them with their analytical exact value. To solve the problem by splitting the short-time transition probability, the ion contribution to P_τ is given by (24) when λ_k is replaced by $Zk(k + 1)$. We stress, once again, that P_τ^{i} is exact and its approximate sum works as being exact too. The integral propagator P_τ^{e} has the form of (16), for $Z = 0$ in the previous coefficients to keep only e/e contributions.

In both advancing schemes analysed here, the time step τ may be relatively larger than the reasonable values that can be taken in a finite-difference advancing scheme. In fact, for both

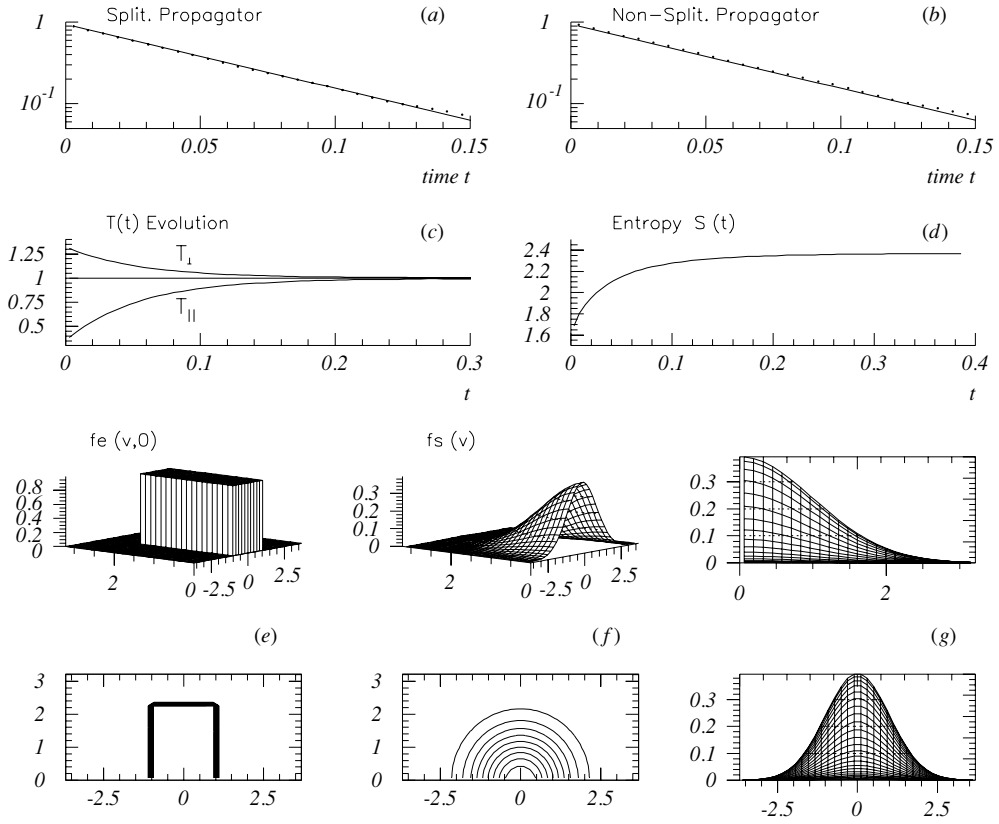

Figure 1. Time evolution of $\log|T_\perp - T_\parallel| = \log|\Delta|$ (dots) for the problem treated in section 4, using the split propagator (*a*) and the full propagator (*b*) where line means analytical solution. The time step is $\tau_r/10$ with $Z = 1$ in a 35×50 grid. The evolution of $T_\perp$ and $T_\parallel$ and the entropy increase are plotted in (*c*) and (*d*) for 150 iterations. Initial (histogram-type) $f_e(\mathbf{v}, 0)$ in frames (*e*) and surfaces and contour lines for steady state $f_s(\mathbf{v})$ in (*f*) and (*g*).

solutions, τ is about a 10–20% of the theoretical (or previously predicted) relaxation time τ_r. For any initial condition $f_e(\mathbf{v}, 0)$, a numerical Maxwellian isotropic distribution is obtained with almost no difference between both methods. The behaviour of the temperature gap Δ agrees with the predicted exponential decay even for large values of the time step τ (a half of τ_r). The solution given by the split propagator is more accurate than that provided by the compact form of P_τ described above. The time evolutions of Δ in both advancing schemes are given in figure 1, where they may be compared with the analytical evolution while the initial energy is kept constant using a small parameter ϵ_n, as given in (27). The expected entropy increase is also observed when entropy is defined as usual $S = -\int f \log f \, d\mathbf{v}$.

5. Application to classical transport coefficients' calculus

When an external force $\mathbf{F}$ is present and space inhomogeneities are introduced, (4) takes the form

$$\frac{\partial f_e}{\partial t} + \mathbf{v} \cdot \frac{\partial f_e}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m_e} \cdot \frac{\partial f_e}{\partial \mathbf{v}} = C^{e/e} + C^{e/i} = C(f_e, f_e) = \mathbf{L}_{FP} f_e, \tag{32}$$

where we have used a more standard notation (C) for the collision operators, assuming plasma neutrality and massive ions at rest. We shall consider the computation of classical transport coefficients when temperature gradients and electric field exist. In this case, we seek for a non-homogeneous FPE to apply the integral numerical solution when $\rho \neq 0$.

As it is well known [15, 17], the steady-state solution of (32) is usually carried out assuming that the distribution function can be expressed as $f_e = f_e^0(v) + f_e^1(v, \cos\theta)$, where f_e^0 stands for the Maxwellian distribution, and f_e^1 obeys

$$f_e^0\left(\frac{mv^2}{2kT} - \frac{5}{2}\right)\frac{\mathbf{v}}{T}\cdot\frac{\partial T}{\partial \mathbf{r}} - f_e^0\frac{e}{kT}\mathbf{E}\cdot\mathbf{v} = -K\left(f_e^1, f_e^0\right) - K\left(f_e^0, f_e^1\right) = -C^{\text{lin}} \tag{33}$$

in an inertial motionless reference system. In (33), $K = -K\left(f_e^1, f_e^0\right) - K\left(f_e^0, f_e^1\right)$ will represent the linearized parts of the full collision operator, C, which we will call C^{lin} for simplicity. For those cases in which $\mathbf{E}$ and ∇T have the same space orientation, we may write the equation in the classical form (33), also followed by Spitzer,

$$\rho_{\text{SPT}} = f_e^0\left(\frac{mv^2}{2kT} - \frac{5}{2}\right)\frac{v_\parallel}{T}\frac{\partial T}{\partial z} - f_e^0\frac{q}{kT}v_\parallel E = -C^{\text{lin}}\left(f_e^0, f_e^1\right). \tag{34}$$

In this well-known formulation of the non-homogeneous term, the temperature gradient factor is fixed in such a way that the average particle flux of the electrons vanishes in the absence of an electric field $\mathbf{E}$.

To look for a physical test of our non-linear propagator, we will compare the result of (34) with the case in which the collisional term is exactly evaluated instead of being approximated. For very small values of the $\mathbf{E}$ and ∇T, the solutions of both equations should coincide.

A comparison between the linearized method and our exact calculation is better understood if we consider (34) as the stationary limit of the following differential equation:

$$\frac{\partial f_e}{\partial t} = \rho_{\text{SPT}} + C^{\text{lin}}\left(f_e^0, f_e - f_e^0\right). \tag{35}$$

As already mentioned, the first step in developing a non-linear kinetic approach is to solve the preceding equation with the same source term $\rho_{\text{SPT}} = \rho$ (that includes $\mathbf{E}$ and ∇T), but substituting the linearized collision operator C^{lin} for the non-linear collision operator $C(f_e, f_e) = \mathbf{L}_{\text{FP}} f_e$. When its time evolution comes to an end, our solution for f_e should be very close to the classical one obtained through a series expansion in Sonine polynomials [15].

We may now use (2) to approximate the non-homogeneous Fokker–Planck equation in the limit of short time steps. The simplest scheme is provided by the advancing formula

$$f_e(\mathbf{v}, t+\tau) = \int d\mathbf{v}'[f_e(\mathbf{v}', t) + \tau\rho(\mathbf{v}', t)]P_\tau(\mathbf{v}, \mathbf{v}'|t) \tag{36}$$

for short τ time steps. From (7), we obtain for energy and rate momentum transfers

$$\langle \dot{v}_\parallel \rangle = \left\langle D_\parallel^{\text{e/e}} + D_\parallel^{\text{e/i}} \right\rangle + \int v_\parallel \rho \, d\mathbf{v} = -\frac{n_i L^{\text{e/i}}}{4\pi}\left\langle \frac{v_\parallel}{v^3}\right\rangle + \int v_\parallel \rho \, d\mathbf{v}, \tag{37}$$

$$\frac{1}{2}\langle \dot{v}^2 \rangle = \frac{1}{2}\int v^2 \rho \, d\mathbf{v} \qquad \text{with} \qquad \dot{n} = \int \rho \, d\mathbf{v}. \tag{38}$$

In previous equations, use is made of average energy conservation in e/e and e/i collisions for very heavy ions. The presence of $\mathbf{E}$ has been included in $\rho = \rho_{\text{SPT}}$ instead of using $D_i = D_i^{\text{e/e}} + D_i^{\text{e/i}} - qE_i/m$. Once the stationary state is reached, $\int \rho \, dv^3 = 0$, (37) and (38) give the relations

$$\int v_\parallel \rho \, dv^3 = -\frac{nZL^{\text{e/e}}}{4\pi}\left\langle \frac{v_\parallel}{v^3}\right\rangle_{\text{ST}} \qquad \text{and} \qquad \frac{1}{2}\int v^2 \rho \, d\mathbf{v} = 0. \tag{39}$$

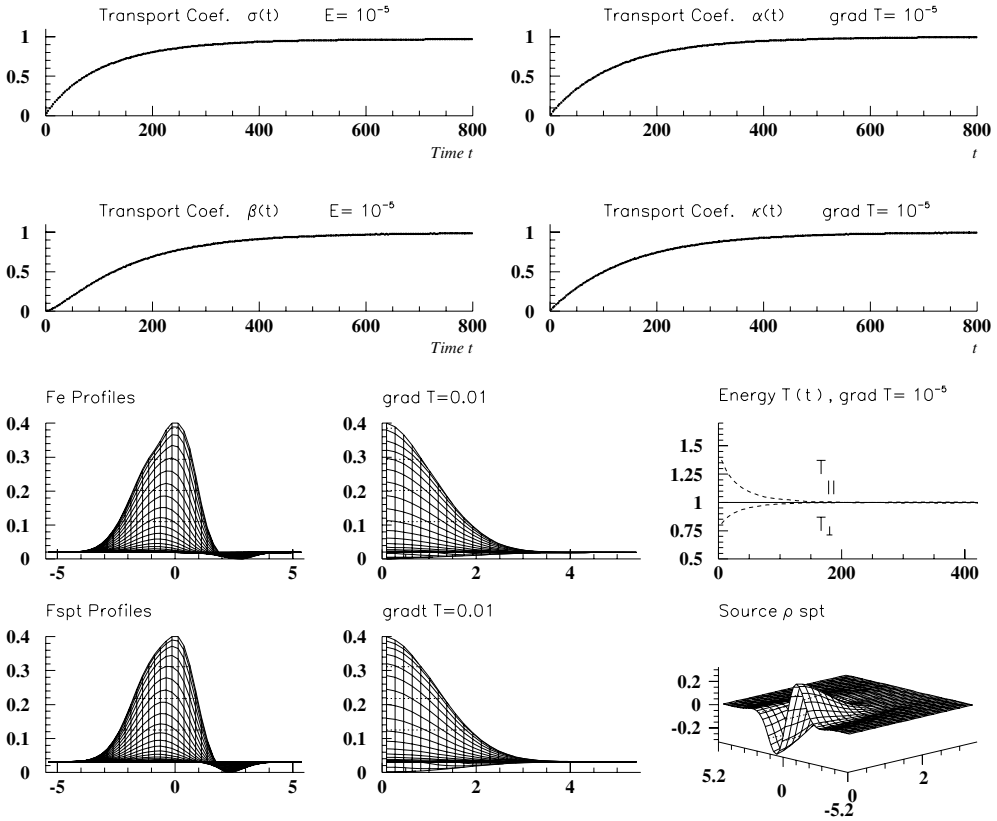

Figure 2. Normalized transport coefficients evolution for small fields E and $|\nabla T|$. The profiles for our f_e can be compared with Spitzer's solution profiles f_{SPT}. In both cases, negative distribution tails appear for large $|\nabla T|$ (here 0.01) because of the unphysical source ρ_{SPT}, but this effect is less sharp for our integral solution. Time evolution for $T_\perp$, $T_\parallel$ and the form of the source term ρ_{SPT} in (34) are also shown.

For Spitzer's equation with no thermal gradient and $\rho = \rho_{SPT}$, as defined in (34), in the stationary state the relations

$$-\frac{qEn}{m} = \frac{nZL^{e/e}}{4\pi}\left\langle\frac{v_\parallel}{v^3}\right\rangle, \qquad \frac{1}{2}\int v^2\rho_{SPT}\,\mathrm{d}\mathbf{v} = 0 \qquad \text{and} \qquad \frac{qE}{m}\langle v_\parallel\rangle = 0 \tag{40}$$

hold. This, however, implies $\langle v_\parallel\rangle = 0$ for $t \to \infty$, an exact result which would seem to contradict the coherence of the classical scheme if no thermal gradient is used to keep a null current $j = -en_e\langle v_\parallel\rangle$. In fact, its results would be just valid in the extreme zero field and zero current case, whereas exact coincidence with Spitzer–Harm's result is only achieved for very weak fields, as expected.

Our analysis shows that in steady state $\dot{n} = 0, \langle\dot{v_\parallel}\rangle = \left\langle D_\parallel^{e/i} - qE/m\right\rangle = 0$ and $1/2\langle\dot{v^2}\rangle = -qE/m\langle v_\parallel\rangle$, which explains the progressive increase in energy of the system with time, as observed in our results when the electric field is not low enough to make it undetectable. This question will be further considered in the context of a fully non-linear approach as a subject for future investigations.

We now proceed to describe the outcome of our analysis. For the sake of clarity, transport coefficients are computed taking the corresponding Spitzer–Harm ones as units. We use the same notation and definitions as in [17] to calculate the electric current and the heat flux as

$\mathbf{j} = \sigma\mathbf{E} + \alpha\nabla T$ and $\mathbf{Q} = -\beta\mathbf{E} - \kappa\nabla T$ when a field or a temperature gradient is present in ρ. We obtained full agreement within the expected computational errors.

Figure 2 shows the evolution of transport coefficients (first four frames) when the run is started with a Maxwellian for f_e at temperature T. For this case, a 35×50 grid was used and 250 time steps were sufficient to reach practical stationary state. The asymptotic or $t_{250} \cong t_\infty$ coefficients obtained were then $99 \pm 2\%$ of Spitzer's, with no further appreciable change in longer times.

In order to appreciate the time scale evolution, figure 2 also presents (seventh frame) a run started with an asymmetric Maxwellian also at average temperature T, but with $T_\parallel \neq T_\perp$. The temperature equilibration time, until a common temperature is reached for f_e, provides the time scale for steady state. This time slightly depends on the strength of the temperature gradient and on the electric field magnitude, too.

Finally, figure 2 also illustrates the difference between the linearized and the exact treatment of (32), in the case of large temperature gradients. This is not a realistic case for the definition of transport coefficients, because of large negative tails in the distribution function. It is interesting, however, that our solution, which uses no linearization of the collision operator, tends to correct these unphysical negative values in a good direction. A full correction, that is, absence of negative amplitudes, is only obtained with an exact flux-balance definition of the source term ρ, but this is out of the scope of this work, being a subject for future applications of our numerical integral method.

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