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Integral Kinetic Method for One Dimension: The Spherical Case

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The integral method to numerically calculate the time evolution of kinetic systems is discussed and improved for one-dimensional problems. The new approach is applied to the solution of the spherically symmetric one-component plasma kinetic evolution. The results are compared with those obtained by means of the finite-difference solution to the equivalent Fokker–Planck kinetic equation.

KEY WORDS: Kinetic; plasma; Fokker–Planck equation; numerical approximation; integral method.

1. INTRODUCTION

One of the challenges in contemporary physics is to discover efficient ways to describe natural processes using our present computational facilities.

In the plasma physics case to which this work is mainly addressed, kinetic studies are generally carried out using the Fokker–Planck expression for the collisional term. Furthermore, the coefficients for this equation are usually expressed in the form derived by Rosenbluth *et al.*[1] because of its simplicity in the applications. This form of the equation clearly shows the considerable complexity of the problem, since the mentioned coefficients are integrodifferential functionals of the time-dependent distribution function itself.

Except for the Maxwellian solution corresponding to thermodynamic equilibrium, no exact analytic solutions to the kinetic equation are known. The problems are solved in an approximate way, which invariably means taking recourse at some stage to numerical computation. It should be

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mentioned that the first computational analysis of the time evolution of an arbitrary initial distribution to equilibrium was carried out by MacDonald *et al.*[2] using a simple explicit scheme. The Fokker–Planck equation was chosen to correspond to the simplified spherically symmetric case.

The more general situation in which the geometry has cylindrical symmetry is usually treated through a multipole expansion, also introduced in ref. 1, and implies very serious computational problems. Thus, related physical cases of modern interest in plasma studies, such as the interaction of collisional plasmas with electromagnetic waves, are generally solved using approximations to the Fokker–Planck equation. Even at this stage, the programs are very complex and present considerable conservation difficulties.[3,4]

Looking for possible improvements in the distribution-function time-evolution description, a reasonable step is to examine just why the Fokker–Planck equation is used, and what principles stand behind it. Clearly, obtaining differential equations is a crucial step for analytic calculations. Arriving at closed expressions through integral methods is in general much harder. When computational methods are used, it is not so clear that differential equations are the best route for the description of physical phenomena, particularly if there are integral principles from which they derive.

It must be said in this respect that in the physics literature two types of Fokker–Planck equations are considered. For those cases in which the first and second moments are constant or depend on the independent variables (considering for simplicity the one-dimensional case), the Fokker–Planck equation is frequently derived from integral probabilistic equations of the type[5]

$$f(a, t+\Delta t)=\int_A P(a, t+\Delta t \mid a', t)\, f(a', t)\, da' \tag{1}$$

Rigorous derivations of the Fokker–Planck equation are then available, and the transition probability for small time increments takes the form[5]

$$P(a, t+\Delta t \mid a', t)=\frac{1}{2[D(a')\pi\, \Delta t]^{1/2}} \exp\left\{-\frac{[(a-a'-A(a')\,\Delta t)]^2}{4D(a')\,\Delta t}\right\} \tag{2}$$

Here A and $2D$ are defined in the usual way as the first and second moments of P per unit time:

$$A=\langle \Delta a \rangle$$

$$2D=\langle \Delta a\, \Delta a \rangle$$

When the Fokker–Planck equation is strictly nonlinear, as in the plasma physics case and other kinetic systems, where the moments are integrodifferential functionals of the time-dependent distribution function itself, no rigorous derivation from a probabilistic equation exists, and the equation is commonly justified by other means. Even in this case, however, there is a strong belief that the difficulties are technical rather than physical, and that a similar equation to (1) is at operation. This assumption is explicitly made in popular textbooks (see, for example, ref. 6).

In the present work we explore the possibility that starting with an integral equation of type (1), the computational solution to the kinetic evolution is simpler than the computational solution to the corresponding Fokker–Planck equation, and the physical evolution more transparent. The basic step is of course to choose the adequate form for the transition probability P in (1). For those cases in which the variation of the moments is slow in time, something that is seen to hold in reality (showing that the nonlinearity is of a milk kind), we believe it is justified to use for P the same expression (2), where now the first and second moments must be recalculated at each time step from the evolving values of the distribution function.

The reason behind our assumption is clearly that for slow changes of the moments in the system evolution, the transition probability is almost constant. So in fact "piecewise in time," the evolution is a succession of situations for which the Fokker–Planck equation has coefficients which are almost constant in time and depend only on the independent variables, so they can be derived from equations of type (1) and transition probabilities (2). The continuous path evolution would be approximated by a "polygonal path" which presumably would tend to the exact solution as the time increment tends to zero.

It has already been shown in previous papers[7,8] that an integral computation of Eq. (1) with P given by (2) describes indeed the evolution of arbitrary initial velocity distributions toward equilibrium, just as the Fokker–Planck method does. Furthermore, the numerical scheme can be defined so that exact conservation of both density and energy holds for any length of time. Considering that the Maxwell distribution is a (unique) analytical stationary solution of (1), with P given by (2) (this fact being true also in case the moments depend on the distribution as in our problem), it is hardly surprising that a numerical scheme preserving the only two additive constants of the motion evolves also to a Maxwellian distribution within the numerical inaccuracies.

Even if the method has shown promising results, work must be done before its potential advantages are fully exploited.

In order to formulate the problem along those lines that are best

suited for an integral procedure, we start by defining a numerical approximation which does not completely coincide with the one generally used with finite differences. We depart in this sense from our first quoted works, where we followed the usual assumptions made in the finite-difference numerical approach. Such is the substitution of the continuous set of points of a variable within an interval in which a function takes certain values, by a discrete set defining the numerical grid.

A related but essentially different approximation is presented here. The new formulation does not change the basic ideas that motivate the method, but demands a reappraisal of the numerical techniques to be used in practice.

Together with the detailed description of the new numerical techniques, a very fundamental improvement for the practical use of the integral method is the suppression of unnecessary angular integrations that were carried out in refs. 7 and 8.

In order to make this possible, the transition probability function must be defined for the weighted density in the corresponding space where the angular variable is irrelevant. The redefinition of the moments to be used in (1) is simple but not trivial for this case.

With the new formulation, we have already been able to derive extremely efficient results for the case with cylindrical symmetry. This is the ultimate motivation for our work and justifies the effort in its development. These results will be published elsewhere.

In the present work, where an overall description of the method is intended, it is more convenient to describe its application to the simple spherically symmetric problem. One reason is that the solution to this problem is well known and presents no difficulties through the Fokker–Planck approach. It is thus easy to check our results against the ordinary differential numerical methods used for its solution. The second reason is that the integral method is particularly unsuited for this case, because the distribution function to be time advanced is the weighted function $F(v, t) = v^2 f(v, t)$. In order to compare with differential results, which solve in fact for $f(v, t)$, we must divide by v^2. This of course is bound to produce considerable uncertainties at the origin. It is thus a considerable success of the method that it can be favorably applied even to this case.

It should be mentioned that for the cylindrically symmetric case the distribution function is only weighted in the form $v_r f(v, t)$. Therefore, the actual value of $f(v, t)$ at the axis is subject to much less numerical uncertainty than $f(v, t)$ at the origin in the spherical case studied in this paper. This is one reason why the integral method can compete with the differential method all the better when the situation is less symmetric.

The paper is organized as follows. In Section 2 we introduce the new

approach that seems adequate for a numerical method calculating integrals of a distribution function multiplied by an integral nucleus. The new approach is addressed to the calculation of transition probabilities in problems defined by first and second moments.

Section 3 deals with setting up a practical scheme to advance the time-dependent distributions.

The general method obtained is applied in Section 4 to the solution of the particular problem chosen, whose differential version is the time advancement of Eq. (17).

Section 5 summarizes the results obtained and the advantages of the method compared to the usual finite-difference results.

2. THE BASIC MATHEMATICAL AND PHYSICAL APPROXIMATION

In the finite-difference approach to computing differential equations, the continuum is replaced by a discrete set of points in which the functions are assigned a value. Outside this discrete set of points, the functions are not defined, although it is assumed that functionals such as an integral can be calculated, with the understanding that the value at a point represents a mean value within a grid interval.

The situation is different in integral methods such as the one described in refs. 7 and 8. Here one is not necessarily restricted to assigning values only to a discrete set of points. Although for reasons of simplicity it is advisable to assign a constant value to functions within each grid interval, as well as to the integral nucleus multiplying the function itself, the quantities thus defined can be considered piecewise continuous and defined at all points within the interval. This has not only a mathematical significance, but also a physical meaning, in the sense that if the function represents, for instance, the distribution of particle velocities, we assume that there are the same number of particles for any equal subintervals within a grid interval. In fact it can be said that at this stage, taking all functions defined within a grid interval as constant is the only approximation considered in the method. One might even eventually consider linear or parabolic functions within the grid intervals for a better approximation, but we believe it is computationally simpler and probably more accurate for equivalent computation times to just subdivide the original grid for improved accuracy, keeping the mentioned constant-functions approximation.

We will now illustrate the above considerations in the light of Eq. (1), which constitutes our starting point. For the case to be considered a, a' stand for the particle velocities defined within the grid boundaries, and will

refer in the present paper to the scalar variable $v=(v_x^2+v_y^2+v_z^2)^{1/2}$ since just the spherically symmetric case will be considered in the applications.

If we followed the approximation taken in finite-difference methods, as was done in refs. 7 and 8 for simplicity, the function $f(a, t)$ might be decomposed in the form

$$f(a, t) \sim \sum f(a_I, t)\, \delta(a-a_I) \tag{3}$$

so that once the analytical expression for the transition probability is known, the integration can be immediately carried out.

As just mentioned, in an integral method it is both possible and more convenient to calculate the evolution of each of the continuous (constant) functions, which will be now defined within each grid interval at a certain fixed time, as follows:

$$\begin{aligned} &f_I(a)=f_I \qquad \text{for} \quad a_I-\frac{\Delta a}{2}<a<a_I+\frac{\Delta a}{2} \\ &f_I(a)=0 \qquad \text{otherwise} \end{aligned} \tag{4}$$

The border points for each interval have a zero contribution to the integral (1), so they need not be considered.

The function defined in (4) will be called a square pulse. Its time evolution through Eq. (1) will clearly constitute the basis of the method, since any function can be decomposed (following our basic approximation) into a set of square pulses.

As was stressed in the Introduction, we will restrict ourselves to those probability functions $P(a, t+\Delta t \mid a, t)$ whose moments can be calculated, and in particular to situations in which neglecting moments higher than second order per unit time is justified, and the transition probability can be expressed by means of (2). It will be convenient for the following to rewrite P in the form

$$P(a, t+\Delta t \mid a', t)=\frac{1}{2\sigma\sqrt{\pi}} \exp\left\{-\frac{[a-a'(t+\Delta t)]^2}{2\sigma}\right\} \tag{5}$$

Where we have defined $\sigma=(D\Delta t)^{1/2}$ and the expression $a'(t+\Delta t)$ is used to mean

$$a'(t+\Delta t)=a'+A(a')\,\Delta t \tag{6}$$

Since the transition probability at each grid interval is thus defined by the local values of the two moments, that is, by A and D, it would seem that in principle the evolution of each square pulse might be predicted with all

generality by means of a sufficiently detailed set of functions formed by applying (2) to a generic square pulse, that is, by functions $F_I(a, \sigma, A)$.

There are two reasons why we have not found it advisable to follow this procedure for the numerical implementation of our method.

First of all, from a practical point of view, it is extremely difficult to create a reliable scheme that approximates the functions $F_I(a, \sigma, A)$ in the grid space, particularly at the boundaries. But also, one cannot actually consider the functions $F_I(a, \sigma, A)$ as a set of completely independent entities. It is true that the diffusion D contained in σ can be given an arbitrary value at each grid interval. But the same cannot be said for A, since its actual value is well known to depend in the general case on the D derivative (a term sometimes called the spurious drift). So in the numerical approximation in which derivatives are formed by linear combinations of values at adjacent grid intervals, the actual A value at I must be made to depend on the values we assign to D at grid points $I+1$ and $I-1$. In other words, in the numerical approximation the functions $F_I(a, \sigma, A)$ cannot be defined as strictly local entities, independent of one another.

There is one very convenient way of doing away with these problems, to be fully described in next section. It consists in splitting the time step into two different operations which we will call diffusion and convection. This is computationally much simpler than doing both operations at a time as suggested above. For the strictly diffusive step, it is quite natural to define a set of functions $F_I(a, \sigma)$ at each grid interval expressing the time evolution of a "square pulse" $f_I(a)$ for a certain D and t. These functions $F_I(a, \sigma)$ are strictly local entities. Also, implementing their evolution in a convenient numerical scheme is not difficult. Once this is done, it is also numerically very easy to carry out a "convective step," which amounts to relocating the diffused square pulses to translated positions at distances $A\Delta t$, where A is calculated at each grid point.

Splitting the time step in the mentioned way implies of course that one is commiting a certain error. It can be shown, however, that the error is of order Δt with respect to the exact zeroth-order result. We have checked this procedure in other, simpler numerical schemes, particularly the Ornstein–Uhlenbeck process, with excellent results. The final stationary solution approximates the exact result with all the desired accuracy for refined grids and reasonable time steps. An independent check is that it makes no practical difference in the system evolution when the order of both operations is commuted.

We will now describe how these approximations have been applied to our general problem.

3. IMPLEMENTING THE TIME ADVANCING SCHEME

It will be sufficient, as said above, to deal with a generic square pulse $f_I(a)$, since our distribution functions $f(a, t)$ are assumed to be always approximated by a set of $f_I(a)$ specified in (4).

Their time evolution is easily calculated by use of the transition probability P:

$$F_I(a, t) = \int_{-\infty}^{\infty} P(a, t + \Delta t \mid a', t)\, f_I(a')\, da' \tag{7}$$

If we use the transition probability defined in (5), the integration can be immediately performed, with the result

$$F_I(a, \sigma) = \frac{f_I}{2}\left[\operatorname{Erf}\left(\frac{a - a_I'(t + \Delta t) + \Delta a/2}{2\sigma_I}\right) - \operatorname{Erf}\left(\frac{a - a_I'(t + \Delta t) - \Delta a/2}{2\sigma_I}\right)\right]$$

Equation (7) constitutes the basis of our numerical treatment of the problem. Figure 1 shows typical shapes of $F_I(a, \sigma)$ for different σ values or, equivalently (for fixed diffusion coefficient D), at different times when just diffusion is present and $a_I = 0$.

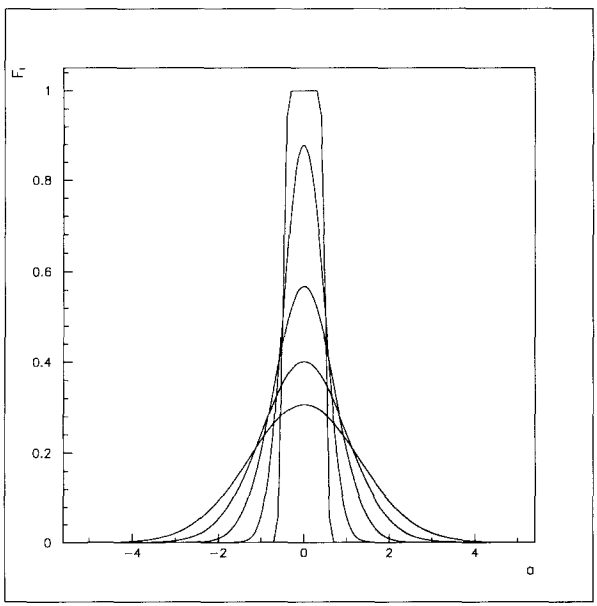

Fig. 1. Exact diffusive evolution of a "square pulse" distribution. For long times the resulting distribution approximates a Gaussian. It can be appreciated that the total diffusion up to distances spanning 4 grid intervals at each side of the square pulse can account for practically all the total norm even when the initial square pulse has lost over two-thirds of its initial norm.

In the general case in which we have diffusion plus convection, i.e., when the position of the diffusive curve center a'_I changes with time, the $F_I(a, \sigma)$ shapes will be identical to the ones shown, only shifted to the new position of its center after time Δt, which we have simply called here $a'_I(t + \Delta t)$ in order not to introduce explicitly the convective term A in this generic illustrative description.

We have already explained, however, in Section 2 that it is more convenient to split this combination of diffusion + translation process just described into its two constitutive parts.

It is convenient at this point to call attention to one fact. In a discrete description, and for no matter what numerical scheme, translating the value of a function at a grid point or interval I to a new position, say J (i.e., "convection"), inevitably produces some information spread, since in general the value at the original I will be distributed into two new locations. The smaller the time step, the more pronounced the cumulative dispersive effect will be. Diffusion, on the other hand, can be faithfully described in our particular integral scheme for any time step, as shown in Fig. 1. Thus, for our scheme, large time increments are from this point of view to be preferred. We will qualify in the next section this fact from other practical limitations.

We now proceed to examine in detail the two basic operations.

3.1. Diffusion

In order to calculate the diffusive contribution of $F_I(a, \sigma)$ to other grid intervals, we just need to integrate this function for different σ values along the different intervals adjacent to I.

Let us recall that almost universally numerical differential schemes just consider diffusion from the grid interval I to $I \pm 1$ at each time step. One is not restricted to such "3-point schemes" in an integral numerical method.

It is to be expected that in practice some limit must be fixed for the convenient number of contributing points. For reasons that now will become clear "9-point schemes" are probably the best choice balancing simplicity, accuracy, and generality in diffusive processes.

Since the time evolution of $F_I(a, \sigma)$ is "universal" once the grid spacing is chosen, because only its normalization changes from point to point, all one needs to have, in order to implement the method numerically, is a set of constants which will be defined for $D = 1$ and different times specified by k, as

$$C_1(\sigma_k) = \int_{a_I + \Delta a/2}^{a_I + 3\Delta a/2} [F_I(a, \sigma_k)/f_I]\, da \tag{9}$$

In general

$$C_J(\sigma_k) = \int_{a_I + J\Delta a/2}^{a_I + (J+1)\Delta a/2} [F_I(a, \sigma_k)/f_I]\, da \tag{10}$$

These functions are shown in Fig. 2, where they have been plotted as functions of a continuous σ, although the dots correspond to equal time increments (recall that σ is proportional to $\sqrt{t}$).

It can be seen in Fig. 2 that for $\sigma = 1$, about 80% of the initial central interval diffuses to the set of nine grid points, with completely negligible amounts going into the next two, not considered in our approximation.

The time step corresponding to the huge diffusive loss inherent to $\sigma = 1$ will be in general much larger than the time steps considered in other numerical schemes. Therefore it can be said that taking $\sigma = 1$ and limiting to 9 the number of neighboring intervals into which the diffusive contribution is evaluated are reasonable upper limits if we wish to set up an efficient scheme for diffusive processes with an integral method.

The numerical program should start by reading a table with the $C_J(\sigma)$ values and proceed to adjust the actual diffusion for a certain σ by linear interpolation.

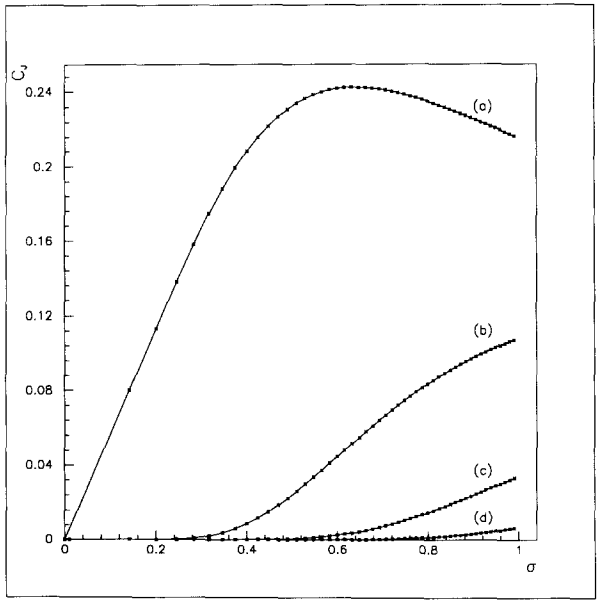

Fig. 2. (a–d) Percentage of initial square pulse norm going into grid intervals respectively first-, second-, third-, and fourth-rank neighbors to the initial square pulse occupying one grid interval.

It should be noted that $C_1(\sigma)$ is amazingly linear up to $\sigma \leqslant 0.25$, which corresponds to a central norm loss of about 25%.

This justifies the linear interpolation for small σ values, where the table points (which are taken proportional to time intervals) are sparse, while at large σ values the points are sufficiently close to minimize the errors. It also shows that a 3-point integral scheme can be considerably accurate if $\sigma \leqslant 0.25$ for each time step. However, the numerical method we are describing is so simple to implement and so fast that there does not seem to be much purpose in thus limiting the time step.

3.2. Convection

Once the diffusive part of the problem is solved, we must consider convection. A detailed discussion of the general problem (diffusion + convection) in the light of the transition probability is now in order.

Let us start our discussion by expressing the first moment with the two terms constituting the quantity A: the so-called "friction" force term and the "diffusive" force term (spurious drift)

$$A(a) = B(a) + \frac{1}{2}\frac{\partial D(a)}{\partial a} \tag{11}$$

In those cases in which external forces exist, these external forces would be included in the term B together with the corresponding "friction forces." The two contributions to A appearing in (11) are best understood in terms of Langevin's equation for each set described by a:

$$\frac{da}{dt} = B(a) + [D(a)]^{1/2}\, \Gamma(t) \tag{12}$$

where $\Gamma(t)$ are Gaussian random variables satisfying

$$\langle \Gamma(t) \rangle = 0, \qquad \langle \Gamma(u)\, \Gamma(v) \rangle = 2\delta(u - v) \tag{13}$$

From these equations, Eq. (11) is well known to follow in first-order approximation in Δt, and Γ^2.

It should be mentioned that within the assumptions made in the Introduction to justify our definition of the transition probability in the nonlinear kinetic case, the Langevin description would be in fact equivalent to our integral formulation and to the Fokker–Planck approach in the sense that they all contain in different forms (for each instant t) the same information about the statistical ensemble. The information is contained in the

first and second moments A and D, which must be reevaluated at each time step.

When we try to implement the situation described by any of these equations with a time-advancing numerical scheme, we find that it is of course impossible to have infinitesimally small time steps. Also, the function D is no longer continuous through the range of a, so rigurously speaking, the numerical realization is not possible: we can only approximate it.

Let us try to outline what kind of approximations can be made that are physically interesting for our purpose.

A very important consequence of having for the numerical description a finite correlation time in (11) is that the expectation value of $\langle(\Delta a)^2\rangle$ is no longer exactly 2D. For those cases where just diffusion is present, this may not seem very important. But particularly when we also have the convective friction term, the physical relevance of the numerical treatment becomes somewhat impaired.

We can see why, if we consider, for example, an isolated system. For such systems, the transition probability P should preserve the number of particles and the total energy. We would also like our numerical schemes to preserve these quantities. However, exact energy conservation depends on the delicate balance between diffusion and convection. In general, convection, as provided in (11), depends on friction but also on diffusion, so a defective evaluation of diffusion is bound to affect the mentioned necessary balance in our approximate "direct" calculation. Thus, energy will no longer be conserved unless some other action is taken as explained below. Lack of energy conservation is of course what we find in practice. Even if we force the norm to be exactly conserved, energy is not.

We will see in next section that one of the features making integral methods attractive is that they are sufficiently flexible to allow corrective actions capable of continuously readdressing the system to an energy-conserving time evolution.

For the numerical implementation of the convective process, now consisting in a translation of each grid content to a new location, we use the simplest choice of two-diagonal matrices. Writing a numerical algorithm capable of placing the content of a grid interval in different (generally two) grid positions with no loss of norm is a trivial matter. Since the time increments used for diffusion are generally very large, the information spread resulting from the convective process is now minimized.

There are several approximations inherent to this factoring prescription.

In the first place, we are taking for convection at time $t+\Delta t$ its constitutive values of friction and diffusion that belong to time t. In general

these values are assumed to change only slowly, so this first-order approximation is justified.

Second, and more important, for large convective values we must assume that the value of convection calculated in grid point I will be valid for grid point J, even when J is several grid intervals apart. In cases such as the Ornstein–Uhlenbeck process where convection is proportional to a, the errors might be inadmissible close to the origin for large convective values. Therefore, even if the numerical process introduces no technical difficulties, the results must be always judged taking into account the approximations made, and the time increment should be chosen so that the approximation obtained is acceptable.

4. ADVANCING IN TIME A SPHERICALLY SYMMETRIC PLASMA DISTRIBUTION

We will now test the physical and numerical integral approach through the solution of a particular problem.

The transition probability P for kinetic processes governed by Coulomb forces is defined at a certain time t by a diffusion matrix and a convective vector which can be expressed through the Rosenbluth potentials,[1]

$$\Phi(\mathbf{v}, t) = -\frac{1}{4\pi}\int \frac{f(\mathbf{u}, t)}{|\mathbf{v}-\mathbf{u}|}\, d^3u$$

$$\Psi(\mathbf{v}, t) = -\frac{1}{8\pi}\int f(\mathbf{u}, t)|\mathbf{v}-\mathbf{u}|\, d^3u$$

Through these definitions (in the convenient form adopted by Trubnikov[9]) the first and second moments are expressed as

$$D_{ik}(\mathbf{v}, t) = \frac{1}{2}\langle \Delta v_i\, \Delta v_k\rangle = -L^{e/e}\frac{\partial^2 \Psi}{\partial v_i\, \partial v_k}$$

$$A_i(\mathbf{v}, t) = \langle \Delta v_i\rangle = -2L^{e/e}\frac{\partial \Phi}{\partial v_i} \tag{14}$$

$$i, k = 1, 2, 3$$

where $L^{e/e} = \lambda(4\pi e^2/m_e)^2$ and λ stands for the well-known "Coulomb logarithm" used in plasma physics.

It has been shown elsewhere[7,8] that the general three-dimensional transition probability[5]

$$P(\mathbf{v}, t+\Delta t \mid \mathbf{v}', t) = \frac{1}{(4\pi\Delta t)^{3/2}\{\mathrm{Det}[D_{sl}(\mathbf{v}', t)]\}^{1/2}} \times \exp - \frac{[v_j - v_j' - A_j(\mathbf{v}', t)\,\Delta t][D^{-1}(\mathbf{v}', t)]_{jk}[v_k - v_k' - A_k(\mathbf{v}', t)\,\Delta t]}{4\Delta t} \tag{15}$$

can be used to advance in time a distribution function. For the case of initial spherical distribution, the evolution leads to a Gaussian with good approximation. The problem is thus solved in fact with much more generality than is actually needed, since a difficult angular integration must be performed in spherical coordinates, even for the simple case of spherical symmetry.

There is therefore in the above approach a severe penalty for the integral method compared with the differential schemes, because the equivalent differential Fokker–Planck equation reduces to a simple form in which no trace of the angular variables remains. It is thus a considerable success that the integral method works properly, and its power shows in that it can reach a stationary solution with exact energy conservation. Yet, in practice, when conservation of energy is not essential, the differential method is simpler for the mentioned reason.

In the present paper we set up a different approach to the same problem.

If we are dealing at all times with a spherically symmetric situation, we should try to find a spherically symmetric transition probability operator that describes the changes taking place in the distribution function of velocities from time t to time $t+\Delta t$. This should alleviate the integration problem, converting it into a strictly one-dimensional operation.

Clearly, carrying out the angular integration in (15) if we write it in spherical coordinates will not give us the desired operator, because the transition would take place from a distribution $v'^2 f(v')$ to a distribution $f(v)$.

What we need is an expression for P, operating the transition from $v'^2 f(v')$ to $v^2 f(v)$. Let us see how this expression can be found.

The only basic requirement is to calculate first and second moments of P. Once these are obtained, the expression for P will be the standard one described in (2).

One simple way to proceed is to write down a one-dimensional Fokker–Planck equation for the distribution $F(v, t) = v^2 f(v, t)$. It is not

hard to achieve this if we use well-known properties of Φ and Ψ to write the ordinary spherically symmetric equation in dimensionless units:

$$\frac{\partial f}{\partial t}=\frac{1}{v^2}\frac{\partial}{\partial v}\left[v^2\left(\frac{\partial \Phi}{\partial v}f-\frac{\partial^2 \Psi}{\partial v^2}\frac{\partial f}{\partial v}?\right]\right. \tag{16}$$

in the form

$$\frac{\partial F}{\partial t}=\frac{\partial}{\partial v}\left[2\left(\frac{\partial \Phi}{\partial v}+\frac{1}{v^2}\frac{\partial \Psi}{\partial v}\right)F-\frac{\partial}{\partial v}\left(\frac{\partial^2 \Psi}{\partial v^2}F\right)\right] \tag{17}$$

Although this equation is identical to (16), it is written in "Fokker–Planck form." This means that we can immediately identify the first and second moments of P, $\langle \Delta v\rangle$, and $\langle \Delta v\, \Delta v\,\rangle$, as

$$-\left(\frac{\partial \Phi}{\partial v}+\frac{1}{v^2}\frac{\partial \Psi}{\partial v}\right) \qquad \text{and} \qquad -\left(2\frac{\partial^2 \Psi}{\partial v^2}\right)$$

just readinig off the coefficients of the first and the second term in the RHS.

Once this has been achieved, we can use the general theory developed above for the construction of an integral numerical scheme.

Before doing so, however, it is convenient to make some comments about the nature of the problem.

From the viewpoint of numerical treatment of partial differential equations, (17) appears extremely hard to solve because of its boundary condition at the origin, where both the function and its derivative vanish.

It is thus rather ironic that there exists the alternative (16) to Eq. (17) which happens to be much simpler to solve from the point of view of numerical computation. For it is (17) that is written in the explicit Fokker–Planck form, while (16) is obviously not. Unfortunately, however, while (16) is easy to solve numerically with differential methods, it is unsuitable for our integral procedure, which is based on knowledge of the transition probability operator (2).

In any case, the difficulties of the problem are a test for the capacity of the method to cope with very general situations. It is interesting that the integral method for solving the equivalent to Eq. (17) allows us in a very direct way to follow the physics of the situation and the limitations of the numerical approximations that are made. This is a consequence of having the evolution described by its two basic features, diffusion and convection, which are blurred in the simpler description (16), but quite clear in (17).

We will now describe the results of numerical computation by our integral method, applied to Eq. (17). Since the initial conditions should be lost in the subsequent evolution, we will always take for simplicity a step function for $f(v)$ at time $t=0$, with the grid large enough so that the tails

are vanishingly small at the grid edge, and no appreciable norm is lost in the iteration.

As might be expected, the evolution takes place without any particularly distinctive feature except at the origin.

Since the method can run expediently with any desirable time step, let us see what it shows in practice. One immediately realizes that reasonable changes in the time step have no great consequence for diffusion, because diffusion changes with the square root of time. Convection on the contrary changes dramatically, since it increases linearly with time. In particular, at the origin, its content can jump a number of grid points, literally emptying out the central grid intervals at each time step. This is, however, unphysical, as mentioned in our general discussion, since we are extrapolating the large values convection reaches at the center (in fact it becomes divergent) to regions where it would be much smaller. So we can wildly overestimate convection and end up in very few time steps at solutions having no relation with reality.

On the other hand, if one takes very small time steps, diffusion is primed with respect to convection, which becomes insignificant. There is here a clear case of the mentioned loss of information associated inevitably with convection in numerical schemes and seldom referred to.

When small convection steps are repeated many times, they amount in practice to diffusion. (Consider the origin content: each time step some of it advances to a further grid interval. Progressively it ends up having a Gaussian shape which for small time increments can be centered at the origin itself. Only if convection is large enough is it centered at further intervals. Thus, if there is diffusion from, say, the second interval toward the origin, the "small time interval effect" can make the origin grow abnormally.)

One thus observes (see Fig. 3A) for too small Δt the inability of the scheme to convect away the diffusion accumulating at the central region, which is seen to grow with an unphysical slope. This is incidentally the same type of solution which obtains with differential scheme solutions of Eq. (17) because of their inability to cope properly with the central boundary conditions. (These schemes are unable to reach the situation described above for large Δt in which large convection overtakes diffusion. The reason lies in that these cases must be described by means of transition matrices having nonzero diagonals far from the central ones, and such matrices are not present in ordinary differential numerical descriptions.)

It is thus quite understandable that the time increment must be chosen carefully if we wish to reproduce the balance between diffusion and convection which takes place at the origin when the physical Gaussian solution is reached.

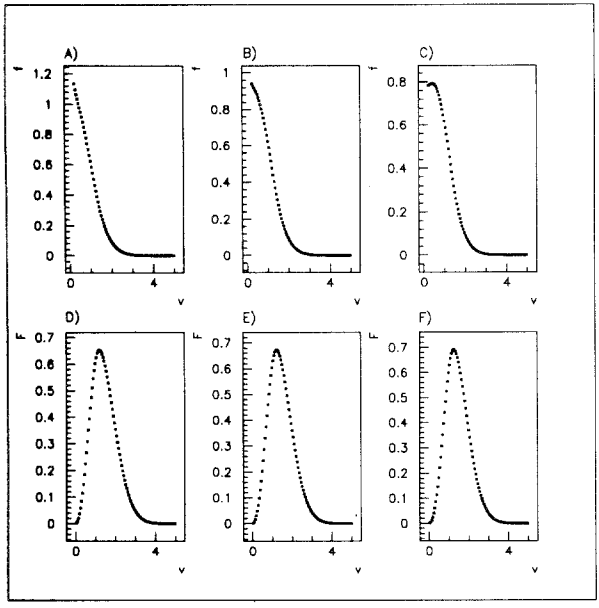

Fig. 3. Stationary solutions of Eq. (1) corresponding to Eq. (17) for different advancing time increments. (A–C) Solutions corresponding to the expected Gaussian shapes in $f(v) = F(v)/v^2$. (D–F) Solutions corresponding to $F(v)$. The time intervals chosen were respectively $\Delta T =$ 0.0015, 0.00175, 0.0020. The $f(v)$ values for the first grid interval are stationary but have large errors (they fall out of scale in A). These errors do not appear in the $F(v)$, which is the actual function advanced in (1). The reason for the different central behavior in A–C is explained in the text.

There is more, however, to the problem if we are looking for a completely satisfactory solution. Since our system is an isolated one, its evolution being governed by self-diffusion and convection in velocity space, energy is physically conserved. Calculating the evolution of energy in the numerical solution shows generally an energy increase. This is associated with the numerical inaccuracy in matching the proper amount of convection to balance the energy increase associated with diffusion, as was mentioned in Section 3.

The solution to this problem can be found, as was done elsewhere,[7,8] in an adjustment of convection by means of some parameter.

The adjustment is made at each time step so that the system is constantly reconducted to its energy-conserving path. When this procedure converges, the solution obtained is unique and leads to a Gaussian as expected.

In practice, we multiply the friction part of diffusion by a convenient function obtained after some adjustment, which we will call the "correla-

tion function" since it should adjust the proper numerical amount of friction to the amount of numerical diffusion. It contains one single parameter adjusting itself at each time step in the energy-conserving direction.

The correlation function $C(v)$ used for the runs shown in Fig. 3 is

$$C(v) = [1 + c(t) \exp(av^b)]^{1/2} \tag{18}$$

where a, b are fixed numbers and the self-adjusting parameter $c(t)$ is calculated in the program at each time step as a function of the energy error $E(0) - E(t)$ by

$$c(t + \Delta t) = c(t) + \{k[E(0) - E(t)]\}^3$$

The energy evolution with this convenient "ansatz" (certainly not unique), with k a constant number, becomes oscillatory with decreasing amplitude until it completely stabilizes at $c(t)$ values close to 1.

We have already discussed the theoretical justification for this numerical procedure. In the particular problem we are considering, there is another reason to believe that some adjustment of the "local" numerical scheme is necessary. By local we understand transitions to only close positions in the grid.

The point is that for the set of particles of lowest energy, there may be an incompatibility between two different assumptions: the physical assumption of small momentum transfer in all transitions, and the numerical assumption that limits interaction to particles occupying neighboring boxes.

In fact, the particles in any of these boxes can spread to the set of three contiguous grid intervals with conservation of particle number and energy, except at the origin, where this is impossible. Thus, in order to have overall numerical energy conservation, there must be some interaction between the lowest energy particles and some particles further out (not immediately close) in the grid. Many possibilities are then open, which of course modify the whole numerical description of the overall interaction.

We stress that this problem is of course also present in the numerical differential description with finite differences, which also does not conserve energy.

A great practical advantage of our integral method is that taking corrective actions as the one just described is straightforward and causes no numerical difficulties because of the positive-definite nature of all the processes. It is not clear that a similar corrective action can be taken in practice for the differential description. The reason is that integration of transition probabilities deals always with positive numbers, while differen-

tiation does not. Avoiding numerical instabilities introduced by a corrective function in a differential method is probably difficult.

In any case, our main point is that a corrective "correlation function" is not only justified in practice, but also deeply rooted in the physics of the problem. Somehow a strict locality of interactions in velocity space must be relaxed. In particular the lowest energy particles can be removed from their grid position by high-energy particles losing small amounts of energy, which redefines the interaction in the whole grid. This "second-order effect" is essential for the conservation of energy and is carried out successfully by our corrective "correlation function."

5. DISCUSSION OF NUMERICAL RESULTS, AND CONCLUSIONS

Some of the numerical results have already been described in relation to Fig. 3. Other points will now be conveniently detailed.

The outcome of the numerical problem solving the integral equation (1), equivalent to the differential equation (17), is contained in Fig. 3. There is one large difference between the solutions to Eqs. (16) and (17), in that in the latter one the grid points correspond to equal densities in velocity space. Thus, in order to obtain Figs. 3A–3C from Figs. 3D–3F, we must divide by v^2. Clearly, the points close to the origin must be expected to have very large errors, although in reality these errors correspond to a vanishingly small population. If the time increment is changed, the shape corresponding to Figs. 3D–3F is practically unchanged. The behavior of the origin in Figs. 3A–3C, on the other hand, changes appreciably. For smaller time increments the points close to the origin are enhanced, and for larger time increments they are depressed. Except for these few points, the rest of the curve is, for a large range of time increments, a Gaussian. The reasons for this numerical behavior have been extensively discussed in Section 4.

The total energy time evolution is shown in Fig. 4. As mentioned above, although there is considerable freedom in the choice of the correlation function, and our choice was guided by the phenomenological criterion of optimizing the results, it is clear that the problem is physically meaningful and we plan to study which functions $C(v)$ can be expected to best correct the errors introduced by the numerical approximation.

In practice, a correlation function $C(v)$ can be considered adequate when it does not perturb the distribution function shape, and preserves its smooth evolution toward the Gaussian equilibrium. On the other hand, the dynamic process of varying $c(t)$ must be tuned to obtain a damped oscillatory behavior. Both objectives were achieved quite satisfactorily with

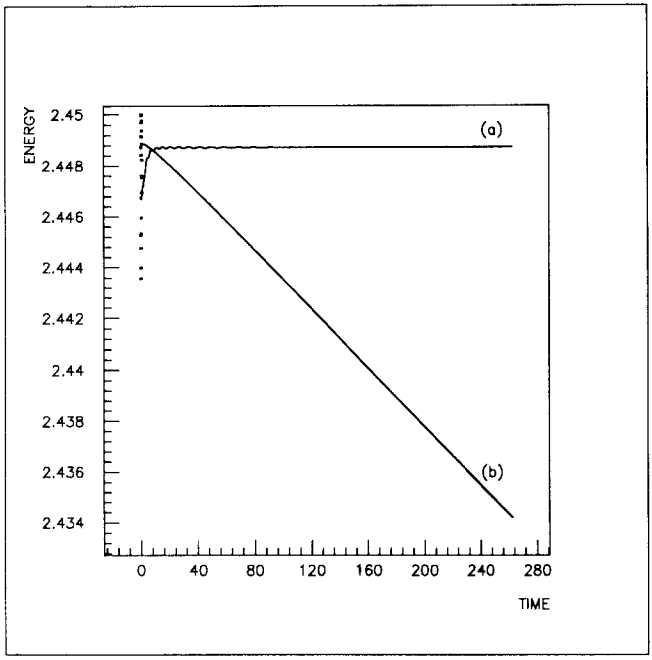

Fig. 4. Energy evolution for integral and differential numerical solutions. (The initial oversized transient oscillatory behavior in the integral solution is expected to be suppressed in improved choices of the "correlation parameter"). (a) Integral solution, (b) differential solution.

(18) in the results shown in Fig. 4. Besides conserving energy exactly, it shows energy conservation throughout the whole evolution, and absolute final stability for any length of computation times at exactly the initial energy.

The most significant success of the numerical method can be seen in Fig. 5. The tail behavior is very good, as shown in the general tendency of the function $F(v^2, t)/v^2$ to a Gaussian throughout the whole v domain in the logarithmic representation.

Finally, we should comment about the computational efficiency of the method.

The comparison is not completely fair in this case, since Eq. (17) does not seem soluble by ordinary numerical differential methods because of the origin boundary condition. Since its equivalent, the simpler equation (16), is the closest one that can be solved, we have chosen it to benchmark computation times.

The differential equation was solved with a predictor (explicit)–

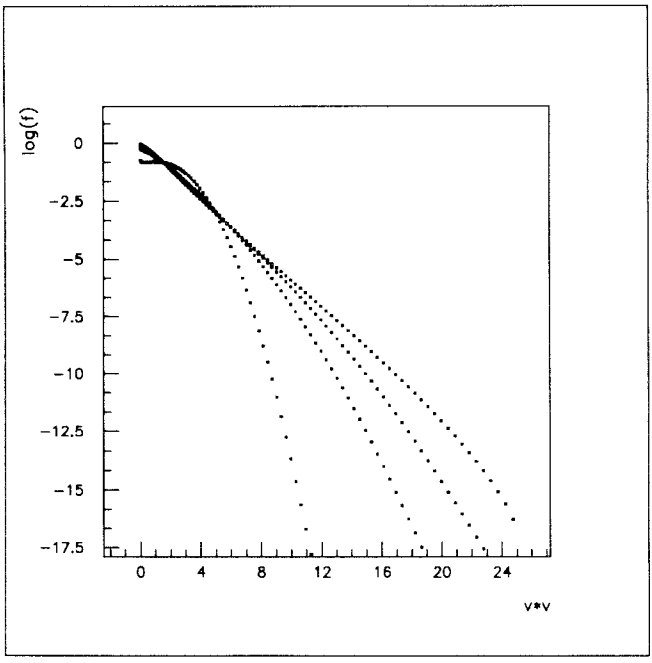

Fig. 5. Time evolution of $\log f(v)$ vs. v^2 for $\Delta t = 0.00175$ for 200, 1000, 2000, and 10,000 iterations. After 10,000 iterations the situation is stationary.

corrector (Crank–Nicholson) method, in which the nonlinear coefficients are calculated at half time step to preserve the second-order precission of this scheme. The time increments were the same in both cases. The computation times were in the ratio 5/6 in favor of the differential scheme. This should be attributed to the differential scheme being a 3-point scheme, while the integral scheme was our standard 9-point scheme with the time evolution split into a diffusive and a convective part.

Although the (nonoptimized) computation times are practically equal, there is an interesting difference to be remarked. The integral method diffusion is "exact" (in the numerical approximation) for each time step, while the diffusion produced in the finite-difference numerical solution is not. In fact, the diffusion for each grid interval is proportional to $\Delta t/(\Delta v)^2$ per time step in the finite-difference method, while it is proportional to the square root of this quantity in the integral method, as diffusion should always be [see in this relation our comments to Eq. (9), and Fig. 1].

It is only in the asymptotic time, after many time steps, that the differential method starts diffusing proportionally to the square root of time, while the integral method does so from the first time step. This fact

explains the apparent difference in the time evolution of both methods. Although the time steps are equal, the integral method advances faster because in practice $[\Delta t/(\Delta v)^2]^{1/2} \gg \Delta t/(\Delta v)^2$, and diffusion proceeds at a quite faster rate. Therefore, also the integral time scheme is in fact computationally much more efficient than the differential one. This fact is clearly shown in the logarithmic scale comparison of both methods (Fig. 6) after 1000 steps for the same time increment. Obviously the integral method advances much faster.

In conclusion, considering the three equivalent formulations of nonlinear kinetic processes, the time-dependent integral transition probability (1), the Fokker–Planck differential equation, and Langevin's stochastic method, it seems that the first one deserves strong attention as an alternative for approximate numerical methods, particularly because some of the technical difficulties associated with the numerical solution of differential equations (stability, boundary conditions, conserved quantities) seem to find clear, almost trivial possibilities for solution. This greater

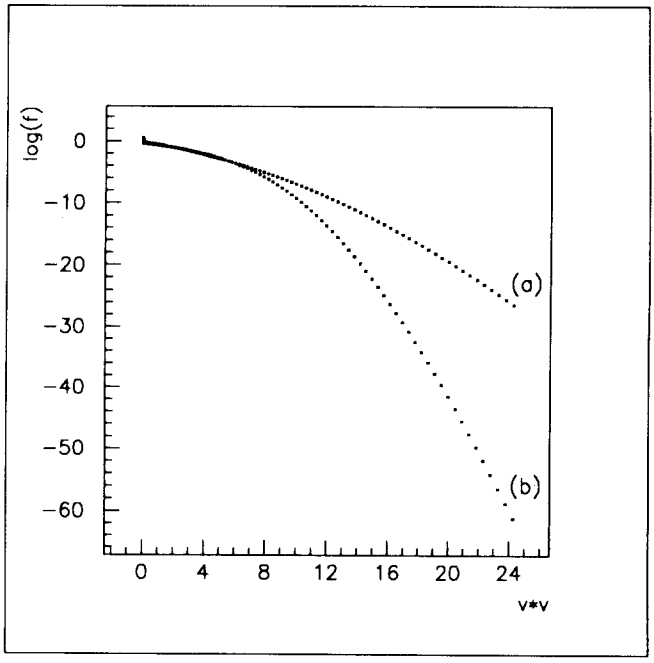

Fig. 6. Logarithmic scale distribution functions vs. v^2 after 1000 iterations. Diffusive evolution is faster in (a) the integral method than in (b) finite-difference schemes for the same time step $\Delta t = 0.00175$, as explained in the text.

flexibility allows one to concentrate on new ways to preserve in the numerical solution essential aspects of the physical processes, such as energy conservation.

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