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A Particle Method for Collisional Kinetic Equations. I. Basic Theory and One-Dimensional Results

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A new method is introduced for describing the collisional term in the framework of a particle scheme. The equations of motion of the particles contain an additional term which takes into account the collisions. Numerical techniques are shown to compute this extra term and to solve the equations. Exact results concerning stability and consistency of the schemes for the diffusion equation are derived. Some numerical results for the one-dimensional case are reported.

1. INTRODUCTION

Particle methods have been extensively used for solving a large variety of problems in many different areas [1, 11]. There is an increasing interest in treating collisional equations. In plasma physics the statistical effects of Coulomb collisions among ionized particles is described by a Fokker–Planck operator which introduces a "friction" and a "diffusion" in velocity space [7]. In semiconductor physics the collisions between the carrier and the lattice are described by a linear integral operator acting in the wave vector space [23]. Binary collisions in rarefied gas are described by the Boltzmann equation, through a nonlinear integral collisional operator [6].

The present particle schemes usually incorporate collisions by making a Monte Carlo simulation of the collision process [5, 16]. This approach is quite general and it reflects the physics of the process. The main drawback of the method is that it introduces large statistical fluctuations and an extremely large number of particles is required for an accurate simulation. Other more mathematical approaches have been proposed by several authors [8, 10, 13, 19, 17]. In [19], for example, position and velocity of the "macroparticle" satisfies the usual equation of motion of the collisionless case and the collisions affect the "weight" of the particles transferring mass from one particle to another.

Our approach is somehow different from the previous ones. The idea underlying the method is the following: we approximate the initial distribution in the phase

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space with a set of equi-weighted particles for each species. Then we move the particles according to equations of motion which are the equations for the collisionless case plus an additional term which is responsible for the change in the density function due to collisions. The method is a Lagrangian description of the kinetic equation and has the advantage of being deterministic and of automatically rezoning the irregular grid which has been determined by the particles. In this respect the technique has some resemblance with moving grid methods [2, 22] and moving finite element method [15, 9, 14]. The other advantage is that the contribution of the collisions is described by an additional term in the equations of motion that can be added to an existent code which treats the collisionless case.

In these paper we illustrate the general features of the method and make some applications to one-dimensional space homogeneous problems. In the case of the diffusion equation we show some rigorous results on the stability and consistency of the method. In a following paper, we shall treat multi-dimensional space inhomogeneous case and make applications to a variety of collisional operators.

The plan of the paper is the following: in Section 2 we describe the method and derive the equations of motion. In Section 3 we describe the one-dimensional space-homogeneous case and show how to treat boundary conditions and source terms (particle "creation" and "annihilation"). In Section 4 we apply the method to the one-dimensional heat equation and show some numerical results on the rate of convergence of the scheme. In Section 5 we show some result on the stability and consistency of the method applied to the diffusion equation. In Section 6 we apply the method to simplified models of a Fokker–Planck equation, a linear integro-differential equation (master equation) and a Boltzmann-like elquation (Kac equation). Finally, in Section 7 we draw conclusions.

2. Derivation of the Method

We consider a generic kinetic equation for a single specie:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = I[f], \tag{2.1}$$

where $f(\mathbf{x}, \mathbf{v}, t)$ is the density function in the phase space, $\mathbf{F}$ is the acceleration field, and $I[f]$ is a generic collisional operator.

We associate to the equation the initial condition:

$$f(\mathbf{x}, \mathbf{v}, 0) = f_0(\mathbf{x}, \mathbf{v}). \tag{2.2}$$

The acceleration field $\mathbf{F}$ may be an external field or a functional of f. In the latter

case we must supplement Eq. (2.1) with an equation relating $\mathbf{F}$ with f. In the Vlasov–Maxwell case, for example, it is

$$\mathbf{F} = \frac{e}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \tag{2.3}$$

and Eq. (2.1) is coupled with Maxwell's equations for $\mathbf{E}$ and $\mathbf{B}$.

In the collisionless case, Eq. (2.1) reduces to the Vlasov equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = 0. \tag{2.4}$$

It can be written in the "characteristic form,"

$$\frac{df}{dt} = 0, \tag{2.5}$$

on the "characteristic lines" $\mathscr{C}$ defined by:

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{v}, \\ \frac{d\mathbf{v}}{dt} &= \mathbf{F}. \end{aligned} \tag{2.6}$$

The solution of the Vlasov equation is given in a parametric form,

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= f_0(\mathbf{x}^0, \mathbf{v}^0), \\ \mathbf{x} = \mathbf{x}(\mathbf{x}^0, \mathbf{v}^0, t), &\qquad \mathbf{v} = \mathbf{v}(\mathbf{x}^0, \mathbf{v}^0, t), \end{aligned} \tag{2.7}$$

where the expressions for $\mathbf{x}$ and $\mathbf{v}$ are obtained by integrating equations (2.6). With particle methods one looks for a solution of Eq. (2.4) of the form:

$$f_{(N)}(\mathbf{x}, \mathbf{v}, t) = \sum_{i=1}^{N} w_i \, \delta(\mathbf{x} - \mathbf{x}_i) \, \delta(\mathbf{v} - \mathbf{v}_i). \tag{2.8}$$

This distribution is a weak solution of Eq. (2.4) provided $\mathbf{x}_i(t)$ and $\mathbf{v}_i(t)$ satisfy the characteristic equations (2.6). The initial conditions for equations (2.6) are the points $(\mathbf{x}_i^0, \mathbf{v}_i^0)$, which are determined by approximating the initial distribution (2.2) in an "optimal" way. Equations (2.6) are then solved numerically and the field $\mathbf{F}$ is evaluated self-consistently at each time step. The distribution of points $\mathbf{x}_i(t)$, $\mathbf{v}_i(t)$, interpreted as a discrete measure, is an approximation of the absolutely continuous measure with density $f(\mathbf{x}, \mathbf{v}, t)$. There are rigorous estimates on the error between the numerical discrete solution and the exact solution, which are based on a proper metric in the space of measures [18, 12].

The transformation (2.7), in particular, preserves integrals:

$$\frac{d}{dt}\int_{\mathscr{V}(t)} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v} = 0, \tag{2.9}$$

for any volume $\mathscr{V}$ in the phase space moving according to Eqs. (2.6).

We shall use this property as a starting point for the derivation of our method. Let us consider the full equation (2.1). We look for a transformation

$$\begin{aligned} \mathbf{x} &= \mathbf{x}(\mathbf{x}^0, \mathbf{v}^0, t), \\ \mathbf{v} &= \mathbf{v}(\mathbf{x}^0, \mathbf{v}^0, t), \end{aligned} \tag{2.10}$$

such that the property (2.9) is satisfied, for each volume $\mathscr{V}(t)$ of points moving according to (2.10), with constant $(\mathbf{x}^0, \mathbf{v}^0)$.

By applying the transport theorem to (2.9) we obtain

$$\begin{aligned} 0 &= \frac{d}{dt}\int_{\mathscr{V}(t)} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v} \\ &= \frac{d}{dt}\int_{\mathscr{V}(0)} f(\mathbf{x}(\mathbf{x}^0, \mathbf{v}^0, t), \mathbf{v}(\mathbf{x}^0, \mathbf{v}^0, t), t) J\, d\mathbf{x}^0\, d\mathbf{v}^0 \\ &= \int_{\mathscr{V}(0)} \left[\left(\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} f \cdot \frac{\partial \mathbf{x}}{\partial t} + \nabla_{\mathbf{v}} f \cdot \frac{\partial \mathbf{v}}{\partial t} \right) J + f \frac{dJ}{dt} \right] d\mathbf{x}^0\, d\mathbf{v}^0 \\ &= \int_{\mathscr{V}(0)} \left[\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot \left(f \frac{\partial \mathbf{x}}{\partial t} \right) + \nabla_{\mathbf{v}} \cdot \left(f \frac{\partial \mathbf{v}}{\partial t} \right) \right] J\, d\mathbf{x}^0\, d\mathbf{v}^0 \\ &= \int_{\mathscr{V}(t)} \left[\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot \left(f \frac{\partial \mathbf{x}}{\partial t} \right) + \nabla_{\mathbf{v}} \cdot \left(f \frac{\partial \mathbf{v}}{\partial t} \right) \right] d\mathbf{x}\, d\mathbf{v}, \end{aligned} \tag{2.11}$$

where

$$J = \frac{\partial(\mathbf{x}, \mathbf{v})}{\partial(\mathbf{x}^0, \mathbf{v}^0)} \tag{2.12}$$

is the Jacobian of the transformation and

$$\frac{\partial \mathbf{x}}{\partial t} = \left(\frac{\partial \mathbf{x}}{\partial t} \right)_{\mathbf{x}^0, \mathbf{v}^0 = \text{const}}, \qquad \frac{\partial \mathbf{v}}{\partial t} = \left(\frac{\partial \mathbf{v}}{\partial t} \right)_{\mathbf{x}^0, \mathbf{v}^0 = \text{const}} \tag{2.13}$$

The relation

$$\frac{dJ}{dt} = J \left(\nabla_{\mathbf{x}} \cdot \frac{\partial \mathbf{x}}{\partial t} + \nabla_{\mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} \right)$$

has been used. From the arbitrariness of $\mathscr{V}$ it follows:

$$\frac{\partial f}{\partial t}+\nabla_{\mathbf{x}}\cdot\left(f\frac{\partial \mathbf{x}}{\partial t}\right)+\nabla_{\mathbf{v}}\cdot\left(f\frac{\partial \mathbf{v}}{\partial t}\right)=0. \tag{2.14}$$

Equation (2.1) can be written in the form

$$\frac{\partial f}{\partial t}+\nabla_{\mathbf{x}}\cdot(f\mathbf{v})+\nabla_{\mathbf{v}}\cdot(f\mathbf{F})=I[f] \tag{2.15}$$

because $\nabla_{\mathbf{x}}\cdot\mathbf{v}=0$, $\nabla_{\mathbf{v}}\cdot\mathbf{F}=0$. Subtracting (2.14) from (2.15) we obtain

$$\nabla_{\mathbf{x}}\cdot\left[\left(\mathbf{v}-\frac{\partial \mathbf{x}}{\partial t}\right)f\right]+\nabla_{\mathbf{v}}\cdot\left[\left(\mathbf{F}-\frac{\partial \mathbf{v}}{\partial t}\right)f\right]=I[f]. \tag{2.16}$$

The equations of motion are therefore

$$\frac{\partial \mathbf{x}}{\partial t}=\mathbf{v}+\frac{1}{f}(\nabla_{\mathbf{x}}\times\mathbf{A}+\mathbf{h}), \tag{2.17}$$

$$\frac{\partial \mathbf{v}}{\partial t}=\mathbf{F}+\frac{1}{f}(\nabla_{\mathbf{v}}\times\mathbf{B}+\mathbf{k}), \tag{2.18}$$

where $\mathbf{A}$ and $\mathbf{B}$ are arbitrary vectors and $(\mathbf{h}, \mathbf{k})$ satisfy the equations:

$$\nabla_{\mathbf{x}}\cdot\mathbf{h}+\nabla_{\mathbf{v}}\cdot\mathbf{k}=-I[f], \tag{2.19}$$

$$\nabla_{\mathbf{x}}\times\mathbf{h}=0, \qquad \nabla_{\mathbf{v}}\times\mathbf{k}=0. \tag{2.20}$$

Equations (2.19)–(2.20) do not define uniquely the two fields $\mathbf{h}$ and $\mathbf{k}$. If the operator $I[f]$ acts in velocity space (which is often the case) then a natural choice is

$$\begin{aligned}\mathbf{h}&=0,\\ \nabla_{\mathbf{v}}\cdot\mathbf{k}&=-I[f].\end{aligned} \tag{2.21}$$

Equations (2.17)–(2.18) define a transformation of the form (2.10) that has the property (2.9). If such a transformation is computed then the function $f(\mathbf{x}, \mathbf{v}, t)$ can be reconstructed: from (2.11) it follows that

$$f(\mathbf{x}, \mathbf{v}, t)=f(\mathbf{x}^0, \mathbf{v}^0, 0)/J(\mathbf{x}^0, \mathbf{v}^0, t). \tag{2.22}$$

Such a transformation, of course, is not unique and this is expressed by the arbitrary quantities in Eqs. (2.17)–(2.18). Making a particular choice for the fields $\mathbf{A}$, $\mathbf{B}$, $\mathbf{h}$, $\mathbf{k}$ merely means defining a particular parametrization of the solution (2.22). This arbitrary nature could be used to make the more convenient choice in each

particular case. A choice which appears to be natural is an irrotational flow given by

$$\mathbf{A} \equiv 0, \qquad \mathbf{B} \equiv 0, \tag{2.23}$$

together with conditions (2.21).

If the case of no boundary in the velocity space equations (2.21) can be solved in terms of Green's functions of the Laplacian operator,

$$k = -\int_{-\infty}^{v} I(\mathbf{x}, v', t)\, dv', \tag{2.24}$$

$$\mathbf{k} = \frac{1}{2\pi} \int_{R^2} \frac{I(\mathbf{x}, \mathbf{v}', t)(\mathbf{v} - \mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|^2}\, d\mathbf{v}', \tag{2.25}$$

$$\mathbf{k} = \frac{1}{4\pi} \int_{R^3} \frac{I(\mathbf{x}, \mathbf{v}', t)(\mathbf{v} - \mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|^3}\, d\mathbf{v}', \tag{2.26}$$

in the case, respectively, of one, two, and three dimensions in velocity space. Here $I[f]$ is considered a function of $(\mathbf{x}, \mathbf{v}, t)$.

Before considering the numerical discretization of the method let us make a remark on the regularity of the transformation (2.10). Suppose that $f(\mathbf{x}, \mathbf{v}, t)$ is defined in a set $\Omega \times [0, T]$, where Ω is an open set $\Omega \subseteq R^d$ (d is the dimension of our phase space). If f vanishes then the equations of motion have a divergent term, and the transformation (2.10) is no longer regular because the jacobian J diverges. Furthermore, the kind of singularity depends on the way f vanishes. In order to avoid this problem it is possible to regularize the transformation in the following way. Let $\phi(\mathbf{x}, \mathbf{v}, t)$ be a positive integrable function. Then we define a class of transformation of the form (2.10) imposing the property:

$$\frac{d}{dt} \int_{\gamma(t)} \psi(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v} = 0, \tag{2.27}$$

with $\psi(\mathbf{x}, \mathbf{v}, t) = f(\mathbf{x}, \mathbf{v}, t) + \phi(\mathbf{x}, \mathbf{v}, t)$.

Then, proceeding in the same way as before, we get the equations of motion for $\mathbf{x}(\mathbf{x}^0, \mathbf{v}^0, t)$, $\mathbf{v}(\mathbf{x}^0, \mathbf{v}^0, t)$

$$\frac{\partial \mathbf{x}}{\partial t} = \frac{f}{f + \phi} \mathbf{v} + \frac{1}{f + \phi} (\nabla_{\mathbf{x}} \times \mathbf{A} + \mathbf{h}), \tag{2.28}$$

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{f}{f + \phi} \mathbf{F} + \frac{1}{f + \phi} (\nabla_{\mathbf{v}} \times \mathbf{B} + \mathbf{k}), \tag{2.29}$$

where (2.19) is replaced by

$$\nabla_{\mathbf{x}} \cdot \mathbf{h} + \nabla_{\mathbf{v}} \cdot \mathbf{k} = -I[f] - \partial\phi/\partial t, \tag{2.19'}$$

Given the transformation, the function is reconstructed:

$$f(\mathbf{x}, \mathbf{v}, t) = \psi(\mathbf{x}^0, \mathbf{v}^0, 0)/J(\mathbf{x}^0, \mathbf{v}^0, t) - \phi(\mathbf{x}, \mathbf{v}, t). \tag{2.30}$$

If Ω is a compact domain then ϕ can be a constant. If Ω is unbounded then ϕ can be chosen in such a way to control the singularity of the transformation.

We mention here an alternative formulation of the equations, which has the advantage that it does not require the local evaluation of the function f. Let us consider a generic volume $\mathscr{V}$ in the phase space and let us denote by $(\hat{\mathbf{x}}, \hat{\mathbf{v}})$ the "center of mass" of such a volume:

$$\hat{\mathbf{x}} \int_{\mathscr{V}} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathscr{V}} \mathbf{x} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}, \tag{2.31}$$

$$\hat{\mathbf{v}} \int_{\mathscr{V}} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathscr{V}} \mathbf{v} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}. \tag{2.32}$$

Suppose that all the points of $\mathscr{V}$ move according to the transformation (2.10). Then, by taking the time derivatives of (2.31) and (2.32) we obtain, proceeding in a similar way as before,

$$\frac{d\hat{\mathbf{x}}}{dt} \int_{\mathscr{V}} f\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathscr{V}} \frac{\partial \mathbf{x}}{\partial t} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}, \tag{2.33}$$

$$\frac{d\hat{\mathbf{v}}}{dt} \int_{\mathscr{V}} f\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathscr{V}} \frac{\partial \mathbf{v}}{\partial t} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}, \tag{2.34}$$

where Eq. (2.14) has been used. Here $\hat{\mathbf{x}} = \hat{\mathbf{x}}(t)$ and $\hat{\mathbf{v}} = \hat{\mathbf{v}}(t)$ and $\partial \mathbf{x}/t$, $\partial \mathbf{v}/t$, defined in (2.13), are evaluated as functions of $(\mathbf{x}, \mathbf{v}, t)$. Note that

$$M_{\mathscr{V}} \equiv \int_{\mathscr{V}} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v} \tag{2.35}$$

does not depend on time. Substituting (2.17)–(2.18) and (2.23) into (2.33)–(2.34) gives the equations of motion,

$$\frac{d\hat{\mathbf{x}}}{dt} = \hat{\mathbf{v}} + \frac{\int_{\mathscr{V}} \mathbf{h}(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}}{M_{\mathscr{V}}}, \tag{2.36}$$

$$\frac{d\hat{\mathbf{v}}}{dt} = \hat{\mathbf{F}} + \frac{\int_{\mathscr{V}} \mathbf{k}(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}}{M_{\mathscr{V}}}, \tag{2.37}$$

where $\mathbf{h}$ and $\mathbf{k}$, defined in (2.17)–(2.18), satisfy Eqs. (2.19)–(2.20) and

$$\hat{\mathbf{F}} \equiv \frac{\int_{\mathscr{V}} \mathbf{F}(\mathbf{x}, \mathbf{v}, t) f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{x}\, d\mathbf{v}}{M_{\mathscr{V}}}.$$

We will discuss later how to obtain a numerical scheme from these equations.

General Considerations on the Discretization of the Equations

The equations of motion of the particles are, from (2.17)–(2.18) and (2.21),

$$\dot{\mathbf{x}}_i = \mathbf{v}_i, \tag{2.38}$$

$$\dot{\mathbf{v}}_i = \mathbf{F}_i + \frac{\mathbf{k}_i}{f_i}, \tag{2.39}$$

where $\mathbf{x}_i(t) = \mathbf{x}(\mathbf{x}_i^0, \mathbf{v}_i^0, t)$, $\mathbf{v}_i(t) = \mathbf{v}_i(\mathbf{x}_i^0, \mathbf{v}_i^0, t)$, $\mathbf{F}_i = \mathbf{F}(\mathbf{x}_i, \mathbf{v}_i, t)$, $\mathbf{k}_i = \mathbf{k}(\mathbf{x}_i, \mathbf{v}_i, t)$, $f_i = f(\mathbf{x}_i, \mathbf{v}_i, t)$, and $\{\mathbf{x}_i^0, \mathbf{v}_i^0\}_{i=1}^N$ is the initial location of the particles. The dot denotes the time differentiation. In a particle scheme an approximation of the right-hand side of the equations is computed as a function of all the particle locations. The term $\mathbf{F}_i$ can be computed in the usual way (particle–particle, particle–mesh schemes, etc. [11, 1]).

The new problem is the computation of $\mathbf{k}_i$ and f_i. This will be one of our main concerns.

Let us consider first the space-homogeneous case. If I is an integral operator then its numerical values are computed as $I[f_{(N)}(\mathbf{v}, t)]$, where $f_{(N)}$ is a sum of δ-distributions of the form

$$f_{(N)}(\mathbf{v}, t) = \sum_{i=1}^{N} w_i \delta(\mathbf{v} - \mathbf{v}_i).$$

The computation of $I[f_{(N)}(\mathbf{v}_i, t)]$ at each time step is a $O(N^2)$ computation. The explicit expression (2.24)–(2.26) (or similar expression for compact domains) can be used in order to compute $\mathbf{k}_i$. The overall computation is thus $O(N^2)$.

The value of the function f_i can be reconstructed in different ways. Usually f_i is obtained by taking the convolution of $f_{(N)}$ with some suitable base function (generally, a piecewise linear or quadratic function) [11, 1]. An alternative approach is based on the relation between particle methods and quadrature formulas, as will be explained in a following paper. *Voronoi diagrams* seem suitable for handling the irregular mesh of the particles and have already been used in 2D hydrodynamical computations [3, 4]. They also provide a discrete approximation of differential operators (laplacian, divergence, gradient) on the irregular mesh given by the particles, and this is particularly useful when the operator I contains differential terms. There are fast algorithms that create a 2D Voronoi diagram in $O(N \log N)$ computations and update it in only $O(N)$ operations. By means of these diagrams and of an appropriate quadrature formula it is possible to compute an approximate expression for f_i (taking care of open polygons). There are interesting physical cases where the phase space is bounded, as in the kinematic description of carriers in a crystal. In this case the physical domain of the "momentum" $\hbar\mathbf{k}$ of the carriers can be restricted to the first Brillouin zone [23].

A possible way to overcome the problem of the unbounded domain is to use a mapping of R^d onto the unit cube $[0, 1]^d$ and analyze the distribution function in the unit cube.

Once a system of ODEs of the form (2.38)–(2.39) is obtained, a standard technique can be used to solve it numerically. In the general spatial non-homogeneous case, the problem can be treated according to the following fractional-step scheme:

1. A regular grid in space is introduced which divides the domain into "cells."

2. The contribution of collisions is then computed separately in each cell and the particles are moved (in velocity) according to this term.

3. The particles are moved according to the (collisionless) equations of motion.

We are presently working on such a scheme, treating a diffusion operator and a linear integral operator. The results will be presented in a subsequent paper.

3. The One-dimensional, Space Homogeneous Case

In this section we shall consider the initial-value problem,

$$\frac{\partial f}{\partial t} = I[f], \tag{3.1}$$

$$f(v, 0) = f_0(v), \tag{3.2}$$

where f is supposed to be a non-negative integrable function in $R \times [0, \infty)$ and $I[f]$ is a generic collisional operator acting on f. This is the simplest prototype of a collisional kinetic equation, where we dropped all the other terms. It is instructive to rederive the method in this simple case. We define a Lagrangian coordinate V in the following way:

$$V \equiv \int_{-\infty}^{v} f(v', t)\, dv'. \tag{3.3}$$

If f is strictly positive, this relation is invertible. Suppose that this is the case and consider v as a function of V and t. Differentiating Eq. (3.3) with respect to t and V we obtain

$$0 = f(v, t)\frac{\partial v}{\partial t} + \int_{-\infty}^{v} \frac{\partial f}{\partial t}(v', t)\, dv', \tag{3.4}$$

$$1 = f(v, t)\frac{\partial v}{\partial V}. \tag{3.5}$$

Making use of (3.1) the "equation of motion" is written as

$$\frac{\partial v}{\partial t} = -\frac{\partial v}{\partial V}\int_{-\infty}^{v} I[f](v', t)\, dv'. \tag{3.6}$$

A numerical scheme is obtained in the following way. Let

$$\bar{V} \equiv \int_{-\infty}^{+\infty} f(v, t)\, dv. \tag{3.7}$$

The quantity $\bar{V}$ is a constant if $I[f]$ does not contain any net source term, i.e., if

$$\int_R I[h](v)\, dv = 0 \tag{3.8}$$

for any function $h(v)$ of the proper class. For the moment we suppose that this is the case.

We define the initial position of the "particles,"

$$V_i = \int_{-\infty}^{v_i^0} f_0(v)\, dv, \qquad i = 1, ..., N, \tag{3.9}$$

where

$$V_i \equiv \bar{V} \frac{2i-1}{2N}. \tag{3.10}$$

The Jacobian $\partial v/\partial V$ is discretized as

$$(v_{i+1} - v_{i-1})/(V_{i+1} - V_{i-1}) = (v_{i+1} - v_{i-1})(N/2\bar{V}). \tag{3.11}$$

If $I[f]$ is an integral operator, it is approximated by substituting to f a sum of Dirac distributions:

$$f \approx \frac{\bar{V}}{N} \sum_{i=1}^{N} \delta(v - v_i). \tag{3.12}$$

The alternative scheme based on the evolution equations for the mean is obtained in the following way. Let us define the quantities v_j, $\hat{v}_i$:

$$\frac{\bar{V}}{N} = \int_{-\infty}^{v_j} f(v, t)\, dv, \qquad j = 0, ..., N, \tag{3.13}$$

$$\hat{v}_i \int_{v_{i-1}}^{v_i} f(v, t)\, dv = \int_{v_{i-1}}^{v_i} v f(v, t)\, dv, \qquad i = 1, ..., N. \tag{3.14}$$

Taking the time derivative of Eq. (3.14), integrating by parts and making use of Eq. (3.6) we obtain

$$\frac{d\hat{v}_i}{dt} = -\frac{N}{\bar{V}} \int_{v_{i-1}}^{v_i} \int_{-\infty}^{v} I(v', t)\, dv'\, dv, \tag{3.15}$$

and, in the evaluation of the integral, $f(v, t)$ is substituted by

$$f(v, t) \approx \frac{\bar{V}}{N} \sum_{i=1}^{N} \delta(v - \hat{v}_i(t)). \tag{3.16}$$

In principle, Eqs. (3.15) can be solved only if $v_i(t)$ are known. In a numerical scheme we need to express v_i as a function of $\hat{v}_i$, in order to close the system of equations. Note that the "total momentum," $P \equiv \int_{-\infty}^{+\infty} vf(v, t)\, dv$, is exact when f is approximated by (3.16). The disadvantages of this formulation consist in the more complicated form of the equations of motion and in the need of a suitable approximation of v_i in terms of $\hat{v}_i$.

Source Terms and Boundary Conditions

In view of application of this method to other problems, we describe how to treat boundary conditions. Let us consider the initial-boundary value problem for the function f: $[0, 1] \times [0, +\infty] \to R$:

$$\frac{\partial f}{\partial t} = I[f] + s(v, t), \tag{3.17}$$

$$f(v, 0) = f_0(v), \tag{3.18}$$

$$f(0, t) = g(t), \qquad f(1, t) = h(t). \tag{3.19}$$

Equation (3.6) becomes

$$\frac{\partial v}{\partial t} = \frac{1}{f}(k - S), \tag{3.20}$$

where

$$k(v, t) \equiv -\int_0^v I[f](v', t)\, dv', \qquad S \equiv \int_0^v s(v', t)\, dv'. \tag{3.21}$$

At the initial time $t = 0$ the equation is described by N^0 points defined by

$$(i - \tfrac{1}{2})C = \int_0^{v_i} f_0(v)\, dv, \qquad i = 1, ..., N^0, \tag{3.22}$$

where $C \equiv \int_0^1 f_0(v)\, dv / N^0$. We discretize the time and define v_0^n and v_{N+1}^n:

$$g(t^n) = \frac{C}{(v_1^n - v_0^n)}, \qquad h(t^n) = \frac{C}{(v_{N+1}^n - v_N^n)}. \tag{3.23}$$

Equation (3.20) is discretized in the form

$$v_i^{n+1} = v_i^n + F_i^n \Delta t, \qquad i = 0, ..., N^n + 1, \tag{3.24}$$

where

$$F_i^n \equiv \frac{v_{i+1}^n - v_{i-1}^n}{2C} [k_i^n - S(v_i^n, t^n)], \qquad i = 1, ..., N^n \tag{3.25}$$

and

$$F_0^n = F_1^n, \qquad F_{N^n+1}^n = F_{N^n}^n.$$

If $v_0^{n+1} > 0$ then we say that a new particle has been created at the left boundary. If $v_1^{n+1} < 0$ then we say that the particle has been annihilated. A similar procedure is applied at the right boundary. If Δt is small enough then only one particle can be created or destroyed at a boundary per each time step. If Δt is not small enough then this procedure can be generalized and more that one particle can be created or annihilated per time step. An application of this method will be shown in the next section for the heat equation.

We remark that particles are created or destroyed only at the boundary, even in presence of an internal source. This is because the information is carried by the relative distance between the "particles" and not by their absolute location.

4. The Diffusion Equation: Numerical Results

We apply the method to the one-dimension diffusion equation. This application is important for many reasons. It is a simple case for which exact results on consistency and stability can be obtained and it is a deterministic way of introducing diffusion in a particle method (without changing the weights of the particles).

As in the case of finite difference schemes, explicit schemes suffer a limitation in the step size. The problem can be overcome by an implicit version of the method which guarantees unconditional stability.

Let us consider the equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial x}\left(\nu \frac{\partial f}{\partial x}\right), \tag{4.1}$$

where ν is the viscosity.

In terms of the Lagrangian coordinate $X \equiv \int f(x, t)\, dx$, the equation can be written in the form:

$$\frac{\partial x}{\partial t} = -\frac{\nu}{f}\frac{\partial f}{\partial x}, \tag{4.2}$$

$$\frac{\partial x}{\partial X} = \frac{1}{f}. \tag{4.3}$$

The discretization of the equations in X yields the system of ODEs,

$$\dot{x}_i = v_i\left(\frac{1}{x_i - x_{i-1}} - \frac{1}{x_{i+1} - x_i}\right), \qquad i = 1, ..., N, \tag{4.4}$$

where $v_i = v(x_i, f_i)$. The function f is reconstructed according to $f_i = \text{const}/(x_{i+1} - x_{i-1})$ and x_0 and x_{N+1} are determined by the boundary conditions. For periodic boundary conditions (period = 1) it is

$$\begin{aligned} x_0 &= x_N - 1, \\ x_{N+1} &= x_1 + 1. \end{aligned} \tag{4.5}$$

For unbounded domain x_0 and x_N go to infinity,

$$x_0 = -\infty, \qquad x_{N+1} = +\infty, \tag{4.6}$$

and in the case of a boundary value problem they are given by Eq. (3.23).

The *Forward–Euler* scheme relative to the system (4.4) is given by

$$x_i^{n+1} = x_i^n + v_i^n\left(\frac{1}{x_i^n - x_{i-1}^n} - \frac{1}{x_{i+1}^n - x_i^n}\right)\Delta t. \tag{4.7}$$

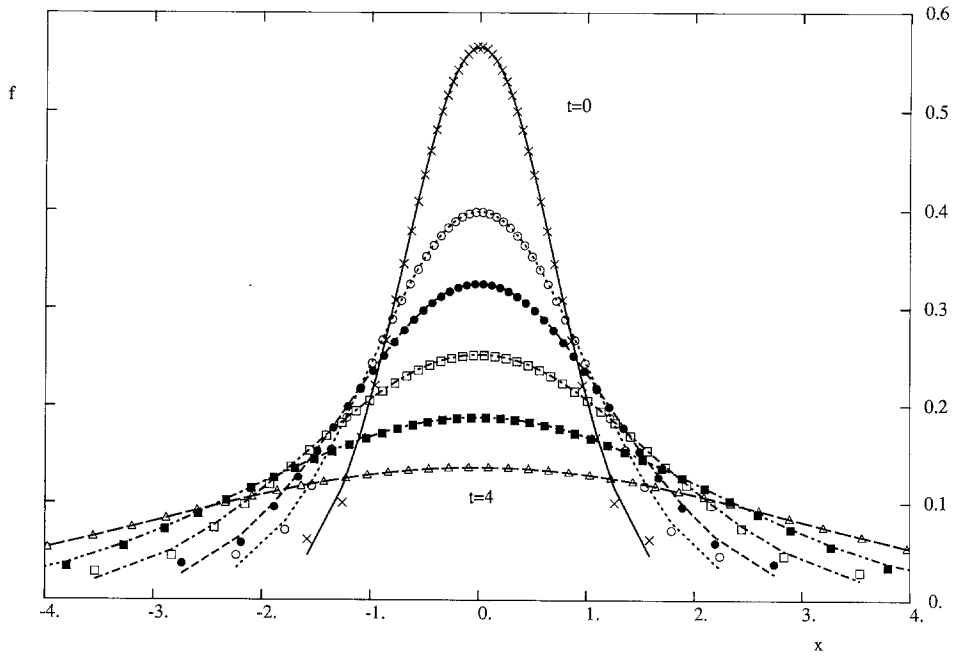

FIG. 1. Comparison between the exact (lines) and numerical (marks) solution for the diffusion equation at different times. The Forward–Euler scheme has been used with 40 particles and time step $\Delta t = 0.001$. The initial profile is gaussian. The output times are: $t = 0$, 0.25, 0.5, 1.0, 2.0, 4.0.

A stability analysis (see Section 5) shows that the scheme is stable if

$$\Delta t \leqslant \frac{1}{2} \min_i \left\{ \frac{(x_i - x_{i-1})^2}{v_{i-1/2}} \right\}. \tag{4.8}$$

In Fig. 1 we compare the numerical results with the exact solution. The boundary conditions (4.6) have been used. The lines represent the exact solution,

$$f(x, t) = \frac{1}{2\sqrt{\pi(t + t_0)}} \exp\left[-\frac{x^2}{4(t + t_0)} \right]$$

at different values of the time. The marks are the computed solution, reconstructed according to (3.5), (3.11). We used the scheme (4.7) with the following values of the parameters: $\Delta t = 0.001$, $N = 40$, $t_0 = 0.25$, $v = 1$. The output times are: $t = 0$, 0.25, 0.5, 1, 2, 4.

In Fig. 2 the stability condition is not satisfied in a part of the profile and oscillations develop. The continuous line is the exact solution and the dotted line represents the numerical solution after 10 time steps.

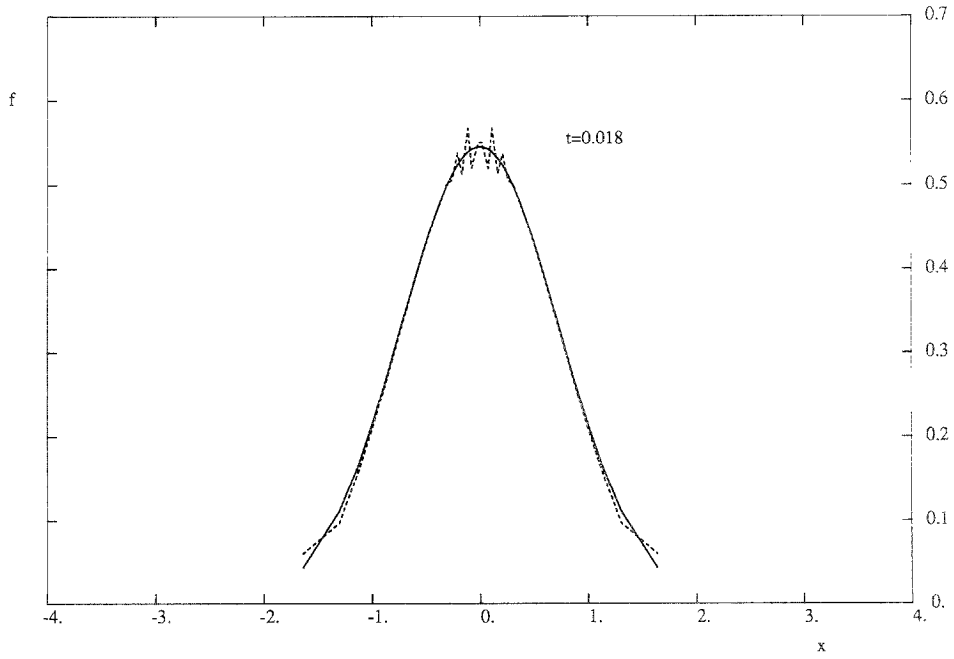

FIG. 2. Instabilities developed near the top of the profile after 10 time steps, when stability condition is not satisfied. The time step is $\Delta t = 0.0018$ and $\min(\hat{x}^0_{i-1} - \hat{x}^0_i)^2 = 0.001953$; $v = 1$.

In Fig. 3 the solution of the initial-boundary value problem (4.1), (3.18)–(3.19) with

$$f_0(x) = c_0(1-x) + c_1 x, \qquad g(t) \equiv a, \qquad h(t) \equiv b,$$
$$s(x) = \sigma\delta(x - \tfrac{1}{2}), \qquad \nu = \nu(x) = \nu_0(1 + \mu x) \tag{4.9}$$

is shown. The parameters used in the calculations are:

$$c_0 = 1.5, \qquad c_1 = 2, \qquad a = 3, \qquad b = 4,$$
$$\sigma = 5, \qquad \nu_0 = 0.15, \qquad \mu = 10.$$

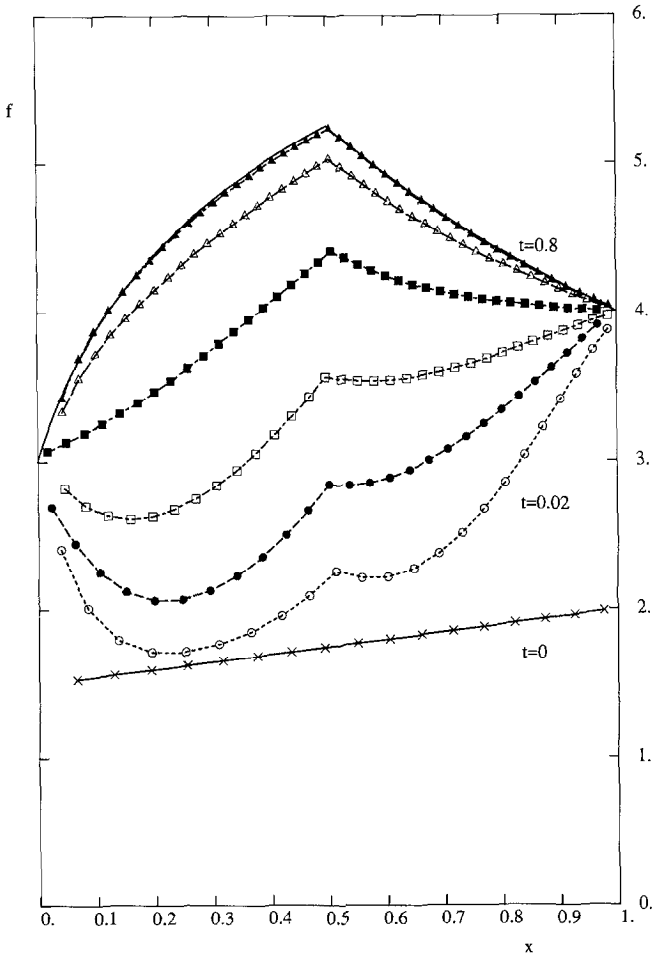

FIG. 3. Initial-boundary value problem for the heat equation, with a source term and a non-constant conductivity. The initial profile is the straight line on the bottom of the figure. A localized source is put at $x = 0.5$. The number of particles is proportional to the area below the profile and ranges from 18 (initial condition) to 45 for large time. The continuous line on the top is the stationary solution. The output times are: $t = 0$, 0.02, 0.05, 0.1, 0.2, 0.4, 0.8.

Δt is computed at each time step imposing the criteria that the stability condition be marginally satisfied. The number of particles varies from 18 to 45 and the numerical solution approaches the exact steady solution for large times. Note that the stability restriction (4.8) ensures that at most one particle per time step is created or annihilated at each boundary.

A fully implicit scheme for system (4.4),

$$x_i^{n+1} = x_i^n + v_i^{n+1}\left(\frac{1}{x_i^{n+1} - x_{i-1}^{n+1}} - \frac{1}{x_{i+1}^{n+1} - x_i^{n+1}}\right)\Delta t, \tag{4.10}$$

requires the solution of a non-linear system at each time step. A scheme which is easier to handle is obtained from (4.10) with the replacement:

$$v_i^{n+1}\,\frac{x_{i+1}^{n+1} - 2x_i^{n+1} + x_{i-1}^{n+1}}{(x_i^{n+1} - x_{i-1}^{n+1})(x_{i+1}^{n+1} - x_i^{n+1})} \to v_i^n\,\frac{x_{i+1}^{n+1} - 2x_i^{n+1} + x_{i-1}^{n+1}}{(x_i^n - x_{i-1}^n)(x_{i+1}^n - x_i^n)}.$$

The scheme reads:

$$x_i^{n+1} = x_i^n + v_i^n\,\frac{x_{i+1}^{n+1} - 2x_i^{n+1} + x_{i-1}^{n+1}}{(x_i^n - x_{i-1}^n)(x_{i+1}^n - x_i^n)}\,\Delta t. \tag{4.11}$$

In the next section we shall prove that this scheme is unconditionally stable. Now we shall study the rate of convergence for this scheme as $N \to \infty$. The error between the numerical solution and the exact solution is computed in the following way: Let

$$X_i^n \equiv \int_{-\infty}^{x_i^n} f(x, t^n)\,dx.$$

We define the error ε_N^n as

$$\varepsilon_N^n \equiv \max_{1 \leqslant i \leqslant N} |X_i^n - X_i|,$$

where X_i is the Lagrangian coordinate and does not depend on time.

We compute ε_N^n for various N and for a fixed time t. In Fig. 4 we plot the error ε as a function of $1/N^2$ in the case of the heat equation with unbounded domain. Here $v = 1$ and the initial condition is the gaussian:

$$f(x, 0) = \frac{1}{2\sqrt{\pi}}\,e^{-x^2/4}.$$

The computation was performed up to a fixed time ($t = 1$) and the equations of motion in the form (2.28)–(2.29) have been used, with $\phi = (2/\pi)/(1 + x^2)$. The scheme (4.11) with $\Delta t = 0.0001$ has been used. It is apparent that the scheme is

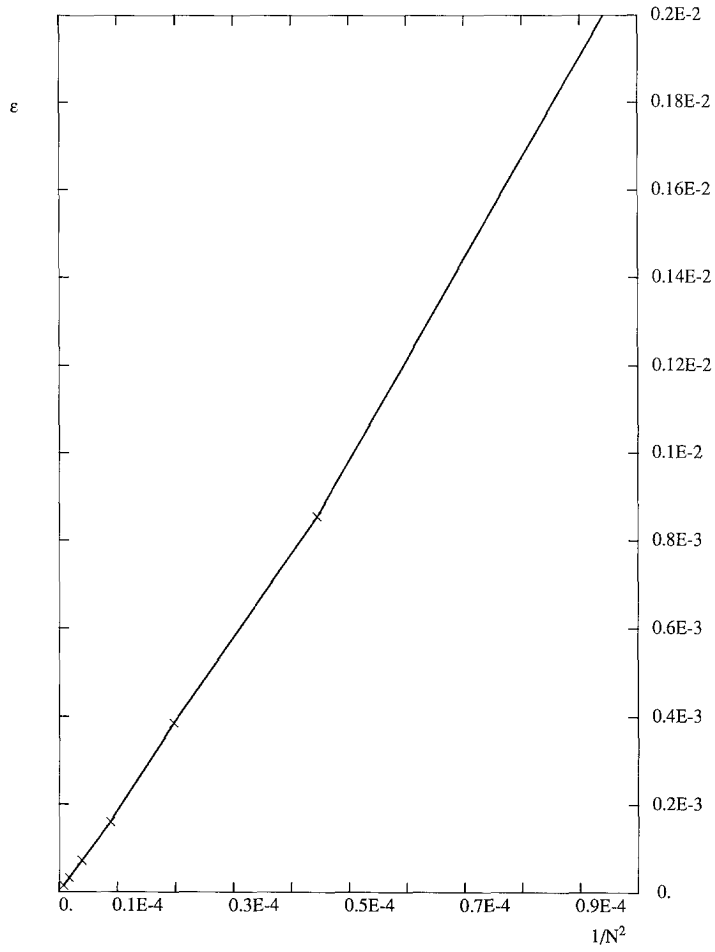

FIG. 4. Rate of convergence of the numerical scheme for the diffusion equation inunbounded domain: ε_N versus $1/N^2$.

second-order accurate with respect to N, while it is first order in time, as expected. The order of accuracy in time depends on the scheme used for solving the ODEs system (4.4). In the next section we shall make a theoretical analysis of the periodic case.

5. THE DIFFUSION EQUATION: THEORETICAL RESULTS

We shall discuss first the properties of the system of ODEs obtained by the "space discretization" and then we shall study the stability and consistency proper-

ties of some simple numerical scheme. In the case $v \equiv 1$ and for periodic boundary conditions the ODEs system for the particles is

$$\dot{x}_i = \frac{1}{x_i - x_{i-1}} - \frac{1}{x_{i+1} - x_i}, \qquad i = 1, ..., N, \tag{5.1}$$

where

$$x_i \in [0, 1], \qquad i = 1, ..., N,$$

and

$$\begin{aligned} x_0 &= x_N - 1, \\ x_{N+1} &= x_1 + 1. \end{aligned} \tag{5.2}$$

The number of particles is obviously conserved. The lengths of the intervals, $y_i \equiv x_{i+1} - x_i$, satisfy the system

$$\dot{y}_i = \frac{2}{y_i} - \frac{1}{y_{i+1}} - \frac{1}{y_{i-1}}, \qquad i = 1, ..., N, \tag{5.3}$$

where $y_{N+1} = y_1$. The following properties hold:

(i) the minimum length of the intervals y_i is a non-decreasing function of time;

(ii) the maximum length of the intervals y_i is a non-increasing function of time;

(iii) the uniform distribution, $x_i = i/N$, $i = 1, ..., N$, is a stable solution of (5.1).

Proof. (i) and (ii). Let k and j denote the indices such that

$$y_k = \min_{1 \leqslant i \leqslant N} y_i, \qquad y_j = \max_{1 \leqslant i \leqslant N} y_i.$$

Then, from (5.3), $\dot{y}_k \geqslant 0$, and $\dot{y}_j \leqslant 0$, therefore the shortest interval cannot decrease and the largest cannot increase.

(iii) That the uniform distribution is a solution of (5.1) is evident. In order to prove stability let us define an "energy":

$$\mathscr{E} \equiv \sum_{i=1}^{N} \frac{1}{y_i}. \tag{5.4}$$

Then

$$\dot{\mathscr{E}} = \sum_{i=1}^{N} -\frac{1}{y_i^2} \dot{y}_i = \sum_{i=1}^{N} \frac{1}{y_i^2} \left(\frac{1}{y_{i+1}} - \frac{2}{y_i} + \frac{1}{y_{i-1}} \right),$$

and, summing by parts,

$$\dot{\mathscr{E}} = \left(\frac{1}{y_{N+1}} - \frac{1}{y_N}\right)\frac{1}{y_N^2} - \frac{1}{y_1^2}\left(\frac{1}{y_1} - \frac{1}{y_0}\right) - \sum_{i=1}^{N-1}\left(\frac{1}{y_i} - \frac{1}{y_{i+1}}\right)^2\left(\frac{1}{y_i} + \frac{1}{y_{i+1}}\right)$$
$$= -\sum_{i=0}^{N-1}\left(\frac{1}{y_i} - \frac{1}{y_{i+1}}\right)^2\left(\frac{1}{y_i} + \frac{1}{y_{i+1}}\right) \leqslant 0, \tag{5.5}$$

because $y_0 = y_N$ and $y_1 = y_{N+1}$. This proves the stability of the uniform distribution and the uniqueness of the stationary solution (expressed in terms of y_i).

We shall consider now the problem of the consistency of the particle scheme with the original diffusion equation.

Let $x = \varphi(X, t)$ be the transformation which satisfies

$$\frac{\partial x}{\partial t} = -\frac{\partial}{\partial X}\left[\left(\frac{\partial x}{\partial X}\right)^{-1}\right] \tag{5.6}$$

(obtained from (4.2)–(4.3) for $\nu = 1$), and let $x_i \equiv \varphi(X_i, t)$. The discrete version of (5.6) is given by Eq. (5.1). For each point x_i we define R_i as

$$\frac{\partial}{\partial X}\left[\left(\frac{\partial x}{\partial X}\right)^{-1}\right]_{X = X_i} = \frac{1}{x_{i+1} - x_i} - \frac{1}{x_i - x_{i-1}} - R_i. \tag{5.7}$$

We shall prove that, under regularity assumptions on the function f and its derivatives, the system (5.1) is consistent with Eq. (5.6) and the accuracy is second order in $1/N$.

For simplicity we shall denote by a prime the differentiation with respect to X.

THEOREM. *Under the assumptions*

$$\frac{1}{C} < f < C, \qquad |f_x| < C, \qquad |f_{xx}| < C, \qquad |f_{xxx}| < C, \tag{5.8}$$

the estimate

$$\max_{1 \leqslant i \leqslant N} |R_i| < \frac{15}{4} C^{16} \frac{\bar{X}^2}{N^2} + \frac{13}{6} C^{17} \frac{\bar{X}^3}{N^3} \tag{5.9}$$

holds, where $\bar{X} \equiv \int_0^1 f(x, t)\, dx$.

Proof. It is

$$R_i = \frac{\varphi_i''}{\varphi_i'^2} - \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\varphi_i - \varphi_{i-1})(\varphi_{i+1} - \varphi_i)}$$
$$= \left[\varphi_i'' \frac{\varphi_{i+1} - \varphi_i}{\Delta X}\frac{\varphi_i - \varphi_{i-1}}{\Delta X} - \varphi_i'^2 \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{\Delta X^2}\right]$$
$$\times \left[\varphi_i'^2 \frac{\varphi_{i+1} - \varphi_i}{\Delta X}\frac{\varphi_i - \varphi_{i-1}}{\Delta X}\right]^{-1}, \tag{5.10}$$

where

$$\varphi_i^{(k)} \equiv \frac{\partial^k \varphi}{\partial X^k}(X_i, t), \qquad k = 0, 1, ...,$$

and

$$\Delta X \equiv \frac{1}{N} \int_0^1 f_0(x)\, dx.$$

From the Taylor expansion of $\varphi(X)$ it follows that

$$\frac{(\varphi_{i+1} - \varphi_i)(\varphi_i - \varphi_{i-1})}{\Delta X^2} - \varphi_i'^2$$
$$= \left[\frac{1}{3}\varphi_i''' \varphi_i' - \frac{1}{4}\varphi_i''^2 + \frac{1}{24}\varphi_i'(\varphi_{\zeta_-}^{(4)} - \varphi_{\zeta_-}^{(4)})\, \Delta X\right] \Delta X^2 \tag{5.11}$$

and

$$\frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{\Delta X^2} - \varphi_i'' = \frac{1}{12}\varphi_\xi^{(4)} \Delta X^2, \tag{5.12}$$

where, with an abuse of notation, $\varphi_\xi \equiv \varphi(\xi, t)$. It is $X_{i-1} < \xi, \zeta_\pm < X_{i+1}$. Substituting (5.11) and (5.12) into (5.10) and making use of the theorem of the mean, it follows that

$$\frac{R_i}{\Delta X^2} = \left\{ -\frac{\varphi_\xi^{(4)}}{12\varphi_{\xi_+}'\varphi_{\xi_-}'} + \frac{\varphi_i''\varphi_i'''}{3\varphi_i'\varphi_{\xi_-}'\varphi_{\xi_-}'} - \frac{\varphi_i''^3}{4\varphi_i^2\varphi_{\xi_+}'\varphi_{\xi_-}'} + \frac{\varphi_i''(\varphi_{\zeta_+}^{(4)} - \varphi_{\zeta_-}^{(4)})}{24\varphi_i\varphi_{\xi_+}'\varphi_{\xi_-}'} \Delta X \right\}, \tag{5.13}$$

where $X_{i-1} < \xi_- < X_i < \xi_+ < X_{i+1}$.

The relations between the derivatives of φ and f are

$$\begin{aligned} \varphi' &= f^{-1}, \\ \varphi'' &= -f^{-3} f_x, \\ \varphi''' &= 3f^{-5} f_x^2 - f^{-4} f_{xx}, \\ \varphi^{(4)} &= -15 f^{-7} f_x^3 + 10 f^{-6} f_x f_{xx} - f^{-5} f_{xxx}. \end{aligned} \tag{5.14}$$

From (5.8) it follows:

$$\begin{aligned} &|\varphi| < C, \qquad |1/\varphi'| < C, \\ &|\varphi''| < C^4, \\ &|\varphi'''| < 3C^7 + C^5, \\ &|\varphi^{(4)}| < 26C^{10}. \end{aligned} \tag{5.15}$$

Using relation (5.15), we get the estimate:

$$R_i < \left(C^{14} + \frac{5}{2} C^{12} + \frac{1}{4} C^{16} + \frac{13}{6} C^{17} \Delta X \right) \Delta X^2$$

$$< \frac{15}{4} C^{16} \frac{\bar{X}^2}{N^2} + \frac{13}{6} C^{17} \frac{\bar{X}^3}{N^3} \tag{5.16}$$

Q.E.D.

We shall consider now some simple numerical scheme for the system (5.1). As we shall see, explicit schemes suffer a limitation on the time step due to stability conditions. This problem can be easily overcome with implicit or linearly implicit schemes.

Let us consider first the Forward–Euler scheme:

$$x_i^{n+1} = x_i^n + \Delta t \left(\frac{1}{x_i^n - x_{i-1}^n} - \frac{1}{x_{i+1}^n - x_i^n} \right). \tag{5.17}$$

We shall perform a linear stability analysis for this scheme. Let $\{\mathring{x}_i^n\}$ and $\{x_i^n\}$ be two solutions of system (5.17). The linearized equation for the "error" $e_i^n \equiv x_i^n - \mathring{x}_i^n$ is

$$e_i^{n+1} = e_i^n + \Delta t \left[\frac{e_{i+1}^n - e_i^n}{(\mathring{x}_{i+1}^n - \mathring{x}_i^n)^2} - \frac{e_i^n - e_{i-1}^n}{(\mathring{x}_i^n - \mathring{x}_{i-1}^n)^2} \right]. \tag{5.18}$$

Equation (5.18) may be written in a vector form

$$\mathbf{e}^{n+1} = A \mathbf{e}^n, \tag{5.19}$$

where, in the periodic case, A is the matrix

$$A = \begin{pmatrix} 1 - z_1 - z_N & z_1 & 0 & \cdots & 0 & z_N \\ z_1 & 1 - z_1 - z_2 & z_2 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ z_N & 0 & 0 & \cdots & z_{N-1} & 1 - z_{N-1} - z_N \end{pmatrix} \tag{5.20}$$

and

$$z_i \equiv \Delta t / (\mathring{x}_{i+1}^n - \mathring{x}_i^n)^2. \tag{5.21}$$

Because A is real and symmetric, the characteristic condition for stability states that all the eigenvalues should not exceed one:

$$|\lambda_k| \leqslant 1, \qquad k = 1, ..., N. \tag{5.22}$$

We shall prove the following:

THEOREM. *If*

$$\Delta t \leqslant \tfrac{1}{2} \min_j (\mathring{x}^n_{j+1} - \mathring{x}^n_j)^2, \tag{5.23}$$

then the scheme (5.17) *is linearly stable.*

Proof. The Gershgorin theorem [21] ensures that all eigenvalues of a matrix $A = (a_{ij})$ are contained in the union of the discs,

$$K_i = \left\{ \mu \in C : |\mu - a_{ii}| \leqslant \sum_{\substack{j=1 \\ j \neq i}}^{N} |a_{ij}| \right\}, \tag{5.24}$$

therefore the eigenvalues λ_k have to satisfy one of the conditions:

$$|\lambda_k - (1 - z_i - z_{i+1})| \leqslant z_i + z_{i+1};$$

that is,

$$1 - 2(z_i + z_{i+1}) \leqslant \lambda_k \leqslant 1$$

and, from condition (5.23), it follows that

$$|\lambda_k| \leqslant 1. \qquad \text{Q.E.D.}$$

Figure 2 shows the behaviour of the solution in the region where condition (5.23) is not satisfied. Note that the instability is localized where the value of the function is large enough. This is typical of explicit schemes applied to a non-linear equation.

Note the resemblance of condition (5.23) with the stability condition for the Forward–Euler scheme applied to the heat equation (4.1) with constant ν [20, p. 12]:

$$\nu \Delta t \leqslant \tfrac{1}{2} \Delta x^2.$$

Here Δx is the spatial step of the uniform Eulerian mesh.

Consider now the implicit scheme for system (5.1):

$$x_i^{n+1} = x_i^n + \Delta t \left(\frac{1}{x_i^{n+1} - x_{i-1}^{n+1}} - \frac{1}{x_{i+1}^{n+1} - x_i^{n+1}} \right). \tag{5.25}$$

We shall prove that such a scheme is unconditionally stable. We shall make use of the "maximum principle" [20]; that is we shall prove that for this system a discrete version of properties (i) and (ii) hold.

Let $j(n)$ and $k(n)$ denote two indices such that

$$y^n_{j(n)} \equiv \max_{1 \leqslant i \leqslant N} y^n_i, \qquad y^n_{k(n)} \equiv \min_{1 \leqslant i \leqslant N} y^n_i,$$

with $y_i^n \equiv x_{i+1}^n - x_i^n$. The system satisfied by y_i^n is derived from system (5.25):

$$y_i^{n+1} = y_i^n + \Delta t \left(\frac{2}{y_i^{n+1}} - \frac{1}{y_{i-1}^{n+1}} - \frac{1}{y_{i+1}^{n+1}} \right). \tag{5.26}$$

Let $\bar{j} = j(n+1)$. Then

$$\frac{y_{\bar{j}}^{n+1} - y_{\bar{j}}^n}{\Delta t} = \frac{2}{y_{\bar{j}}^{n+1}} - \frac{1}{y_{\bar{j}-1}^{n+1}} - \frac{1}{y_{\bar{j}+1}^{n+1}} \leqslant 0,$$

and hence

$$y_{j(n)}^n \geqslant y_{j(n+1)}^n \geqslant y_{j(n+1)}^{n+1}.$$

The proof that $y_{k(n+1)}^{n+1} \geqslant y_{k(n)}^n$ is analogous. This proves the stability of the implicit scheme (5.25). As a corollary, it follows that the distance between the particles cannot shrink to zero, that is $y_i^n > 0$, $i = 1, ..., N$; $n = 0, 1, ...$ It is easy to prove that system (5.25) is energetically stable. We use again the *energy* definition (5.4):

$$\mathscr{E}^n \equiv \sum_{i=1}^{N} \frac{1}{y_i^n}. \tag{5.27}$$

It is

$$\begin{aligned} \frac{\mathscr{E}^{n+1} - \mathscr{E}^n}{\Delta t} &= \frac{1}{\Delta t} \sum_{i=1}^{N} \frac{1}{y_i^{n+1}} - \frac{1}{y_i^n} \\ &= \sum_{i=1}^{N} \frac{y_i^n - y_i^{n+1}}{y_i^{n+1} y_i^n \Delta t} \\ &= \sum_{i=1}^{N} z_i^{n+1} z_i^n (z_{i-1}^{n+1} - 2z_i^{n+1} + z_{i+1}^{n+1}), \end{aligned}$$

where $z_i^n \equiv 1/y_i^n$ and (5.26) has been used. Adding and subtracting the same term we have

$$\begin{aligned} \frac{\mathscr{E}^{n+1} - \mathscr{E}^n}{\Delta t} = & \sum_{i=1}^{N} (z_i^n - z_i^{n+1})(z_{i+1}^{n+1} - 2z_i^{n+1} + z_{i-1}^{n+1}) \\ & + \sum_{i=1}^{N} (z_i^{n+1})^2 (z_{i+1}^{n+1} - 2z_i^{n+1} + z_{i-1}^{n+1}). \end{aligned}$$

Making use of (5.26) in the first term, summing by parts the second and using periodic conditions (5.2) we obtain

$$\frac{\mathscr{E}^{n+1}-\mathscr{E}^n}{\Delta t}=-\frac{1}{\Delta t}\sum_{i=1}^{N}\frac{(z_i^n-z_i^{n+1})^2}{z_i^n}$$
$$-\sum_{i=1}^{N}(z_i^{n+1}-z_{i-1}^{n+1})^2(z_i^{n+1}+z_{i-1}^{n+1})\leqslant 0, \tag{5.28}$$

where $z_0^n=z_N^n$.

With the use of the maximum principle it is easy to prove the stability of the linearly implicit scheme (4.11).

6. Other Examples

Master Equation

This equation can be considered as a special kinetic equation with a linear integral collisional operator, in which the kernel represents the differential cross section between the particles and a known background. The equation is given by

$$\frac{\partial f(x,t)}{\partial t}=\int_R Q(x,x')[f(x',t)-f(x,t)]\,dx', \tag{6.1}$$

$$f(x,0)=f_0(x). \tag{6.2}$$

We applied our method to this equation and derived the following equations of motion for the points,

$$\dot{x}_i=-\frac{x_{i+1}-x_{i-1}}{2}\sum_{j=1}^{N}[S(x_i,x_j)-C(x_j)\,H(x_i-x_j)]\equiv G_i, \tag{6.3}$$

where

$$S(x,y)\equiv\int_{-\infty}^{x}Q(x',y)\,dx',$$
$$C(x)\equiv\int_{-\infty}^{+\infty}Q(x,x')\,dx', \tag{6.4}$$
$$H(x)\equiv\begin{cases}1 & x>0\\ \frac{1}{2} & x=0\\ 0 & x<0.\end{cases}$$

We considered the case of a periodic domain $[0,2\pi]$, with

$$Q(x,x')=1+\cos(x-x'),$$
$$f_0(x)=(1+A\cos x)/(2\pi), \tag{6.5}$$

and the comparison with the exact solutionis shown in Fig. 5. The lines represent the exact solution,

$$f(x, t) = (1 + Ae^{-\pi t} \cos x)/(2\pi)$$

at different times. The marks represent the numerical solution. The equations in the form (2.28)–(2.29) have been used, with $\phi = 1/(2\pi)$. A Forward–Euler discretization in time has been used with $\Delta t = 0.001$. The function has been reconstructed by a fourth-order scheme:

$$f_i = (24/N)/[8(x_{i+1} - x_{i-1}) - (x_{i+2} - x_{i-2})] - \frac{1}{2\pi}. \tag{6.6}$$

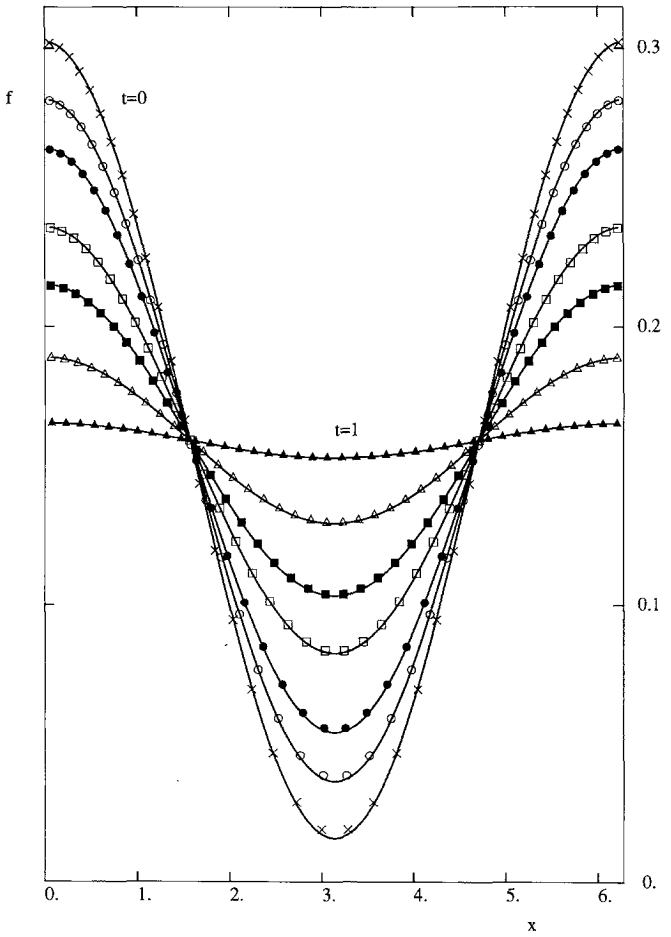

FIG. 5. Master equation on a periodic domain. Comparison between the exact solution (lines) and the numerical solution (marks) for different times. A Forward–Euler scheme has been used with 40 particles and $\Delta t = 0.001$. The output times are: $t = 0$, 0.05, 0.1, 0.2, 0.3, 0.5, 1.0.

Several runs have been made with different numbers of particles and time steps. The error

$$\varepsilon_1(t) = \frac{1}{N} \sum_{i=1}^{N} |f(x_i, t) - f_i(t)|, \tag{6.7}$$

has been computed at a fixed time $\bar{t} = 0.2$ and plotted versus $1/N^2$ for various values of Δt (see Fig. 6), confirming that the rate of convergence is second order in $1/N$ (and, of course, first order in time).

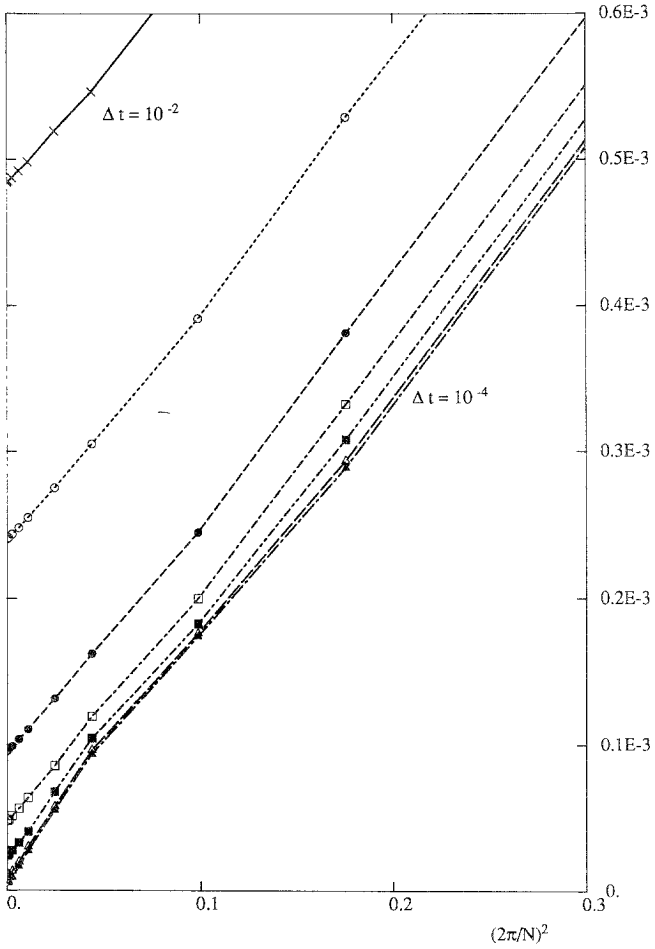

FIG. 6. Rate of convergence of the scheme for the Master equation. Error versus $(2\pi/N)^2$ for different time steps.

Kac Equation

This is a one-dimensional model for a Boltzmann equation:

$$\frac{\partial f}{\partial t} = \int_{-\infty}^{+\infty} dy \int_0^{2\pi} \frac{d\theta}{2\pi} [f(x', t) f(y', t) - f(x, t) f(y, t)] \, dx' \, dy', \tag{6.8}$$

$$\begin{aligned} x' &= x \cos\theta + y \sin\theta, \\ y' &= -x \sin\theta + y \cos\theta. \end{aligned} \tag{6.9}$$

We can interpret this equation in the following way: given two "particles" with coordinates x' and y', they are "rotated," in the phase plane $x - y$, by a collision through an angle θ, which is uniformly distributed. Then the probability density as a function of the rotation angle is

$$P_\theta(\theta) = 1/2\pi \tag{6.10}$$

and, in the coordinate of a particle,

$$P_x(x; R) = \begin{cases} 0 & \text{if} \quad |x| > R \\ \dfrac{1}{\pi \sqrt{R^2 - x^2}} & \text{if} \quad |x| < R, \end{cases} \tag{6.11}$$

where $R^2 = x'^2 + y'^2$.

With this in mind, the collisional operator applied to a set of N particles with coordinates x_j, $j = 1, ..., N$, becomes

$$I[f_{(N)}] = \frac{1}{N^2} \sum_{i,j} P_x(x; R_{ij}) \tag{6.12}$$

with $R_{ij}^2 \equiv x_i^2 + x_j^2$. The equations of motion are given by

$$\dot{x}_i = -\frac{(x_{i+1} - x_{i-1})}{2N} \sum_{jk} \int_{-\infty}^{x_i} P_x(x; R_{jk}) \, dx. \tag{6.13}$$

The system has been solved numerically with a Forward–Euler time discretization scheme. The initial condition is the bi-modal distribution

$$f_0(x) = \frac{2}{\sqrt{\pi}} x^2 e^{-x^2}.$$

The solution relaxes to the steady gaussian:

$$f(x, \infty) = \left(\frac{1}{3\pi}\right)^{1/2} \exp\left(-\frac{x^2}{3}\right).$$

The result is shown in Fig. 7, where 64 particles have been used. Note that the solution at $t = 15$ practically coincides with the stationary solution.

Model Fokker–Planck Equation

We consider a simplified one-dimensional model for the Fokker–Planck equation:

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial x} + 2xf\right]$$
$$f(x, 0) = f_0(x). \tag{6.14}$$

The equations of motion are given by

$$\dot{x}_i = \frac{1}{x_i - x_{i-1}} - \frac{1}{x_{i+1} - x_i} - 2x_i. \tag{6.15}$$

We use a semi-implicit first-order time discretization, with $\Delta t = 0.002$. The initial conditions are

$$f_0(x) = \begin{cases} 0.5, & 2 < |x| < 3 \\ 0, & \text{otherwise.} \end{cases}$$

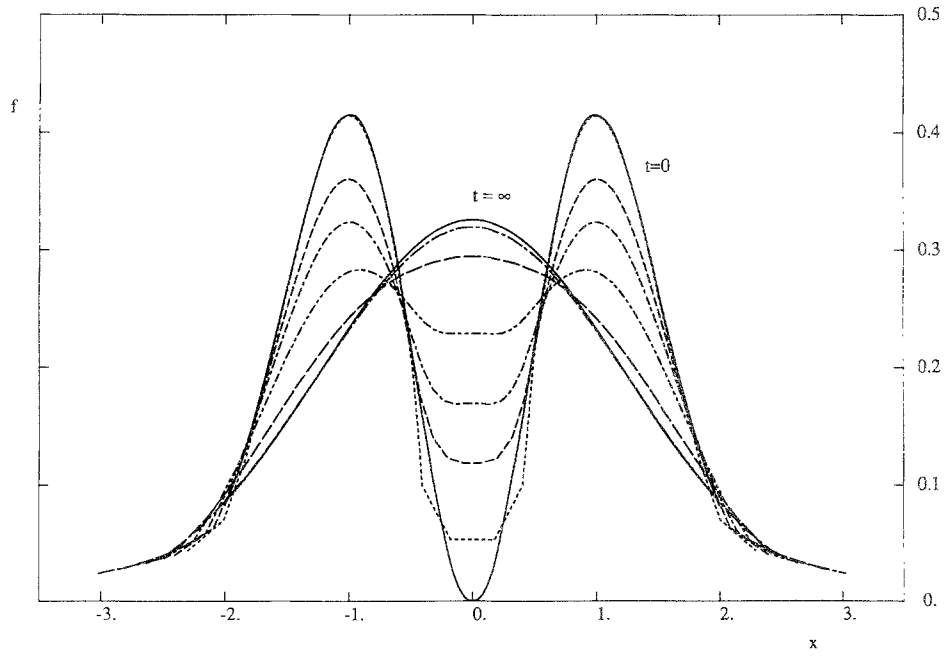

FIG. 7. Numerical solution of the Kac equation. A Forward–Euler scheme has been used with $N = 64$ and $\Delta t = 0.1$ and $A = 0.9$. The output times are: $t = 0$, 0.5, 1, 2, 5, 15.

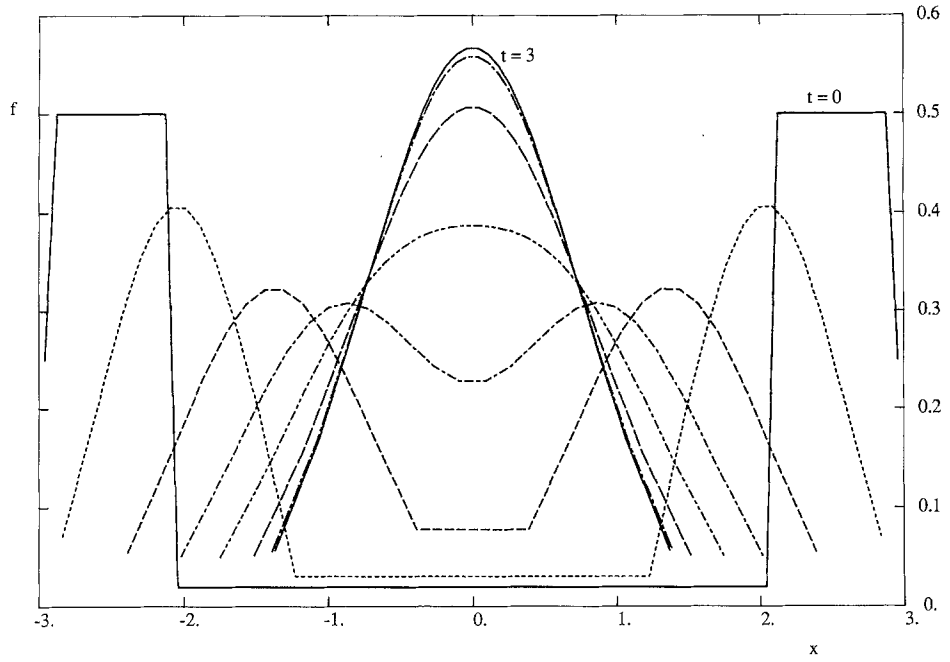

FIG. 8. Numerical solution of the model Fokker–Planck equation: 24 particles have been used

The results are shown in Fig. 8, where the asymptotic solution is the gaussian $(1/\sqrt{\pi})\exp(-x^2)$.

7. CONCLUSIONS

The method presented is an extension of usual particle methods and is suitable to treat a collisional term on the right-hand side of a kinetic equation. The density function is approximated by a set of "particles," suitably distributed in the phase space. The equations of motion of these particles are the usual dynamic equations of the collisionless case plus an additional term which describes the collisions. Note that there is no abrupt change in the position and velocity of the "particles" due to collisions, as in Monte Carlo simulations.

The technique can handle both differential and integral operators. It can be used also for non-linear integral operators, as in the Boltzmann equation. The difference in the various cases essentially consists in the number of operations required per time step. In a space homogeneous case the complexity is $O(N)$ for the diffusion equation, $O(N^2)$ for a linear collisional operator, and $O(N^3)$ for a quadratic integral operator. This disadvantage is compensated by the accuracy that can be

reached by this method. In one dimension second-order schemes are easily derived. In this paper we described the general characteristics of the method and devised numerical schemes for the one-dimensional, space-homogeneous case. We are presently working on multi-dimensional codes, both space-homogeneous and non-homogeneous.

The main difficulty in the multi-dimensional case is the reconstruction of the density function f at each particle location at each time step. This is equivalent to assigning to each point of a set the value of the local "density" of the points. To our knowledge there is no satisfactory way to compute this term in a fast and accurate way in more than one dimension.

The technique applied to the diffusion equation leads to many interesting properties that we briefly mention and that we hope to develop further.

(i) The use of the Lagrangian coordinate shows the equivalence between the usual diffusion equation and the quasi-linear diffusion equation:

$$\frac{\partial F}{\partial t} = F^2 \frac{\partial^2 F}{\partial X^2} \Leftrightarrow \frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2}.$$

Here $F(X, t) = f(x, t)$ and $X = \int_{-\infty}^{x} f(y, t)\, dy$.

(ii) The particle solution of the heat equation can be used to distribute particles according to a given function.

(iii) It can be used to define a "canonical" transformation from a uniform distribution to a given distribution.

(iv) It is a deterministic way to introduce diffusion within a particle scheme.

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