Iterative Solution of the Boltzmann Equation

D. H. Fujii,[1,2] R. O. Barrachina,[1,3] and C. R. Garibotti[1,4]

We define an iterative scheme to solve the nonlinear Boltzmann equation. Conservation rules are maintained at each iterative step. We apply this method to a spatially uniform and isotropic velocity distribution function on the Maxwell and very-hard-particle models. A particular example is evaluated and results are compared with the exact solution. It shows to be a very fast convergent approach.

1. INTRODUCTION

The nonlinear Boltzmann equation (NLBE) was proposed in 1872 by Ludwig Boltzmann. When a spatially uniform gas with no external forces acting on it is considered, the NLBE for the one particle velocity distribution function $f(\mathbf{v}, t)$ reads

$$\frac{\partial f}{\partial t} = B[f, f] \tag{1}$$

where $B[f, f]$ is a bilinear collision operator which depends on the interaction law between the particles, i.e.

$$B[f, f] = \int d\hat{g}' \, d\mathbf{v}_1 \, gI(g, \hat{g} \cdot \hat{g}')[f(\mathbf{v}', t) f(\mathbf{v}'_1, t) - f(\mathbf{v}, t) f(\mathbf{v}_1, t)] \tag{2}$$

$\mathbf{g} = (\mathbf{v} - \mathbf{v}_1)$ and $\mathbf{g}' = (\mathbf{v}' - \mathbf{v}'_1)$ are the relative speeds of particles before and

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[1] Centro Atómico Bariloche, 8400 Bariloche, R.N., Argentina.
[2] Fellow of the Conselho Nacional de Desenvolvimento Cientifico e Tecnológico, Brasil.
[3] Comisión Nacional de Energía Atómica, Argentina.
[4] Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina.

after the collision of cross-section $I(g, \hat{g} \cdot \hat{g}')$; $\hat{g}$ is a unit vector in the direction of g.

Research on the NLBE was induced by the lack of an explicit solution for the associated initial and boundary problem. Recently many authors have suggested approximation methods, which provide a good description of the temporal evolution of the distribution function for some particular interaction models.

Some of the earlier procedures are those related to perturbative methods. A first approach in this direction was presented by Hilbert[1] in 1912 and Enskog[2] and Chapman[3] in 1917. They expanded f as a power series of the Knudsen number.[4] The zero order of this expansion leads to the Euler's equations for an ideal gas; the first order provides the hydrodynamical Navier–Stokes equations. Higher orders give the Burnett equations. Recently, Bobylev[5] used a simplified model and showed that Burnett (second-order) equations do not improve, as hoped, the results obtained with the first-order equations (Navier–Stokes). This is a discussion point about the convergence properties of the approach.

Carleman[6] solved the NLBE for an isotropic gas of elastic spheres and proved the existence of solutions using an iterative method. This is considered one of the most simple cases; however, a general solution is not known.[7]

The distribution function expanded in Hermite's polynomial is presented by Grad.[8] When second-order terms are kept in the expansion the distribution function is determined by thirteen moments. The results of this approximation agree with that of Hilbert, Chapman, and Enskog for some special cases.[9]

In 1951, Wild[10] transformed the NLBE in an iteratively solvable integral equation. He applied the method for a gas with molecules interacting in such a way that the differential scattering cross section is inversely proportional to their relative velocities. The convergence of the method requires the cut-off of small scattering angles. The application of this method is exclusively restricted to this particular pseudo-Maxwellian interaction model. Later on, Arkeryd extended this approach to probe convergence of NLBE solutions for more general interactions.[11]

In Section II we consider an iterative method for solving the NLBE. It is based on a perturbation scheme in terms of the deviation from equilibrium. It is known that the linearized solution of the problem is proper when the deviation from equilibrium is small. Therefore, nonlinear effects—introduced through an iterative procedure—should improve the approximation. An analytical proposal of this method was previously outlined by Cercignani[4] and Shizuta,[12] but examples about the velocity of convergence were not given in the literature.

In Section IIIA, we describe the method for Maxwell molecules. In this case we expand the distribution function in terms of the eigenfunctions of the linearized collision operator, with coefficients that can be iteratively evaluated. The method is also applied to the very-hard-particle model which was introduced by Ernst and Hendriks[13] in 1979. In Section IV, we evaluate a simple example for a particular initial condition.

2. DESCRIPTION OF THE METHOD

The nonlinear Boltzmann equation for the distribution function $f(\mathbf{v}, t)$ of a spacially homogeneous gas can be written as follows

$$\frac{\partial}{\partial t} f(\mathbf{v}, t) - L[f] = A[f, f] \tag{3}$$

with

$$L[f] = B[f, f_0] + B[f_0, f] \tag{4.a}$$

$$A[f, f] = B[f, f] - B[f, f_0] - B[f_0, f] \tag{4.b}$$

f_0 represents the equilibrium distribution function, i.e

$$f(\mathbf{v}, t) \xrightarrow[t \to \infty]{} f_0(v) = \frac{e^{-v^2/2}}{(2\pi)^{d/2}} \tag{5}$$

where d is the phase space dimension. The total number of particles and total energy are conserved

$$\int f(\mathbf{v}, t) \, d\mathbf{v} = 1 \qquad \int f(\mathbf{v}, t) \, \mathbf{v} \, d\mathbf{v} = 0 \qquad \int f(\mathbf{v}, t) \, v^2 \, d\mathbf{v} = d \tag{6}$$

When the deviation from equilibrium

$$R(\mathbf{v}, t) = \frac{f(\mathbf{v}, t) - f_0(v)}{f_0(v)} \tag{7}$$

is small, we can neglect the bilinear terms in $R(\mathbf{v}, t)$ obtaining the linearized Boltzmann equation

$$\frac{\partial}{\partial t} f_1(\mathbf{v}, t) - L[f_1] = 0 \tag{8}$$

Its solution is generally believed to be a good approximation for the distribution function. However, it does not properly describe the time

evolution of the system when the initial deviation from equilibrium is important. In that situation we can calculate a second-order approximation including the bilinear term. Actually we propose an iterative scheme in order to solve the nonlinear Boltzmann equation

$$\frac{\partial}{\partial t} f_l(\mathbf{v}, t) - L[f_l] = A[f_{l-1}, f_{l-1}] \qquad l = 1, 2,... \tag{9}$$

Integration of this equation provides the *l*-iterative approximation for the distribution function.

It is easily shown that the conservation laws (6) and the asymptotic condition (5) are verified by each iteration order. This is a remarkable improvement upon Wild's approach.

3. APPLICATIONS

A. Maxwell Interaction Model

First we study Maxwell models, where the collision rate reads

$$gI(g, \hat{g} \cdot \hat{g}') = \alpha(\hat{g} \cdot \hat{g}') \tag{10}$$

The solution of the NLBE for isotropic initial conditions can be represented by an expansion in Laguerre polinomials[7]

$$f(v, t) = f_0(v) \sum_{n=0}^{\infty} c_n(t) L_n^{(d/2)-1}(v^2/2) \tag{11}$$

when the distribution function belongs to a Hilbert space with norm

$$\|f\|^2 = \int \frac{|f(v, t)|^2}{f_0(v)} d\mathbf{v} < \infty \tag{12}$$

The coefficients $c_n(t)$ satisfy a set of sequentially solvable equations

$$c_0(t) = 1 \tag{13a}$$

$$c_1(t) = 0 \tag{13b}$$

$$c_n(t) = c_n(0) e^{-A_n t} + \sum_{m=1}^{n-1} \mu_{nm} \int_0^t e^{-A_n(t-\tau)} c_m(\tau) c_{n-m}(\tau) d\tau \tag{13c}$$

where

$$A_n = \int_0^\pi \frac{2\pi^{(d-1)/2}}{\Gamma((d-1)/2)} (\sin x)^{d-2} \alpha(\cos x) \left[1 + \delta_{n0} - \left(\frac{1+\cos x}{2}\right)^n \right.$$

$$\left. - \left(\frac{1-\cos x}{2}\right)^n \right] dx \tag{14}$$

$$\mu_{nm} = \binom{n}{m} \int_0^\pi \frac{2\pi^{(d-1)/2}}{\Gamma((d-1)/2)} (\sin x)^{d-2} \alpha(\cos x) \left(\frac{1+\cos x}{2}\right)^m$$

$$\times \left(\frac{1-\cos x}{2}\right)^{n-m} dx \tag{15}$$

The coefficients A_n are the known eingenvalues of the linearized collision operator $L[f]$.[7]

We can formalize the iterative scheme (9) for the moments c_n as follows

$$c_n^{(0)}(t) = \delta_{n0}$$

$$c_n^{(l)}(t) = c_n(0) e^{-A_n t} + \sum_{m=1}^{n-1} \mu_{nm} \int_0^t e^{-A_n(t-\tau)} c_m^{(l-1)}(\tau) c_{n-m}^{(l-1)}(\tau) d\tau \tag{16}$$

In view that the first two moments $c_0^{(l)}$ and $c_1^{(l)}$ are the same for each iteration order, the number of particles and the total energy are conserved in the iterative scheme.

The convergence of $c_n^{(l)}$ to c_n can be proved by an algebraical comparison of (13) with (16), obtaining that

$$c_n^{(l)}(t) = c_n(t) \tag{17}$$

for

$$l \geqslant (n-3)/2 \tag{18}$$

Therefore the partial sums

$$S_N = f_0(v) \sum_{n=0}^N c_n(t) L_n^{(d/2)-1}(v^2/2) \tag{19}$$

of expansion (11) will be exactly reproduced by the approximate solution $f^{(l)}$ for $l \geqslant (N-3)/2$. However, $f^{(l)}$ will contain further information about the higher moments not contained in S_N. Actually, $f^{(l)}$ will converges to f when usual mathematical conditions are fulfilled.

B. Very Hard Particles

The collision rate that defines the bidimensional $(d=2)$ VHP model is

$$gI(g, \cos x) = \tfrac{1}{2} g^2 |\sin x| \tag{20}$$

and the corresponding NLBE reads[13]

$$\frac{\partial}{\partial t} f(\mathbf{v}, t) = \int d\mathbf{v}_1 \int_0^\pi dx \, g^2 |\sin x| \, [f(\mathbf{v}', t) f(\mathbf{v}_1', t) - f(\mathbf{v}, t) f(\mathbf{v}_1, t)] \tag{21}$$

The application of the Laplace transform

$$G(z, t) = 2\pi \int_0^\infty v e^{-zv^2/2} f(v, t) \, dv \tag{22}$$

$$f(v, t) = \frac{1}{4\pi^2 i} \int_{\Gamma - i\infty}^{\Gamma + i\infty} e^{zv^2/2} G(z, t) \, dz \qquad \Gamma > 0 \tag{23}$$

to (21) results in a nonlinear partial differential equation

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial z} + 1 \right) G(z, t) = \frac{1}{z} (1 - G^2) \tag{24}$$

with solution[13]

$$G(z, t) = \frac{1 + (z-1) e^z \beta(z+t)}{(z-1) - e^z \beta(z+t)} \tag{25}$$

where $\beta(z+t)$ can be determined from the initial distribution function.

Following (3) and (4) we obtain the corresponding iterative resolution scheme for the G function

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial z} + 1 \right) G_l(z, t) = \frac{1}{z} \left(1 - \frac{2}{1+z} G_l \right) - \frac{1}{z} \left(G_{l-1}^2 - \frac{2}{1+z} G_{l-1} \right) \tag{26}$$

with

$$G_0(z, t) = \frac{1}{1+z} \tag{27}$$

For $l = 1$ this equation reads

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial z} + 1 \right) G_1(z, t) = \frac{1}{z} \left[1 - \frac{1}{1+z} \left(\frac{1}{1+z} - 2G_1 \right) \right] \tag{28}$$

with solution

$$G_1(z, t) = \frac{1}{1+z}\left[1 + z^2\alpha_1^{(1)}(z+t)\frac{e^z}{1+z}\right] \tag{29}$$

The arbitrary function $\alpha_1^{(1)}$ is determined from the initial conditions $G(z, 0)$

$$\alpha_1^{(1)}(z) = \left(\frac{1+z}{z}\right)^2 e^{-z}\left[G(z, 0) - \frac{1}{1+z}\right] \tag{30}$$

A general solution can be easily proved

$$G_l(z, t) = \frac{1}{1+z}\left[1 + z^2\sum_{n=1}^{2^{l-1}}\alpha_n^{(l)}(z+t)\left(\frac{e^z}{1+z}\right)^n\right] \tag{31}$$

From (26) and (31) we obtain

$$\alpha_n^{(l)} = \frac{1}{n-1}\sum_{m=1}^{n-1}\alpha_m^{(l-1)}\alpha_{n-m}^{(l-1)} \qquad n \neq 1 \tag{32}$$

Now we can prove that (31) reproduces the exact solution when $l \to \infty$. Actually, (32) assures that the limit of $\alpha_n^{(l)}$ must be of the form

$$\alpha_n^{(l)} \xrightarrow[l \to \infty]{} \beta^n \tag{33}$$

where β is as in (25). Replacing in (31) we obtain

$$G_l(z, t) \xrightarrow[l \to \infty]{} \frac{1}{1+z}\left\{1 + z^2\sum_{n=1}^{\infty}\left[\beta(z+t)\frac{e^z}{1+z}\right]^n\right\} \tag{34}$$

which can be compared with the expansion of (25) in powers of β.

Now, we will write the solution G_l in a suitable form for deriving the transformed solution.
Defining

$$U(z) = \frac{1+z}{z^2}\left[G(z, 0) - \frac{1}{1+z}\right] \tag{35}$$

and denoting a polynomial in x of degree m by $P_m(x)$, we have

$$\alpha_n^{(l)}(z) = \{[(1+z)/e^z]\,U(z)\}^n\,P_{2^{l-1}-n}(U) \tag{36}$$

This relation can be proved by induction in (32). Replacing in (31), we see that G_l contains the initial conditions $U(z+t)$ up to a 2^{l-1} power.

Actually, the singularities of G_l are those introduced by the initial condition.

For an initial condition with k poles located in σ_i, G_l is shown to be a proper rational function of $1/z$, i.e., one in which the degree of the numerator is smaller than the degree of the denominator. In this case

$$G_l(z, t) = \sum_{n=1}^{1+2^{l-1}} A_n^{(l)}(t) \left(\frac{z}{1+z}\right)^n + \sum_{n=1}^{2^{l-1}} \sum_{i=1}^{k} B_{n,i}^{(l)}(t) \left[\frac{z(\sigma_i + t)}{z + \sigma_i + t}\right]^n \tag{37}$$

The coefficients $A_n^{(l)}$, $B_{n,i}^{(l)}$ are directly given by the iterative method. The associated distribution function is

$$f_l(v, t) = e^{-v^2/2} \sum_{n=1}^{1+2^{l-1}} A_n^{(l)}(t) L_n^{(0)}(v^2/2)$$

$$+ \sum_{n=1}^{2^{l-1}} \sum_{i=1}^{k} B_{n,i}^{(l)}(t) e^{-v^2(\sigma_i + t)/2} L_{n-1}^{(0)}[v^2(\sigma_i + t)/2] \tag{38}$$

This expression looks quite similar to the modified Laguerre expansion proposed by Hendriks and Ernst[7] for Maxwell interaction model. However, a set of sequential equations for the recurrent determination of the coefficients $A_n^{(l)}$ and $B_n^{(l)}$, could not be found.

IV. RESULTS AND DISCUSSION

Now we check the method by comparing the approximate iterative solutions with the exact one for a particular example.

Let us consider a VHP model with a simple initial condition given by the superposition of two Maxwellian,[14] i.e.

$$f(v, 0) = a_1 e^{-\sigma_1 v^2/2} + a_2 e^{-\sigma_2 v^2/2} \tag{39}$$

The conditions of conservation and positivity of the distribution require

$$a_1 = \sigma_1 \frac{\sigma_2 - 1}{\sigma_2 - \sigma_1} \quad \text{and} \quad a_2 = \sigma_2 \frac{\sigma_1 - 1}{\sigma_1 - \sigma_2} \tag{40.a}$$

$$\frac{\sigma_1 + \sigma_2}{\sigma_1 \sigma_2} \geqslant 1 \quad \text{and} \quad \sigma_2 > 1 \tag{40.b}$$

The Laplace transformed initial distribution reads

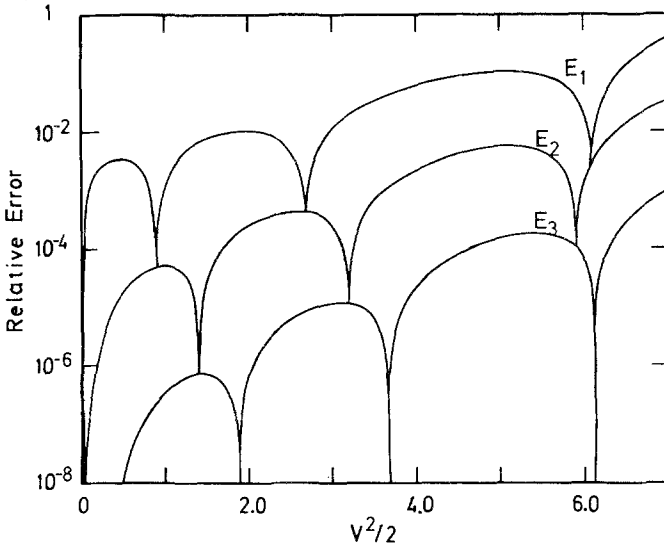$$G(z, 0) = \frac{a_1}{z + \sigma_1} + \frac{a_2}{z + \sigma_2} \tag{41}$$

Fig. 1.   Relative error E_1, E_2, and E_3 of the iterative approach as a function of energy for the VHP model at $t = 0.2$. Initial conditions given by (39) with $\sigma_1 = 20/11$ and $\sigma_2 = 20/9$.

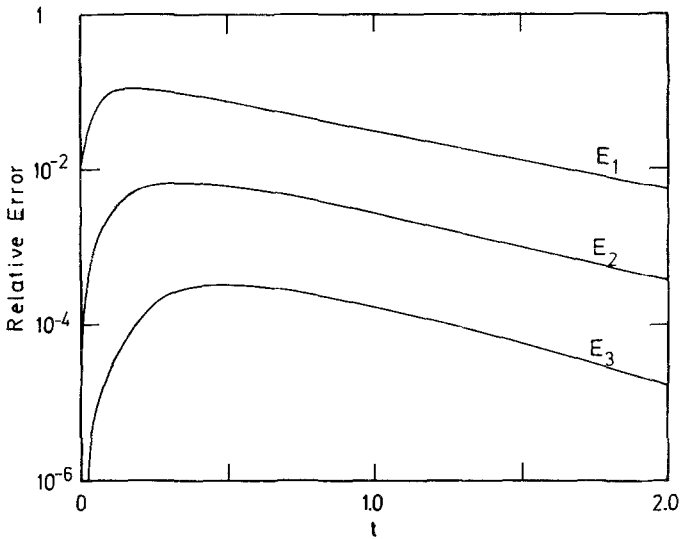
Fig. 2.   Relative error E_1, E_2, and E_3 of the iterative approach as a function of time for VHP model at $v^2 = 10$. Initial condition as in Fig. 1.
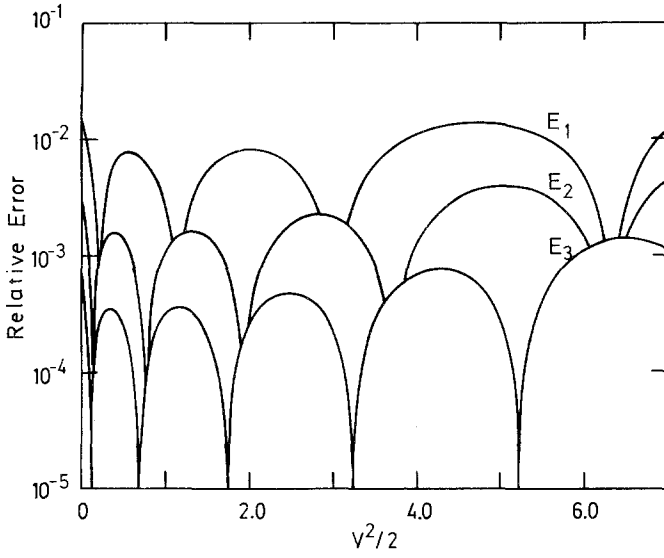
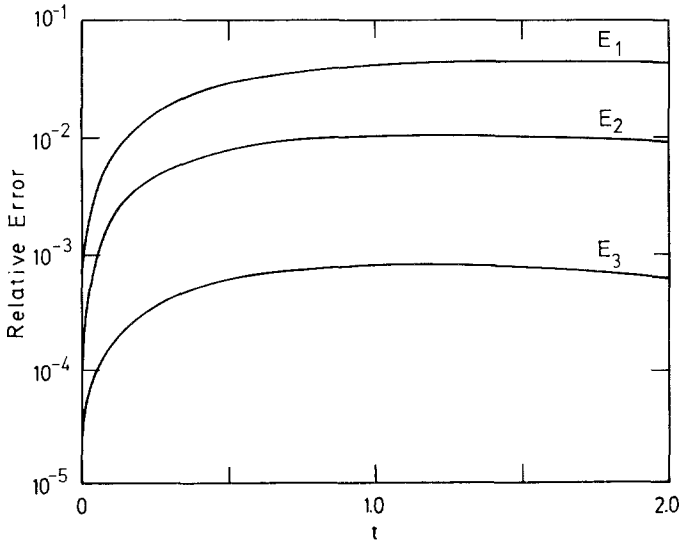Fig. 3.   As in Fig. 1 for the Tjon–Wu model.

Fig. 4.   As in Fig. 2 for the Tjon–Wu model.

Applying (37) we obtain the following expression for the l-order solution of the iterative scheme

$$G_l(z, t) = \sum_{n=1}^{1+2^{l-1}} A_n^{(l)}(t) \left(\frac{z}{1+z}\right)^n + \sum_{n=1}^{2^{l-1}} B_{n,1}^{(l)}(t) \left[\frac{z(\sigma_1 + t)}{z + \sigma_1 + t}\right]^n$$
$$+ \sum_{n=1}^{2^{l-1}} B_{n,2}^{(l)}(t) \left[\frac{z(\sigma_2 + t)}{z + \sigma_2 + t}\right]^n \tag{42}$$

We have calculated the coefficients $A_n^{(l)}$ and $B_{n,i}^{(l)}$ for various values of the initial parameters σ_1 and σ_2. We define the relative error of the l-iterative solution in the following way

$$E_l(v, t) = \frac{f_l(v, t) - f(v, t)}{f(v, t)} \tag{43}$$

where $f(v, t)$ is the exact distribution.

In Fig. 1 we show the results for $\sigma_1 = 20/11$, $\sigma_2 = 20/9$, and time $t = 0.2$. We observed an oscillatory convergence. Considering that the error is outlined by the enveloping curves, we observed a fast convergence of the iterative process. The E_l shows an error 10 times smaller than E_{l-1} over the whole energy range. Figure 2 shows E_l ($l = 1, 2, 3$) for a fixed value of energy. We note that the convergence of the iterative approach is faster at large times and slower for large energies. Actually, the relevance of non-linear contributions is more important at small times. Furthermore, we verify that the iterative solution gives a satisfactory description of the relaxation to the equilibrium process over the whole energy range.

We have also applied the method to the Maxwell model described in Section IIIA with the initial condition given by (39) and the same values of the parameters as in the VHP case. However, in this case, comparison of approximate and exact solutions is hidden by the twofold approximation implicit in (11). Actually, the orders of the iterative scheme and the N truncation of expansion (11) have to be taken into account. In this case, we define E_l as the error of the series with coefficients $c_n^{(l)}$ relative to the series with the exact ones, both truncated to the same order. For the Tjon–Wu model $\mu_{nm} = 1/(n+1)$ we were able to calculate the series up to $N = 18$. We note that at large time the double approximation scheme becomes critical and no conclusion can be stated about the velocity of convergence.

ACKNOWLEDGMENTS

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