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Wild's Solution of the Nonlinear Boltzmann Equation

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The relaxation to equilibrium of a spatially uniform pseudo-Maxwellian gas is considered. A modified Wild expansion is defined for solving the nonlinear Boltzmann equation. The positivity and asymptotic conditions, as well as the conservation rules, are maintained at each truncation order. Some particular examples are evaluated. The comparison with exact solutions illustrates the very fast convergence of this method.

KEY WORDS: Boltzmann equation; Wild expansion; Maxwell molecules.

1. INTRODUCTION

I consider a dilute gas of structureless particles that interact through binary elastic collisions. The temporal evolution of the corresponding one-particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ is characterized by the nonlinear Boltzmann equation. Research on this equation was induced by the lack of an explicit solution for the associated initial and boundary value problem.[1,2] A large number of approximation methods for solving this problem has been suggested.[3] A pioneering approach in this direction is given by the Chapman–Enskog method,[4] which leads to successive refinements (in the Knudsen number) of the hydrodynamic equations. However, the convergence of this approach is a subject of discussion in the literature.[5] Other techniques of solution are based upon the so-called moment methods.[3] In the Grad moment method the distribution function is expanded in Hermite polynomials.[6] Another iterative method for solving the nonlinear Boltzmann equation is a perturbation scheme in terms of the deviation from equilibrium.[7] It is known that the linearized solution is a good approximation when the deviation from equilibrium is small.

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Therefore, nonlinear effects, introduced through an iterative procedure, should improve the approximation.

In order to gain insight into the Boltzmann equation, a great variety of interaction models have been considered in the literature.[3] For instance, Maxwell-type models provide a large simplification of the Boltzmann equation, since their collision probabilities do not depend on the relative velocity of the colliding particles.[2] Within these models, significant progress has been achieved in the study of the exact solutions of the nonlinear equation for spatially homogeneous distributions $f(\mathbf{v}, t)$. In this case the general solution is known within a certain Hilbert space $\mathscr{L}_2(R^d)$ with norm $\int |f(\mathbf{v}, t)|^2/f_{eq}(v)\, d\mathbf{v}$. This solution is given in the form of an expansion in orthogonal polynomials. The time-dependent coefficients in this expansion obey a solvable coupled set of nonlinear equations.[2] This solution has been extensively studied by the sequential resolution of the coupled system up to some order and the numerical evaluation of the resulting truncated series.[8] This procedure is restricted to low values of the velocity, where not too many terms in the series are required. Furthermore, it is very difficult to guarantee the positivity of the truncated series at all times.

In the present paper I introduce an approximation procedure for solving the homogeneous Boltzmann equation for Maxwell-type interaction models. This method is essentially different from the above-mentioned ones. It is based upon a modified version of Wild's approach.[9] I show that the positivity and asymptotic condition as well as the conservation laws are verified by each iteration order. Furthermore, the unphysical restriction to the Hilbert space $\mathscr{L}_2(R^d)$ is eliminated in this method. These are remarkable improvements over other approximate approaches.

In the following section I state the notation to be used. In Section 3 I introduce the method, which separates the distribution function in collision classes with a quite simple analytical structure. In Section 4 I show that the time evolution features of $f(\mathbf{v}, t)$ are mainly given by the first few terms in this expansion. Using this technique, I study the relaxation toward equilibrium of different initial distribution functions. I conclude with a discussion of the results.

2. BASIC CONCEPTS AND NOTATION

The nonlinear Boltzmann equation for the distribution function $f(\mathbf{r}, \mathbf{v}, t)$ of a dilute gas of structureless particles without internal degrees of freedom reads[3]

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{r}} + \frac{\mathbf{F}}{m}\cdot\nabla_{\mathbf{v}}\right) f(\mathbf{r}, \mathbf{v}, t) = B[f, f] \tag{2.1}$$

where

$$B[f, f] = \int d\mathbf{v}_1\, d\hat{\mathbf{n}}\, |\mathbf{v} - \mathbf{v}_1|\, \sigma\left(|\mathbf{v} - \mathbf{v}_1|, \frac{(\mathbf{v} - \mathbf{v}_1) \cdot \hat{\mathbf{n}}}{|\mathbf{v} - \mathbf{v}_1|}\right)$$
$$\times [f(\mathbf{r}, \mathbf{v}', t)\, f(r, \mathbf{v}_1', t) - f(\mathbf{r}, \mathbf{v}, t)\, f(r, \mathbf{v}_1, t)] \tag{2.2}$$

is the bilinear collision operator. σ is the differential cross section for the binary collision $(\mathbf{v}, \mathbf{v}_1) \to (\mathbf{v}', \mathbf{v}_1')$. The incoming and postcollisional velocities are related by the dynamics

$$\mathbf{v}' = \tfrac{1}{2}(\mathbf{v} + \mathbf{v}_1) + \tfrac{1}{2}|\mathbf{v} - \mathbf{v}_1|\, \hat{\mathbf{n}} \tag{2.3a}$$

$$\mathbf{v}_1' = \tfrac{1}{2}(\mathbf{v} + \mathbf{v}_1) - \tfrac{1}{2}|\mathbf{v} - \mathbf{v}_1|\, \hat{\mathbf{n}} \tag{2.3b}$$

Here $\hat{\mathbf{n}}$ is a unit vector in the direction of $\mathbf{v}' - \mathbf{v}_1'$. In view of the possible application to systems of one, two, or three dimensions, we consider the position $\mathbf{r}$ and velocity $\mathbf{v}$ of the particle as vectors of arbitrary dimension d.

When a spatially homogeneous gas with no external forces acting on it is considered, the nonlinear Boltzmann equation in d dimensions reads

$$\frac{\partial}{\partial t} f(\mathbf{v}, t) = B[f, f] \tag{2.4}$$

Conservation of particles, momentum, and energy requires (in appropriate units)

$$\int f(\mathbf{v}, t)\, d\mathbf{v} = 1 \tag{2.5a}$$

$$\int f(\mathbf{v}, t)\mathbf{v}\, d\mathbf{v} = 0 \tag{2.5b}$$

$$\int f(\mathbf{v}, t) v^2\, d\mathbf{v} = d \tag{2.5c}$$

The second conservation law indicates that the temporal evolution of the gas is observed from the center-of-mass reference frame. The H theorem guarantees that the distribution function will approach its equilibrium state,[10]

$$f(\mathbf{v}, t) \xrightarrow[t \to \infty]{} f_{\text{eq}}(v) = (2\pi)^{-d/2}\, e^{-v^2/2} \tag{2.6}$$

Furthermore, if the distribution function is initially nonnegative, then Eq. (2.1) preserves this property at later times.

In order to simplify the complex mathematical structure of the collision term (2.2), one looks for mathematical models of the cross section with a simple dependence on the relative velocity and the scattering angle. Maxwell models provide this simplification. For these models the collision probability does not depend on the relative velocity of the colliding particles:

$$v\sigma(v, \cos\theta) = \alpha(\cos\theta) \tag{2.7}$$

Such a scattering cross section may be obtained from a repulsive potential $V(r) = ar^{-2(d-1)}$. For these Maxwell molecules the probability $\alpha(\cos\theta)$ is a complicated function of its arguments.[3] However, one may define more general mathematical models by a convenient choice of the function $\alpha(\cos\theta)$. For instance, one may define the so-called pseudo-Maxwell models, for which the collision frequency is required to be finite,

$$\mu = \int \alpha(\hat{\mathbf{v}} \cdot \hat{\mathbf{n}})\, d\hat{\mathbf{n}} < \infty \tag{2.8}$$

It is worth mentioning that this condition is not fulfilled by Maxwell molecules, since the total cross section for a repelling $r^{-2(d-1)}$ potential is infinite.

3. DESCRIPTION OF THE METHOD

The purpose of this paper is to tackle the nonisotropic Boltzmann equation for a pseudo-Maxwellian gas. We rewrite Eq. (2.4) in the following way:

$$\left(\frac{1}{\mu}\frac{\partial}{\partial t} + 1\right) f(\mathbf{v}, t) = J[f, f] \tag{3.1}$$

with

$$J[h, g] = \frac{1}{\mu}\int \alpha\left(\frac{(\mathbf{v} - \mathbf{v}_1)\cdot\hat{\mathbf{n}}}{|\mathbf{v} - \mathbf{v}_1|}\right) h(\mathbf{v}', t)\, g(\mathbf{v}_1', t)\, d\mathbf{v}_1\, d\hat{\mathbf{n}} \tag{3.2}$$

In this case the general solution is known within a certain Hilbert space $\mathscr{L}_2(R^d)$ with norm[2]

$$\int |f(\mathbf{v}, t)|^2 / f_{\text{eq}}(v)\, d\mathbf{v} < \infty \tag{3.3}$$

This solution is given in the form of an expansion in terms of the eigenfunctions of the corresponding linearized equation. The time-dependent

coefficients in this expansion can be found sequentially from a solvable coupled set of nonlinear equations. In actual numerical calculations this solution is restricted to moderate values of the velocity $v < v_0$, where not too many terms in the series are required. This v_0 is an increasing function of the truncation order and time.[8] Therefore, it is desirable to improve the numerical convergence, especially for small times and large velocities. Furthermore, it is very difficult to guarantee the positivity of the truncated expansion at all times.

Before proceeding further, it is worth mentioning that there are no physical reasons for restricting considerations to functions in the Hilbert space $\mathscr{L}_2(R^d)$.[2] So we seek solutions in the usual Banach space $L_1(R^d)$ with norm

$$\int |f(\mathbf{v}, t)|\, d\mathbf{v} < \infty \tag{3.4}$$

In this space the collision term (3.2) is a bounded and continuous bilinear operator $J: L_1 \times L_1 \to L_1$. I propose a solution of the previous initial value problem with the following form:

$$f(\mathbf{v}, t) = \sum_{n=0}^{\infty} C_n(t)\, R_n(\mathbf{v}) \tag{3.5}$$

where the factors $R_n(\mathbf{v})$ are defined by induction,

$$R_0(\mathbf{v}) = f(\mathbf{v}, 0) \tag{3.6a}$$

$$R_n(\mathbf{v}) = \frac{1}{n} \sum_{q=0}^{n-1} J[R_{n-q-1}, R_q] \tag{3.6b}$$

These "collision factors" have a very clear physical meaning, as the distribution function of particles that result from a precise number of collisions. Actually, $R_n(\mathbf{v})$ consists of molecules that, belonging to $R_q(\mathbf{v})$ with $q < n$, have made a collision with molecules of $R_{n-q-1}(\mathbf{v})$. Those particles that have not collided since $t = 0$ are described by $R_0(v)$. The first collision factors read explicitly

$$R_0 = f(\mathbf{v}, 0) \tag{3.7a}$$

$$R_1 = J[R_0, R_0] \tag{3.7b}$$

$$R_2 = \tfrac{1}{2} J[J[R_0, R_0], R_0] + \tfrac{1}{2} J[R_0, J[R_0, R_0]] \tag{3.7c}$$

$$\begin{aligned} R_3 = {} & \tfrac{1}{6} J[J[J[R_0, R_0], R_0], R_0] + \tfrac{1}{6} J[J[R_0, J[R_0, R_0]], R_0] \\ & + \tfrac{1}{6} J[R_0, J[J[R_0, R_0], R_0]] + \tfrac{1}{6} J[R_0, J[R_0, J[R_0, R_0]]] \\ & + \tfrac{1}{3} J[J[R_0, R_0], J[R_0, R_0]] \end{aligned} \tag{3.7d}$$

Placing expansion (3.5) into Eq. (3.1), one finds that the coefficients $C_n(t)$ can be exactly evaluated:

$$C_n(t) = e^{-\mu t}(1 - e^{-\mu t})^n \tag{3.8}$$

Then Eq. (3.5) is a representation of the distribution function in the form of a Wild expansion.[9,11] Its partial sums constitute a positive monotonic sequence which, in view of the Lebesgue monotone convergence theorem, converges to a Banach solution of the Boltzmann equation.

The coefficient $C_n(t)$ weights the contribution to the distribution function $f(\mathbf{v}, t)$ of the collision factor $R_n(\mathbf{v})$. We notice in Fig. 1a that this contribution is maximum at

$$t_n = \frac{1}{\mu} \ln(1 + n) \tag{3.9}$$

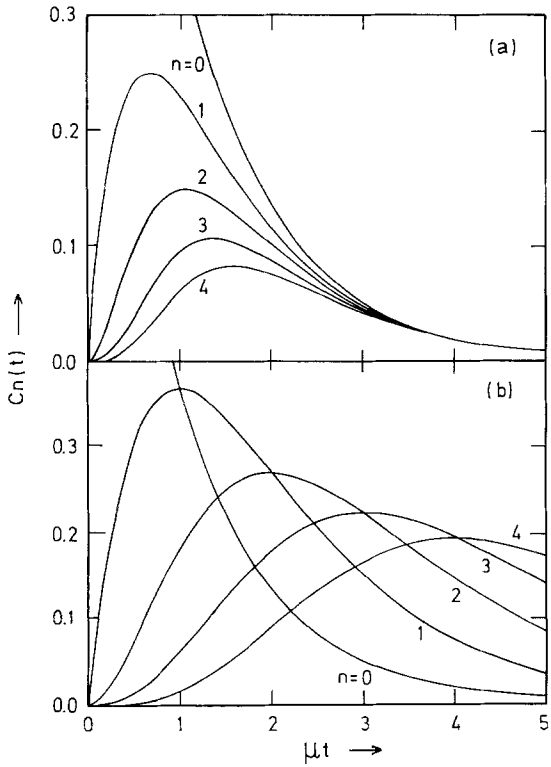

Fig. 1. (a) Time evolution of the coefficients $C_n(t)$ of expansion (3.5) and (b) for the linearized version (3.10).

This is not the case in the linearized version of expansion (3.5):

$$f(\mathbf{v}, t) \approx \sum_{n=0}^{\infty} C_n^{\mathrm{L}}(t)\, R_n^{\mathrm{L}}(\mathbf{v}) \tag{3.10}$$

with

$$R_0^{\mathrm{L}}(\mathbf{v}) = f(\mathbf{v}, 0) \tag{3.11a}$$

$$R_n^{\mathrm{L}}(\mathbf{v}) = J[R_{n-1}^{\mathrm{L}}, f_{\mathrm{eq}}] + J[f_{\mathrm{eq}}, R_{n-1}^{\mathrm{L}}] - f_{\mathrm{eq}}(v) \tag{3.11b}$$

and

$$C_n^{\mathrm{L}}(t) = \frac{1}{n!}\, e^{-\mu t}(\mu t)^n \tag{3.12}$$

where the contribution of the linearized factor $R_n^{\mathrm{L}}(\mathbf{v})$ is dominant after n collision times; namely

$$t_n^{\mathrm{L}} = n/\mu \tag{3.13}$$

It is reasonable to expect that the collision factor $R_n(v)$ will be more independent of the initial distribution function as the number of collisions increases.[9] This idea can be stated more precisely by resumming expansion (3.5). Actually, since

$$\sum_{n=0}^{\infty} C_n(t) = 1 \tag{3.14}$$

we can write

$$f(\mathbf{v}, t) = f_{\mathrm{eq}}(v) + \sum_{n=0}^{\infty} C_n(t)[R_n(\mathbf{v}) - f_{\mathrm{eq}}(v)] \tag{3.15}$$

Now the contribution of the high-order terms in this series is less important, and an approximate solution of Boltzmann equation can be defined by truncating it:

$$f_N(\mathbf{v}, t) = f_{\mathrm{eq}}(v) + \sum_{n=0}^{N} C_n(t)[R_n(\mathbf{v}) - f_{\mathrm{eq}}(v)] \tag{3.16}$$

It is immediately seen that this solution is positive, since $R_n(\mathbf{v}) \geqslant 0$ and $\sum_{n=0}^{N} C_n(t) \leqslant 1$. This is an important improvement over other

approximation methods. Furthermore, the conservation and asymptotic conditions are maintained independently of the truncation order

$$\int f_N(\mathbf{v}, t)\, d\mathbf{v} = 1 \tag{3.17a}$$

$$\int f_N(\mathbf{v}, t)\mathbf{v}\, d\mathbf{v} = 0 \tag{3.17b}$$

$$\int f_N(\mathbf{v}, t)v^2\, d\mathbf{v} = d \tag{3.17c}$$

$$f_N(\mathbf{v}, t) \xrightarrow[t\to\infty]{} f_{\text{eq}}(v) \tag{3.18}$$

It is worth indicating that these conditions are not verified in a direct truncation of Wild's sum (3.5).

Finally, I compare the approximate solution (3.16) with the iterative scheme devised by Wild.[9] He defined a mild solution of Boltzmann equation (3.1) as the limit of the following iteration:

$$f_0^{\text{W}}(\mathbf{v}, t) = e^{-\mu t} f(\mathbf{v}, 0) \tag{3.19a}$$

$$f_N^{\text{W}}(\mathbf{v}, t) = e^{-\mu t}\left\{ f(\mathbf{v}, 0) + \mu \int_0^t J[f_{N-1}^{\text{W}}, f_{N-1}^{\text{W}}]\, e^{\mu t'}\, dt' \right\} \tag{3.19b}$$

It is easy to show that this scheme leads to expansion (3.16).[9] However, the N iteration of this integral equation incorporates, together with the leading Nth collision factor, an enormous amount of superfluous information. Furthermore, it does not satisfy the conservation and asymptotic condition, except in the limit $N \to \infty$. In short, the expansion (3.16) represents a modification to Wild's method that overcomes the former hindrances.

In the following section I show that this representation of the distribution function can be very convenient for the numerical analysis of the relaxation process.

4. NUMERICAL CALCULATIONS

Up to now I have been concerned with the properties of the expansion in collision factors (3.15). Now I check the method by comparing the approximate solution (3.16) with the exact one for a particular example. I test the precision of the method through the BKW mode,[12]

$$f(\mathbf{v}, t) = f_{\text{eq}}(v) \frac{e^{-\sigma\varepsilon/(1-\sigma)}}{(1-\sigma)^{d/2}} \left[1 - \frac{\sigma}{1-\sigma}\left(\frac{d}{2} - \frac{\varepsilon}{1-\sigma} \right) \right] \tag{4.1a}$$

$$\sigma(t) = \sigma(0) e^{-\lambda t}, \qquad 0 \leqslant \sigma(0) \leqslant \frac{2}{2+d} \tag{4.1b}$$

$$\lambda = \frac{\Pi^{(d-1)/2}}{\Gamma[(d-1)/2]} \int \alpha(\cos\theta) \left(1 - \cos^4\frac{\theta}{2} - \sin^4\frac{\theta}{2}\right) d\theta \tag{4.1c}$$

with $\varepsilon = v^2/2$ the energy per thermal unit. This is the only known exact nontrivial solution of Eq. (2.4). Figure 2 displays the first few collision factors R_n for a two-dimensional BKW mode with $\sigma(0) = 1/4$ as a function of the energy. One observes a fast convergence to the equilibrium distribution function when the number of collisions increases. I have also evaluated the relative error for various values of energy and time. Figures 3 and 4 show the relative error of the approximate solution for the same BKW mode in the Tjon–Wu interaction model

$$\alpha(\cos\theta) = \tfrac{1}{4}\mu\,|\sin\theta| \tag{4.2}$$

In Fig. 4 the truncation order was arbitrarily fixed at $N = 4$. The convergence is very good at small and large times. Actually, the truncated expansion (3.16) provides a satisfactory description of the relaxation process over a wide energy range, which rapidly increases with time.

Henceforth, I consider the temporal evolution of an initially nonisotropic distribution, namely

$$f(\mathbf{v}, t) = f_{\text{eq}}(v)\, 2v^2 e^{-v^2/2}[1 - \cos(2\theta)] \tag{4.3}$$

with θ the polar angle of the velocity $\mathbf{v}$. Figure 5 shows the collision factors R_n up to the second order. One can see that the two overpopulated peaks spread in the angular direction for increasing number of collisions, giving rise to a population ring at an energy $\varepsilon = 1$. Once these collision factors are known, the time evolution of the system can be easily evaluated. Actually, such a simple calculation leads to a behavior similar to that of Fig. 7 of ref. 8, which was evaluated with a truncated Laguerre expansion.

5. CONCLUSIONS

I have introduced an expansion of the distribution function in collision factors for a spatially homogeneous pseudo-Maxwellian gas. This modified version of Wild's sum gives a simple physical picture of the evolution of the system. By applying the method to some particular initial condition, I have shown that it is a very suitable approach for the numerical analysis of the relaxation process. Furthermore, it satisfies the conservation laws and the positivity and asymptotic conditions, and eliminates the unphysical restric-

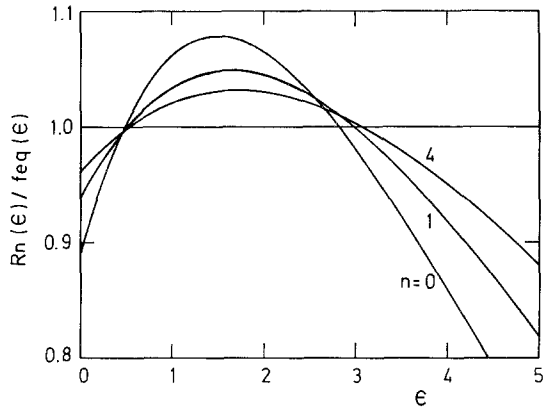

Fig. 2. Collision factors R_n for a two-dimensional BKW mode with $\sigma(0)=1/4$ as a function of the energy $\varepsilon=v^2/2$.

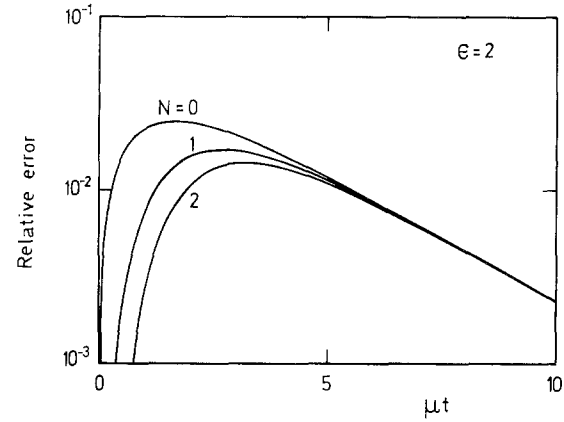

Fig. 3. Relative error of expansion (3.16) for the BKW mode $[\sigma(0)=1/4]$ in the Tjon–Wu interaction model. N is the truncation order.

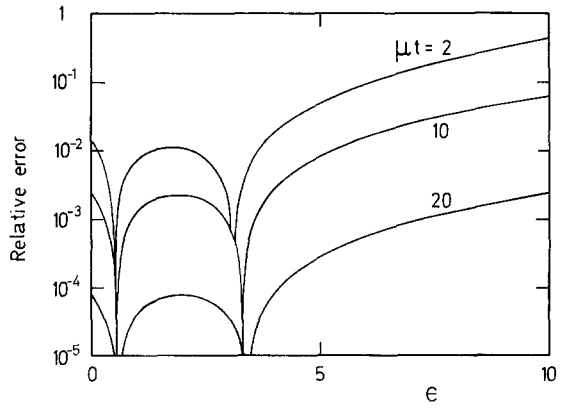

Fig. 4. Relative error of expansion (3.16) truncated at $N=4$ for the case shown in Fig. 3.

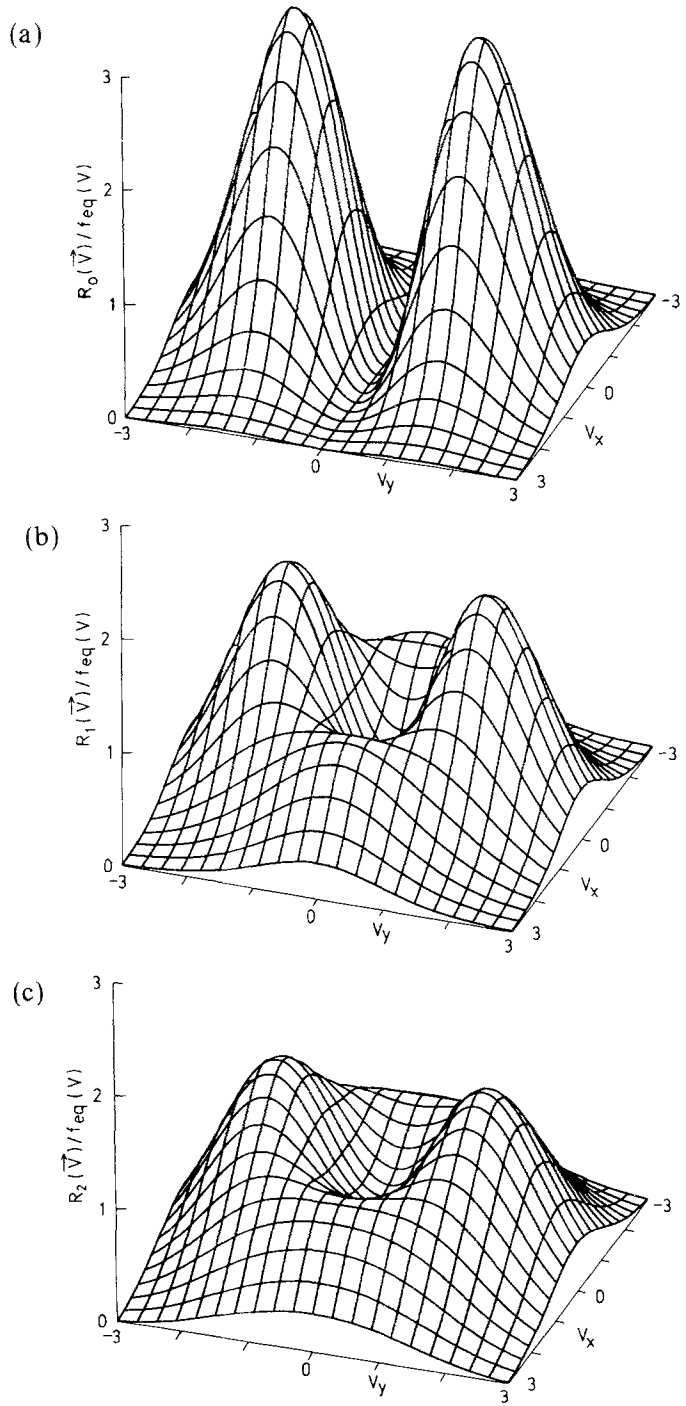

Fig. 5. Collision factors $R_n(\mathbf{v})$ for the distribution function (4.3).

tion to the Hilbert space $\mathscr{L}_2(R^d)$. These are remarkable improvements over other approximation methods. Most of the discussion was restricted to analytical initial distribution functions, even though more complex velocity dependences can be analyzed.

REFERENCES

1. J. L. Lebowitz and E. W. Montroll (eds.), *Non-equilibrium Phenomena I, The Boltzmann Equation* (North-Holland, Amsterdam, 1983).
2. M. H. Ernst, *Phys. Rep.* **78**:1 (1981).
3. C. Cercignani, *Mathematical Methods in Kinetic Theory* (Plenum Press, New York, 1969).
4. S. Chapman, *Phil. Trans. R. Soc. A* **216**:279 (1916); D. Enskog, Dissertation, Uppsala (1917).
5. A. V. Bobylev, *Sov. Phys. Dokl.* **27**:29 (1982).
6. H. Grad, *Commun. Pure Appl. Math.* **4**:331 (1949).
7. D. H. Fujii, R. O. Barrachina, and C. R. Garibotti, *J. Stat. Phys.* **44**:95 (1986).
8. R. O. Barrachina and C. R. Garibotti, *J. Stat. Phys.* **45**:541 (1986).
9. E. Wild, *Proc. Camb. Phil. Soc.* **47**:602 (1951).
10. L. Arkeryd, *Commun. Math. Phys.* **105**:205 (1986).
11. H. P. McKean, *J. Comb. Theory* **2**:358 (1967).
12. A. V. Bobylev, *Sov. Phys. Dokl.* **20**:820, 822 (1976); M. Krook and T. T. Wu, *Phys. Fluids* **20**:1589 (1977).