HIGHER ORDER SOLUTION OF BOLTZMANN'S EQUATION FOR ELECTRONS IN AN ELECTRIC FIELD WITH ISOTROPIC SCATTERING IN ELASTIC AND EXCITING COLLISIONS[1)]

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The analysis of the mathematical structure of the hierarchy resulting for the coefficients of a of 2 l-term expansion of the electron velocity distribution function in Legendre polynomials shows that its general solution at low as well as high energies contains l singular and l non-singular fundamental solutions. A special technique is developed to isolate all non-singular contributions of the general solution and to construct the physically relevant solution of Boltzmann's equation in an arbitrary even order 2 l. Some applications to a model plasma yield with increasing order 2 l converged solutions even for physical situations with large anisotropy in the velocity space. The results are, in part, compared with those from very accurate Monte Carlo simulations.

РЕШЕНИЯ УРАВНЕНИЯ БОЛЬЦМАННА ДЛЯ ЭЛЕКТРОНОВ В ЭЛЕКТРИЧЕСКОМ ПОЛЕ С ИЗОТРОПНЫМ РАССЕЯНИЕМ В УПРУГИХ И ВОЗБУЖДЕННЫХ СОУДАРЕНИЯХ НА ОСНОВЕ ВЫСШИХ ПОРЯДКОВ РАЗЛОЖЕНИЙ

Анализ математической структуры иерархии, получающейся для коэффициентов 2 l-ого члена разложения функции распределения скорости элементов по полиномам Лежандра, показывает, что общее решение при низких и высоких энергиях содержит l сингулярных и l несингулярных фундаментальных решений. В данной работе развит специальный метод, позволяющий выделить, все несингулярные вклады от общего решения и сконструировать физически приемлемое решение уравнения Больцмана в произвольном четном порядке 2 l. Применение этих результатов к модельной плазме дает при увеличении порядка 2 l сходящиеся решения даже для случая большой анизотропии в пространстве скоростей. Проведено также частичное сравнение новых результатов с результатами, полученными на основе метода Монте-Карло.

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I. INTRODUCTION

By solving the electron Boltzmann equation a bridge has been built between the data of elementary processes and the macroscopic properties of the plasma such as transport and rate coefficients of the electrons. But the conclusion from macroscopic properties as, e.g., provided by modern swarm techniques back to the atomic data involved needs an accurate relationship between both these groups of quantities and thus requires a precise solution of the electron Boltzmann equation. Unfortunately the well known Lorentz, i.e. 2-term, approximation fails in several cases of practical interest, which demands a more accurate solution technique of the Boltzmann equation and thus when using the Legendre polynomial expansion of the velocity distribution function, a higher order than the 2-term Lorentz approximation. Several attempts have been undertaken to improve the level of accuracy by such an expansion in [1] and very recently in [2]. Here we outline a well-founded solution technique of the electron Boltzmann equation in an arbitrary even (2 l) order approximation of the Legendre polynomial expansion for a plasma in an electric field $\boldsymbol{E} = E\boldsymbol{e}_z$ and with elastic and exciting electron-neutral particle collisions, a technique which is a logically consequent generalization of the conventional method that solves this equation in a two-term approximation (TTA) by backward integration. Starting from the expansion

$$f(v) = \sum_{n=0}^{2l-1} F_n(v) P_n(v_z/v) \tag{1}$$

of the distribution function $f(v)$ in Legendre polynomials P_n, we obtain from the homogeneous and stationary Boltzmann equation the hierarchy

$$\begin{aligned}
&\frac{1}{3} U \frac{\mathrm{d}}{\mathrm{d}U} f_1 + \frac{1}{3} f_1 + \delta U^2 p \frac{\mathrm{d}}{\mathrm{d}U} f_0 + [\delta(2U_p + U^2 \frac{\mathrm{d}}{\mathrm{d}U} p) - Uq] f_0 + \\
&+ \sum_k (U + U_k^{ex}) q_k^{ex} f_0 (U + U_k^{ex}) = 0, \\
&\frac{n}{2n-1} U \frac{\mathrm{d}}{\mathrm{d}U} f_{n-1} - \frac{n}{2n-1} \frac{n-1}{2} f_{n-1} + \frac{n+1}{2n+3} U \frac{\mathrm{d}}{\mathrm{d}U} f_{n+1} + \frac{n+1}{2n+3} \frac{n+2}{2} f_{n+1} - \\
&- U(p+q) f_n = 0, \\
&1 \leqslant n \leqslant 2l-1, \quad l \geqslant 1, \quad f_{21} \equiv 0
\end{aligned} \tag{2}$$

for the normalized expansion coefficients

$$f_n(U) = 2\pi (2/m)^{3/2} F_n[v(U)]/n_e \tag{3}$$

where $U = mv^2/2$ and n is the electron concentration. Furthermore

$$p(U)=\frac{Q^{el}(U)}{e_0E/N},\quad q_k(U)=\frac{Q_k^{ex}(U)}{e_0E/N},\quad q(U)=\sum_k q_k(U),\quad \delta=2m/M, \qquad (4)$$

where Q^{el} and Q_k^{ex} is the total cross section for elastic collisions and for the k-th exciting collision process with the threshold U_k^{ex}, respectively. With this form of the hierarchy (2) isotropic scattering in elastic as well as exciting collisions is assumed, thus only the total cross sections occur, i.e. the differential ones integrated over the scattering angle. With (3) f_0 is to be normalized according to

$$\int_0^\infty U^{1/2} f_0(U)\,dU=1. \qquad (5)$$

II. GENERAL SOLUTION AND SOLUTION TECHNIQUE

Assuming appropriate power series for $Q^{el}(U)$ at small U and for $Q_k^{ex}(U)$ at energies just above the threshold U_k^{ex} and considering for small U the inscattering terms $f(U+U_k^{ex})$ formally as an inhomogeneity of the linear system of ordinary differential equations, it follows that (2) constitutes a weakly singular differential equation system for small energies with the singular point $U=0$. Using, however, for Q^{el} and Q_k^{ex} asymptotic series representations in U for large energies, (2) becomes a strongly singular differential equation system with the singular point at $U=\infty$ (3).

Because of a different character of the singularities of system (2) separate considerations of the structure of the general solution of the hierarchy are necessary in the region of small and large energies respectively. As a result it was found that the general solution at small as well as that at large energies contains l non-singular (i.e. normalizable) and l singular fundamental solutions. The desired, i.e. physically relevant solution has to be sought within the non-singular part of the general solution (NSPGS) both at low and large energies, with both NSPGS's involving a total of $2l$ free parameters. Therefore the physically relevant solution can be uniquely determined (i) by construction of the NSPGS at low as well as large energies, (ii) by continuous connection of these at an appropriate connection point U_c and (iii) by additional normalization according to (5).

On the basis of these findings a new technique was developed to isolate numerically all contributions to both NSPGS's starting firstly from a sufficiently large energy U_∞ (i.e. from a numerical approximation of the upper singular point) down to the connection point U_c and secondly from the singular point $U=0$ up to U_c to find thus both NSPGS's. This technique leads to the distribution function f in the even order approximation $(2l)$ via l-fold backward and $2l$-fold forward integration of the hierarchy in order to construct both NSPGS's from the singular points to U_c.

Two particular aspects of the numerical technique should still be mentioned. Firstly the l non-singular fundamental solutions at large energies show, with increasing order $2l$, a widely differing exponential behaviour. To preserve despite of this property the linear independence, a special procedure must be applied to enforce repeatedly the linear independence of the l non-singular solutions during the backward integration [4]. Secondly, in order to find numerically all $(2l)$ independent contributions to the NSPGS at small energies an analytical isolation of the independent contributions by appropriate power series representations of the fundamental solutions and of the contributions to the particular solution near the singular point is necessary and was carried out in [4].

III. RESULTS AND DISCUSSION

A model plasma is considered with atoms of a mass M of four atomic units and with energy independent cross sections Q^{el} and Q^{ex} for elastic collisions and for only one excitation process but with a linear increase of the latter from 0 to its final constant value Q^* over a small energy region $U^{ex}\leq U\leq U^{ex}+0.2$ eV. To demonstrate the potential of the new technique, we selected conditions which produce a large anisotropy, i.e. we chose the values $Q^{el}=Q^*=6\times10^{-16}$ cm^2 and $U^{ex}=1$ eV. Using these atomic data for the model, the solution of the hierarchy (2) was performed with increasing order $2l$ up to the converged solution for different field strength values E/N (N denoting the neutral particle concentration). Fig. 1 shows for $E/N=50$ Td (1 Td $=10^{-17}$ V cm^2) as full and dashed curves the first four converged coefficients $f_n(U)$ of the Legendre polynomial expansion obtained in the approximation for $2l=8$ as dependent on the energy. As can be seen for energies somewhat above the threshold, the first contributions f_1, f_2, f_3 to the anisotropic part of the distribution function shown in this figure have larger moduli than the isotropic part f_0. This distinctly reflects the large anisotropy of the velocity distribution function under these conditions. To assess the accuracy of this new technique very accurate Monte Carlo simulations [5] were performed in addition. The results of these simulations obtained for the same first 4 coefficients are in very good agreement with the kinetic results and thus confirm the accuracy of the new method. To illustrate the insuficient description of this physical situation by the conventional TTA, Fig. 2 shows the ratio of the converged $(2l=8)$ first and second coefficient f_0 and f_1 respectively to the corresponding function resulting from the conventional TTA. It is obvious that there are large changes of these functions from TTA to the 8-term approximation which increase to about one order of magnitude at large energies. Because the macroscopic quantities are to be calculated via f_0 and f_1, this result shows the importance of an accurate technique for solving the Boltzmann equation under such conditions, in particular for the

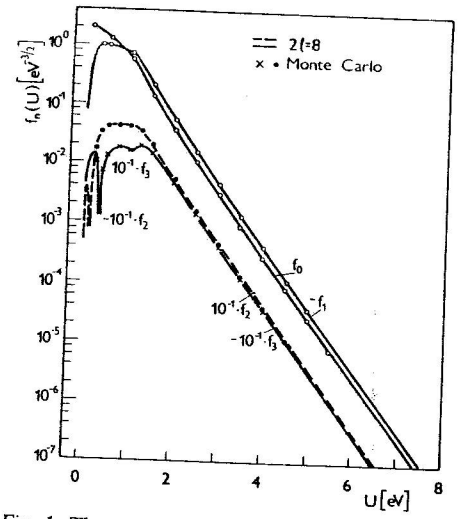

Fig. 1. The converged expansion coefficients f_0, f_1, f_2 and f_3 for the model with $E/N = 50$ Td in comparison with Monte Carlo results.

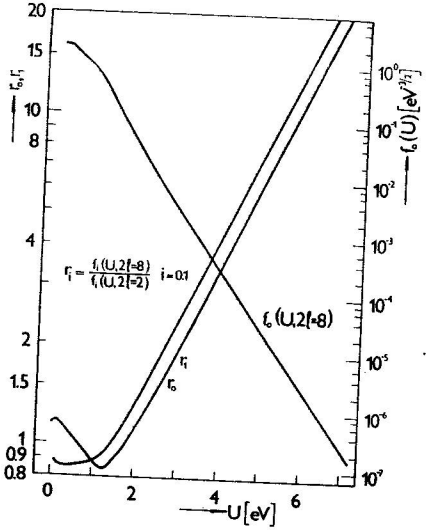

Fig. 2. The ratio of 8-term to 2-term values of f_0 and f_1 for $E/N = 50$ Td.

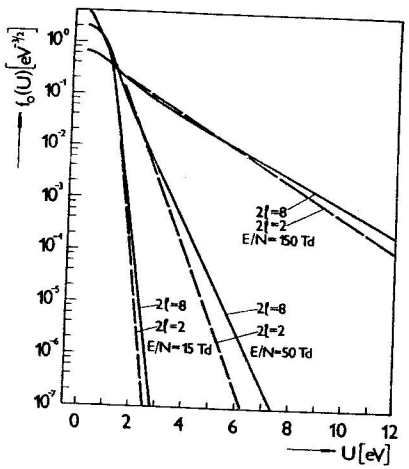

Fig. 3. The change of the isotropic distribution from 2- to 8-term approximation for different E/N.

determination of collision frequencies for additional collision processes with high thresholds, which, however, are not considered here. Fig. 3 compares the 2-term and 8-term results for f_0 at widely differing E/N-values. As expected, the change from the TTA to the converged approximation is markedly dependent on the electric field strength, where changes are largest at medium E/N and decrease with increasing as well as decreasing E/N.

Table 1

Macroscopic quantities with increasing order $2l$ in comparison with Monte Carlo results

	$E/N = 50$ Td			$E/N = 100$ Td		
$2l$	$\bar{U}$	W	$\bar{\nu}^{ex}/N$	$\bar{U}$	W	$\bar{\nu}^{ex}/N$
2	7.458	1.760	8.793	12.47	2.307	23.06
4	7.233	1.641	8.198	12.32	2.173	21.71
6	7.216	1.640	8.195	12.29	2.167	21.66
8	7.217	1.640	8.194	12.29	2.167	21.66
MC	7.217	1.639	8.188	12.28	2.165	21.63

Finally, to demonstrate the changes of some macroscopic quantities with increasing approximation order, leading ultimately to their converged values, Table 1 presents the mean values

$$\bar{U} = \int_0^\infty U^{3/2} f_0(U)\,dU, \quad W = -(1/3)\,(2/m)^{1/2} \int_0^\infty U f_1(U)\,dU,$$
$$\bar{\nu}^{ex}/N = (2/m)^{1/2} \int_0^\infty U Q^{ex}(U) f_0(U)\,dU \tag{6}$$

of the energy (in 10^{-1} eV units), of the drift velocity (10^7 cm s^{-1}) and the excitation frequency (10^{-9} cm^3 s^{-1}) of the electrons for two E/N values, all of which are averaged over the low energy region. The last row gives the corresponding quantities from Monte Carlo simulations. As can be clearly seen, it is possible to achieve the converged macroscopic quantities with an accuracy of about four significant figures by means of a 6- or 8-term approximation and these converged values are in very good agreement with Monte Carlo results.

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