Several Properties of the Matrix Elements of the Collision Integral of the Boltzmann Equation

Andrey Ya. Ender* and Irina A. Ender**

** Ioffe Physico-Technical Institute of RAS, Polytekhnicheskaya St. 26, 194021 St. Petersburg, Russia*
*** Saint-Petersburg State University, University Embankment 6, 199034 Saint-Petersburg, Russia*

Abstract. A new calculating algorithm is advanced, being the major part of the moment method in solving the Boltzmann equation. It is founded on the invariance of the collision integral relative to a choice of basis. In details, the relationships between the matrix elements of the collision integral are studied. Here it is shown, how the constraints for the moment method caused by the Grad criterion can be overwhelmed. Considered are the relationships between the MEs for the oriented particles under a preference direction in a space.

INTRODUCTION

For strongly non-equilibrium flows of rarefied gas, the general Boltzmann equation should be solved, taking in mind the most difficult task of the collision integral calculation. In the moment method of solving the Boltzmann equation, the collision integral is represented a set of its matrix elements (ME). Here, an idea to use the invariance property of the collision integral relative to a choice of a basis system of functions is developed[1, 2]. As a result, the relationships between the MEs are found and an opportunity to calculate not only the linear MEs of the collision integral but the non-linear ones arises at the large indices. It allows to obtain the transport coefficients at arbitrary Knudsen number and to solve both the linear and non-linear problems on a level of the distribution functions (DF) [3].

Following Burnett [4], we use the real spherical non-normalized Hermite polynomials

$$H^i_{r,l,m} = S^{(r)}_{l+1/2}(c^2)c^l Y^i_{l,m}(q,j), \quad Y^0_{l,m}(q,j)=\cos mj\ P^m_l(\cos J), \quad Y^1_{l,m}(q,j)=\sin mj\ P^m_l(\cos J),\ \mathrm{c}=\frac{m}{2kT}(\mathrm{v}-\mathrm{u})^2 \quad (1)$$

Where $S^{(r)}_{l+1/2}(c^2)$ are the Sonine polynomials, $Y^i_{lm}(q,j)$ are the real spherical harmonics, $i=0,1$.

The Hermite polynomials are orthogonal with Maxwellian weight function. Denoting all set of indices in the spherical Hermite polynomials via j, for DF expansion we obtain

$$f(\mathbf{v}) = M(T,\mathbf{u},\mathbf{c})\sum_j C_j H_j(\mathbf{c}) \ , \quad (2)$$

Here, $M(T,\mathbf{u},\mathbf{c})$ is the Maxwellian distribution of a temperature T and a mean velocity $\mathbf{u}$.

One of the general problem braking the development of the moment method is the enormous difficulties in calculating the non-linear (ME) of the collision integral. We find that the ME are interrelated through a number of the relationships, where are the recurrence ones and can be used in calculating the MEs, specially, the non-linear ones [1, 2].

When deducing the recurrence relationships, the collision integral is treated in a set of bases, which are distinct in a temperature T or a value of mean velocity u, or axes direction relative to which the angles q and j in $Y_{lm}(q,j)$ are measured.

RECURRENCE RELATIONSHIPS

From the collision integral invariance relative to a choice in a basis, it follows an equation, from which the ME in one basis is expressed via a subset of the MEs in other basis. Differentiating this equation with respect to the one of the basis parameters, those or others relationships between the ME in the same basis can be obtained.

Usually, the T and $\boldsymbol{u}$ values in (2) are chosen involving the DF properties. When studying the collision integral, we retain these parameters as the free ones.

When expanding in terms of the spherical Hermite polynomials, the Boltzmann equation is substituted with an equivalent system

$$DC_j / Dt = \sum_{j_1, j_2} K^j_{j_1, j_2} C_{j_1} C_{j_2} \tag{3}$$

An operator D/Dt in (3) corresponds to a differential part of the Boltzmann equation. The MEs $K^j_{j_1, j_2}$ of the collision integral $\hat{I}$ are determined as follows

$$K^j_{j_1, j_2} = \int H_j \hat{I}(M(T_0, u_0) H_{j_1}, M(T_0, u_0) H_{j_2})\, d^3\mathrm{v} / g_j \ . \tag{4}$$

Here, $M(T_0, u_0)$ is the Maxwellian, g_j is a square of a norm of the Hermite polynomial

The linear matrix elements (LME) of two kinds $K^j_{j_1,0}$ and K^j_{0, j_2} correspond to the linear collision integral. The MEs of the first kind correspond to a non-equilibrium DF relaxation on the Maxwell background, and the LMEs of the second kind correspond to a Maxwellian relaxation on the non-equilibrium background. Further, non-isotropic LMEs are denoted Λ and the isotropic ones as l , e.g., in the axially symmetric case, $\Lambda^{(2)}_{r, r_2, l} = K^{r,l}_{0,0,r_2,l}$.

The expansion coefficients in the different bases are interrelated via a transfer matrix

$$C^1_j = \sum_{k=0}^{\infty} D_{j,k}(W_1, W_0) C^0_k \ . \tag{5}$$

Here, W is a four-vector $T, \mathbf{u}$. We obtain all main results from a condition of independence of the collision integral on a set of function in terms of which the DF is expanded. From this simple and common invariance principle, it follows an important theorem: The MEs of collision integral in two different bases are expressed via each other as follows

$$K^{i'}_{k', j'}(W_1) = \sum_i D_{i', i}(W_1, W_0) \sum_{k, j} K^i_{k, j}(W_0) D_{k, k'}(W_0, W_1) D_{j, j'}(W_0, W_1) \, . \tag{6}$$

Let a transfer from a basis W_0 to a basis W_1 is accompanied only with a change in temperature and mean velocity value with no change in its direction. Moreover, set, for simplicity, the DF to be axially symmetric. In this case, using $a - u$ representation [5] of the spherical Hermite polynomials, we calculated successfully a matrix D .

If to differentiate an expression (6) with respect to T_1 or u_1 and to set $W_1 = W_0$ ($u_1 = u_0$, $T_1 = T_0$), we obtain some relationships between the MEs. Write these relationships for the particles of different masses.

When differentiating with respect to T , we obtain the “temperature” recurrence relationships, which, in a special case of the power potentials, take a form

$$mK^{r,l}_{r_1, l_1, r_2, l_2} = RK^{r,l}_{r_1, l_1, r_2, l_2} + rK^{r-1,l}_{r_1, l_1, r_2, l_2} - (r_1 + 1) K^{r,l}_{r_1+1, l_1, r_2, l_2} - (r_2 + 1) K^{r,l}_{r_1, l_1, r_2+1, l_2} \ ,$$
$$R = r_1 + r_2 - r + \tfrac{l_1 + l_2 - l}{2} \, . \tag{7}$$

In the case of the power potentials, the MEs are proportional to T^m, where, e.g., $m = 0$ for the Maxwellian molecules, $m = 0.5$ for the hard spheres. For arbitrary interaction potentials, multiplication by m in the left side is substituted by an operator $T\, d / dT$. Note that these relationships interrelate the MEs at fixed l, l_1, l_2. Moreover, the "temperature" relationships do not depend on the masses of the colliding particles. In (7), the indices a and b point out that a mixture of the particles of a and b types is under consideration, and, particularly, under study are the ME of collision integral for a-particles interacting with b-particles.

When differentiating with respect to u, we obtain the "velocity" recurrence relationships

$$\begin{gathered}0 = b(l-1)K^{r,l-1}_{r_1,l_1,r_2,l_2} + g(r-1,l+1)K^{r-1,l+1}_{r_1,l_1,r_2,l_2} - b(l_1)K^{r,l}_{r_1,l_1+1,r_2,l_2} - g(r_1,l_1)K^{r,l}_{r_1+1,l_1-1,r_2,l_2} - \\ \sqrt{m_b / m_a}\left(b(l_2)K^{r,l}_{r_1,l_1,r_2,l_2+1} - g(r_2,l_2)K^{r,l-1}_{r_1,l_1,r_2+1,l_2-1}\right) \\ b(l) = -\frac{l+1}{2l+1}, \qquad g(r,l) = \frac{(r+1)l}{2l+1} \\ .\end{gathered} \tag{8}$$

Here, behavior of particles of the "a" type of m_a mass interacting with particles of the "b" type of m_b mass is considered.

The recurrence relationships (7) and (8) are held not only for the MEs of the general collision integral but, separately, for the gain and loss terms.

The relationships (7) and (8) between the MEs are the recurrence ones which hold in the case, when a system has a preferred direction and the particles are oriented.

When differentiating with respect to the angles determining the axes directions, the relationships for the MEs with different l and m at fixed r. In [11], using these relationships, it is shown that 3D MEs are proportional to the corresponding axially symmetric MEs, and the coefficients of proportionality are easily expressed via the Clebsch-Gordan coefficients.

The above relationships are sufficient for calculation of all MEs if the linear isotropic MEs are taken. There are ever the simple formulas for the latter.

The recurrence relationships (7) are used as well to build up the isotropic non-linear MEs in velocity space of the relaxation problems [1, 2]. The calculation of the non-linear MEs with large indices via direct formulas [6] are very time consuming. Using the MEs with $r \le N_0 = 128$ allows to calculate the DF up to 10 times the thermal velocity by the moment method. Knowledge on the DF in a region of high velocities is of very importance when investigating the processes of physical chemistry.

EXPANSION IN TERMS OF THE SPHERICAL HARMONICS

The moment method has two general faults, i.e., constraints on convergence of DF expansion (Grad criterion) and complications concerning the boundary conditions. These constraints are omitted if the DF is not expanded in terms of the Hermite polynomials with a weight Maxwellian but the spherical harmonics with the coefficients depended on a velocity module, the collision integral being also expanded in terms of the spherical harmonics. Knowledge of the MEs allows to build up the kernels of Fredholm type, which depend, now, only on the absolute values of the velocities for both the linear and non-linear cases. Till now, such kernels were built up analytically only for a hard-sphere model and linearized Boltzmann equation [7, 8]. The expansion of the collision integral in terms of the spherical harmonics suits well when solving the boundary problems as well [9].

For convergence of (2), the Grad criterion needs to be hold:

$$\int f^2(\mathrm{v}) \exp\left(c^2\right) d\mathrm{v} < \infty \,. \tag{9}$$

The restrictions involving the Grad criterion do not arise when expanding the DF in terms of the spherical harmonics but the Sonine polynomials as these ones do be orthogonal with a Maxwellian weight. If the DF is expanded only in terms of the spherical harmonics, the restrictions inherent for the Grad criterion are withdrawn. For brevity, consider the Boltzmann equation for the axially symmetric DF

$$f(\mathbf{v}) = \sum_{l=0}^{\infty} f_l(v) P_l(\cos q) . \tag{10}$$

The equations for f_l at space-homogeneous case without external forces take a form

$$\partial f_l(v,t)/\partial t = \sum_{l_1,l_2} \int_0^{\infty} v_1^2 dv_1 \int_0^{\infty} v_2^2 dv_2 G^l_{l_1,l_2}(v,v_1,v_2) f_{l_1}(v_1,t) f_{l_2}(v_2,t) . \tag{11}$$

A kernel G depends on only the absolute values of the velocities and, as it is shown in [1], is expressed via MEs

$$G^l_{l_1,l_2}(v,v_1,v_2) = M(a,c) \sum_r \sum_{r_1} \sum_{r_2} \frac{1}{s_{r_1,l_1} s_{r_2,l_2}} c^l S^r_{l+1/2}(c) K^{r,l}_{r_1,l_1,r_2,l_2} c_1^{l_1} S^{r_1}_{l_1+1/2}(c_1) c_2^{l_2} S^{r_2}_{l_2+1/2}(c_2) \tag{12}$$

Here, $a = m/2kT$, and $s_{r,l}$ is a square of a norm of the Sonine polynomial.

When using the kernels, it is suitable to consider separately the kernels corresponding to the gain and loss MEs. With formula (12), they are expressed via the gain and loss MEs. The loss MEs are easily found, and the main problem is to find the gain MEs. Note that, describing a behavior of a small admixture on the Maxwellian background (linear problem), a kernel corresponding to a loss term turns out to be a multiplication by a function $k(v)$, and a gain term refers to the linear Fredholm operator with a kernel

$$L_l(v,v_1) = M(a,c) \sum_r \sum_{r_1} \frac{1}{s_{r_1,l_1}} c^l S^r_{l+1/2}(c) K^{r,l}_{r_1,l,0,0} c_1^{l_1} S^{r_1}_{l_1+1/2}(c_1) . \tag{13}$$

It is easily shown that the kernels of a collision operator, in the 3D case, are expressed via the axially symmetric kernels by an analogy with the expression of 3D MEs via the axially symmetric MEs. Thus, all the properties of the collision integral arise in the ME $K^{r,l}_{r_1,l_1,r_2,l_2}$.

Thus, at DF expansion in terms of the spherical Hermite polynomials as well as in terms of the spherical harmonics, the main problem is the ME calculation and, especially, the gain MEs. Clearly, for building-up the kernel, an asymptotical behavior of the MEs at large indices r, r_1, r_2 needs to be known.

To build up such kernels, the detailed study of ME properties is needed and, particularly, their asymptotical behavior at large indices. The first results concerning the ME asymptotic are obtained in [10], in the isotropic case.

It is shown that, in the axially symmetric case, the linear MEs in different l–subspaces $\Lambda_{r,r_1,l}$ with fixed $\Delta = r - r_1$ have the similar asymptotic. For the hard-sphere model, the linear MEs in a function of r at fixed $\Delta + l$ are distinct in only a constant factor.

ORIENTED PARTICLES

Consider the ME in the case with a preferred direction in a space related to the strong external fields, the particles being oriented along such a direction. In this case, the Boltzmann operator symmetry is broken, and many other effects arise which are beyond the standard kinetic theory. Emphasize that we take in mind the neutral particles and the field effects on only a scattering cross-section but not the trajectory of the particles after their collision.

A scattering cross-section depends, now, on not only a scattering angle but also two other angles inherent to a direction between the relative velocity of the particles before their collision and the preferred direction. Hence, the MEs do depend on two angles determining a mean velocity direction of the base Maxwellian. Simultaneously, a relation between the MEs in the different bases (6) is hold.

For such particle, there are no constraints of the Hecke theorem and its generalization on the non-linear case. It signifies, particularly, that the anisotropic DF can arise in a course of relaxation with initially isotropic DF.

At a weak orientation (magnetic field $H \sim 1000\,Oe$), the Senftleben-Beenakker effects [11]-[12] are known, i.e., the effect of the field on the transport coefficients and corresponding intercrossing effects. A strong orientation of particles arises in vicinity of the neutron stars ($H \sim 10^{9} - 10^{12}\,Oe$).

A development of kinetic theory for such particles is very difficult and, till now, nothing but simplified semi-empirical models is advanced.

If, using the invariance relative to changes in T and u, the relationships between the MEs are the same both for oriented and non-oriented particles, it is other deal when concerning the rotations of the reference frame. Under rotation about z-axis through an angle w counterclockwise, an azimuthal angle j of a point in velocity space transforms into $j' = j - w$.

A transfer matrix to a new basis D and the derivatives of D and D^{-1} with respect to w are as follows

$$D(mw) == \begin{pmatrix} \cos mw & \sin mw \\ -\sin mw & \cos mw \end{pmatrix}, \quad \left.\frac{dD(mw)}{dw}\right|_{w=0} = m\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \left.\frac{dD^{-1}(mw)}{dw}\right|_{w=0} = m\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{14}$$

Differentiating (6) with respect to w we obtain the expressions as follows

$$\frac{dK^{i}_{i_1,i_2}}{dw} = m(-1)^{i} K^{1-i}_{i_1,i_2} + m_1(-1)^{i_1} K^{i}_{1-i_1,i_2} + m_2(-1)^{i_2} K^{i}_{i_1,1-i_2}, \tag{15}$$

Here, there are no changes in all the indices r, l, m of ME and are omitted. Only i, i_1, i_2 indices change which correspond to the different real spherical harmonics (1).

With no preferred direction in a system under consideration, the ME does not depend on w, a derivative at the left is zero and the system of equations turns out to be algebraic. A condition of solvability of this uniform algebraic system is

$$m = |m_1 \pm m_2| \tag{16}$$

With preferred direction, a system of differential equations (15) should be solved, and an exclusion (16) is removed. The particular solution of a system (15) is $x_j = a_j \exp(lw)$. If m, m_1 and m_2 are non-zero, there are 8 roots of the characteristic equation, and those are $l = \pm i k_p$. All k_p are integers equal to $m_1 + m_2 + m$, $m_1 + m_2 - m$, $m + m_2 - m_1$, and $m + m_1 - m_2$. Hence, a character of ME dependence on w is determined unambiguously.

From the invariance relative to a basis rotation about y-axis, we obtain a system of ordinary differential equations as follows

$$\begin{aligned} 2\frac{dK^{l,l_1,l_2}_{m,m_1,m_2}(y)}{dy} &= p(l,m-1)K^{l,l_1,l_2}_{m-1,m_1,m_2}(y) - q(l,m+1)K^{l,l_1,l_2}_{m+1,m_1,m_2}(y) \\ - p(l_1,m_1)K^{l,l_1,l_2}_{m,m_1+1,m_2}(y) + q(l_1,m_1)K^{l,l_1,l_2}_{m,m_1-1,m_2}(y) &- p(l_2,m_2)K^{l,l_1,l_2}_{m,m_1,m_2+1}(y) + q(l_2,m_2)K^{l,l_1,l_2}_{m,m_1,m_2-1}(y). \end{aligned} \tag{17}$$

$$p(l,m) = \Theta(l-m-1)(1+d_{m,0}), \quad q(l,m) = \Theta(l-m)\Theta(m-1)(l-m+1)(l+m), \quad \Theta(x) = 1, x \ge 0;\ \Theta(x) = 0, x < 0.$$

Here, the indices i, i_1, i_2, r, r_1, r_2 are omitted and the inequalities $0 \le m \le l$, $0 \le m_1 \le l_1$, $0 \le m_2 \le l_2$. are accomplished.

With no preferred direction, i.e., in the standard kinetic theory, the derivative at the left turns out to be zero, and the system becomes the algebraic one. A condition of solvability of such a system is the generalized Hecke theorem, along which the nonzeros are such MEs for which a condition $|l_1 - l_2| \le l \le l_1 + l_2$ is met. From the solution of a system (17), in this case, the relationships between 3D and axially symmetric MEs are derived

$$K^{l,l_1,l_2}_{m,m_1,m_2} = \breve{Z}^{l,m}_{l_1,m_1,l_2,m_2} K^{l,l_1,l_2}_{0,0,0} \tag{18}$$

For the oriented particles, the solution of differential equations (17) is as follows

$$K^{l,l_1,l_2}_{m,m_1,m_2}(y) = \sum_s \exp(l_s y)\, \overset{s}{K}{}^{l,l_1,l_2}_{m,m_1,m_2} \tag{19}$$

It is maintained that, at fixed l, l_1, l_2, a whole set of l_s can be represented as follows

$$l_s = \pm i(l + l_1 + l_2 - 2s), \qquad s = 0,1,2,\ldots[(l + l_1 + l_2)/2]. \tag{20}$$

In (19), $\overset{s}{K}{}^{l,l_1,l_2}_{m,m_1,m_2}$ do not depend on y and they are the expansion coefficients of the MEs in terms of the exponents.

As a rule, the roots are degenerate and degeneracy degree increases monotonically with a rise in s (at $s = 0$, a root is not degenerate). If there is a root of kr multiplicity, the number of free constants of a solution equals this multiplicity. A rule of selection of general (base) MEs is formulated. Their number includes necessarily the axially symmetric MEs $\overset{s}{K}{}^{l,l_1,l_2}_{0,0,0}$.

If, for usual non-oriented particles, any ME with fixed l, l_1, l_2 is determined via the base one, namely, axially symmetric, then, in the case of the oriented particles, every such ME is determined via a set of the base MEs of which amount equals multiplicity of corresponding root. For example, at $kr = 2$, any ME (if $l_2 > 0$) is represented as follows

$$\overset{s}{K}{}^{l,l_1,l_2}_{m,m_1,m_2} = \overset{s}{H}{}^{l,l_1,l_2}_{m,m_1,m_2}\, \overset{s}{K}{}^{l,l_1,l_2}_{0,0,0_2} + \overset{s}{G}{}^{l,l_1,l_2}_{m,m_1,m_2}\, \overset{s}{K}{}^{l,l_1,l_2}_{0,0,1} \tag{21}$$

The functions $\overset{s}{H}$ and $\overset{s}{G}$, and so on are the expansion coefficients in terms of the base MEs. They are universal and, as the Clebsch-Gordan coefficients, do not depend on the physical properties of molecules.

The additional relationships between the base elements are resulted from the relations following from the collision integral invariance relative to a mean velocity in 3D case. Using these relationships, all the base MEs are expressed via corresponding linear MEs. Thus, a whole deal results in calculation of a few base linear MEs and building-up with aid of the above recurrence relationships of all other MEs. It simplified drastically the ME determination for such a complicated object as a system of oriented particles.

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