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Matrix Elements of the Boltzmann Collision Operator in a Basis determined by an Anisotropic Maxwellian Weight Function including Drift

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Abstract

The matrix elements of the linear Boltzmann collision operator are calculated in a Burnett-function basis determined by a weight function which itself describes a velocity distribution with a net drift and an anisotropic pressure (or temperature) tensor. Three different methods of calculation are described, leading to three different types of formulae. Two of these involve infinite summations, while the third involves only finite sums, but at the cost of greater complications in the summands and the integrals over cross sections. Both elastic and inelastic collisions are treated. Special cases arising from particular choices of the parameters in the weight functions are pointed out. The structure of the formulae is illustrated by means of diagrams. The work is a contribution towards establishing efficient methods of calculation based upon a better understanding of the matrix elements in such bases.

1. Introduction

Recent work by Mason and coauthors (Viehland and Mason 1975, 1978; Lin *et al.* 1979*b*)* and by Forsth (1979) has provided evidence that the calculation of transport coefficients for charged particles moving in neutral gases, in the presence of an electric field, can be improved by expanding the distribution function in polynomials orthogonal with respect to a gaussian weight function which incorporates some of the nonequilibrium features of the charged particle distribution. In many cases it appears that a Maxwellian, with a suitably chosen temperature, different from the gas temperature, provides a sufficiently good weight function. In other cases it may be necessary to include the drift or the anisotropy of the pressure or both in the weight function.

The choice of parameters in the weight function must be related to the intrinsic parameters of the problem, the strength of the electric field and the nature of the gas and charged particles. This is an intricate relationship and requires much investigation on its own. Some of these questions, along with different ways of handling the collision operator, are discussed in the previous accompanying paper (Kumar *et al.* 1980, present issue pp. 343–448; hereinafter referred to as Paper I).

* The cited work of Mason and coauthors is significant for having shown that approximation schemes based on these ideas can be carried out in practice. However, in their papers this basic point gets somewhat obscured since the parameters in the weight functions are found by an elaborate nonlinear iteration and the work is described as a rigorous theory. Professor Mason has since explained that in their use of the word 'rigorous' they mean to imply 'a systematic theory capable of improvement, in contrast to something like a momentum-transfer theory or a free-flight type of calculation'.

The present paper is devoted to the technical problem of calculating the matrix elements of the collision operator in the bases suggested in the works cited above. This is of central importance for the matrix methods of solving the Boltzmann equation. The problem is approached with the aim of showing the structure of these matrix elements in terms of certain coefficients and integrals involving cross sections. These quantities have their own independent significance and may be studied separately. This is intended to facilitate both the theoretical analysis and computational evaluation of these matrix elements.

The paper is largely self-contained and should be understandable on its own. It is based upon techniques introduced in an earlier paper (Kumar 1967) and follows the principles outlined in Section 12 of Paper I. A recourse to these papers is necessary only if the reader wants to know how certain mathematical devices arise and why certain alternatives are to be preferred.

The arrangement of the paper is as follows: The first part (Sections 2–5) deals with elastic collisions. In Section 2, the notation is introduced and the derivation of the matrix elements in the gas-temperature basis is briefly recapitulated. The gas-temperature basis is determined by an isotropic Maxwellian weight function without drift and with the same temperature as the neutral gas. In Section 3, this representation is related to that in the general basis, including drift and anisotropy, by means of a similarity transformation. In Section 4, the matrix elements in the general basis are calculated by expanding the neutral distribution also in a general basis. In Section 5, the same quantities are calculated by a different treatment of the gaussian factors in the collision integral, and the formulae involving finite summations are obtained.

The second part (Section 6) deals with inelastic collisions. The collision operator is taken in the form given by Wang-Chang *et al.* (1964). The derivation follows the same pattern as for the elastic collisions and only the changes required in the formulae are given.

A quick survey of the formulae derived here can be obtained by looking at the diagrams (Figs 1–5). Their use is explained in Section 2*b*. They contain a representation of the formulae and their derivation. Important special cases of two- and three-temperature representations are given in Sections 5*b* and 5*c*.

2. Notation and Preliminaries

The weight function of interest here has the form

$$\bar{w}(\alpha, x) = (\alpha^2/2\pi)^{3/2} (\det \boldsymbol{\tau}) \exp(-\tfrac{1}{2}\alpha^2 x^2), \tag{1a}$$

with

$$\boldsymbol{x} = \boldsymbol{\tau}(\boldsymbol{c} - \boldsymbol{W}), \qquad \alpha^2 = m/kT_0, \tag{1b}$$

where $\boldsymbol{c}$ is the particle velocity and m the particle mass. The parameter α has the dimensions of inverse speed and is defined in terms of the neutral gas temperature T_0 for the sake of convenience. The weight function depends on α, $\boldsymbol{\tau}$ and $\boldsymbol{W}$ as parameters. The 3×3 real nonsingular matrix $\boldsymbol{\tau}$ is dimensionless and the real vector $\boldsymbol{W}$ has the dimensions of velocity.

As a velocity distribution, $\bar{w}(\alpha, x)$ has an average velocity $\boldsymbol{W}$ and a kinetic pressure tensor given by

$$\mathbf{P} = kT_0(\boldsymbol{\tau}^{\mathrm{T}} \boldsymbol{\tau})^{-1}. \tag{2}$$

There is no loss of generality in taking $\mathbf{P}$ or τ to be diagonal. This corresponds to taking the velocity coordinate system along the principal axis of $\mathbf{P}$. The modification needed for taking $\mathbf{P}$ or τ nondiagonal is slight.

As polynomials orthogonal with respect to the weight function $\bar{w}(\alpha, x)$, we choose the Burnett functions $\phi^{(\nu)}(\alpha x)$, $\nu \equiv (v, l, m)$. In the x coordinate system they are proportional to spherical harmonics:

$$\phi^{(\nu)}(\alpha x) \equiv R_{vl}(\alpha x)\, Y_m^{(l)}(\hat{x}), \tag{3}$$

where $\hat{x}$ denotes the unit vector along x. They satisfy the orthogonality relations

$$\int \bar{w}(\alpha, x)\, \phi^{(\nu)}(\alpha x)\, \phi^{[\nu']}(\alpha x)\, \mathrm{d}c = \delta_{\nu\nu'} \equiv \delta_{vv'}\delta_{ll'}\delta_{mm'}. \tag{4}$$

Further information on these polynomials is given in the next accompanying paper (Kumar 1980, present issue pp. 469–79; hereinafter referred to as Paper III). We speak of these Burnett functions as the basis determined by the gaussian weight function $\bar{w}(\alpha, x)$, which in general contains a drift and an anisotropic temperature (or pressure). We shall call this the x basis.

The expansion of the charged particle distribution, of number density n, in the x basis has the form

$$f(c) = n\, \bar{w}(\alpha, x) \sum_{\nu} \phi^{[\nu]}(\alpha x)\, \mathfrak{F}^{(\nu)}, \tag{5a}$$

$$\mathfrak{F}^{(\nu)} = n^{-1} \int f(c)\, \phi^{(\nu)}(\alpha x)\, \mathrm{d}c. \tag{5b}$$

By putting τ equal to the unit matrix $\mathbf{1}$ and $W = 0$ we obtain the c basis, also to be called the gas-temperature basis. The corresponding expansion is called the one-temperature expansion.

The relation between the x and c bases has been worked out in Paper III and is given by the transformation matrix $A(\tau, \alpha W)$:

$$\phi^{(\nu)}(\alpha x) = \sum_{\nu'} [A(\tau, \alpha W)]^{\nu\nu'}\, \phi^{(\nu')}(\alpha c), \tag{6a}$$

$$\bar{w}(\alpha, x)\, \phi^{[\nu]}(\alpha x) = \sum_{\nu'} \bar{w}(\alpha, c)\, \phi^{[\nu']}(\alpha c)\, [A^{-1}(\tau, \alpha W)]^{\nu'\nu}. \tag{6b}$$

It is shown in Paper III that the sum in equation (6a) is a finite sum while that in equation (6b) is an infinite sum.

With the definitions

$$x = \tau(c - W), \qquad x_0 = \tau(c_0 - W), \tag{7a}$$

$$\Gamma^2 = \alpha^2 + \alpha_0^2, \qquad \gamma^2 = \alpha^{-2} + \alpha_0^{-2} = \Gamma^2/\alpha_0^2\alpha^2, \tag{7b}$$

$$\mu = \alpha^2/\Gamma^2 = m/(m+m_0), \qquad \mu_0 = \alpha_0^2/\Gamma^2 = m_0/(m+m_0), \tag{7c}$$

we have the analogue of the transformation to the centre of mass and relative velocities,

$$\Gamma^2 Y = \alpha^2 x + \alpha_0^2 x_0, \qquad y = x - x_0, \tag{8a}$$

$$x = Y + \mu_0 y, \qquad x_0 = Y - \mu y. \tag{8b}$$

The following relation then holds:

$$\phi^{(\nu_1)}(\alpha \boldsymbol{x})\,\phi^{(\nu_2)}(\alpha_0 \boldsymbol{x}_0) = \sum_{Nn} T(\Gamma N, \gamma \boldsymbol{n} \mid \alpha \nu_1, \alpha_0 \nu_2)\,\phi^{(N)}(\Gamma \boldsymbol{Y})\,\phi^{(n)}(\gamma y)\,. \tag{9}$$

The T coefficients here are called Talmi coefficients. They depend on the α's only through the ratio α/α_0 and will sometimes be abbreviated as $T(N, \boldsymbol{n} \mid \alpha \nu_1, \alpha_0 \nu_2)$, $T(N\boldsymbol{n} \mid \nu_1 \nu_2)$ or $T(\alpha/\alpha_0)$, depending on what information is to be emphasized; for their definition and use in kinetic theory see Kumar (1967).

The neutral particles have velocity $\boldsymbol{c}_0$, mass m_0, temperature T_0 and number density n_0. Their distribution $f_0(\boldsymbol{c}_0)$ is Maxwellian,

$$f_0(\boldsymbol{c}_0) = n_0\,\bar{w}(\alpha_0, c_0)\,, \qquad \alpha_0^2 = m_0/kT_0\,. \tag{10}$$

The collision operator is defined by

$$J(f) = \int [f(\boldsymbol{c})\,f_0(\boldsymbol{c}_0) - f(\boldsymbol{c}')\,f_0(\boldsymbol{c}_0')]\,g\,\sigma(g,\chi)\,\mathrm{d}\hat{\boldsymbol{g}}'\,\mathrm{d}\boldsymbol{c}_0\,, \tag{11a}$$

$$\boldsymbol{g} = \boldsymbol{c} - \boldsymbol{c}_0\,, \qquad \boldsymbol{g}' = \boldsymbol{c}' - \boldsymbol{c}_0'\,, \qquad \cos\chi = \hat{\boldsymbol{g}}.\hat{\boldsymbol{g}}'\,, \tag{11b}$$

$$\Gamma^2 \boldsymbol{G} = \alpha^2 \boldsymbol{c} + \alpha_0^2 \boldsymbol{c}_0\,, \quad \Gamma^2 \boldsymbol{G}' = \alpha^2 \boldsymbol{c}' + \alpha_0^2 \boldsymbol{c}_0'\,, \quad \boldsymbol{G} = \boldsymbol{G}'\,. \tag{11c}$$

For any vector $\boldsymbol{a}$, the unit vector in the direction of $\boldsymbol{a}$ is denoted by $\hat{\boldsymbol{a}}$, and the corresponding element of solid angles by $\mathrm{d}\hat{\boldsymbol{a}}$. In Sections 2–5 we deal with elastic collisions only, so that

$$g^2 = g'^2\,. \tag{11d}$$

The cross section $\sigma(g, \chi)$ is assumed independent of, or averaged over, the azimuthal angle.

The matrix element in the $\boldsymbol{x}$ basis is obtained by using the expansion (5a) in equation (11a). Transforming the volume elements in the usual way with equations (11b), (11c) and (11d) we have

$$J_{\nu\nu'} = \int \phi^{(\nu)}(\alpha \boldsymbol{x})\,[\phi^{[\nu']}(\alpha \boldsymbol{x})\,\bar{w}(\alpha, x)\,\bar{w}(\alpha_0, c_0) - \phi^{[\nu']}(\alpha \boldsymbol{x}')\,\bar{w}(\alpha, x')\,\bar{w}(\alpha_0, c_0')]\,\mathrm{d}\mathscr{V}\,, \tag{12a}$$

with

$$\mathrm{d}\mathscr{V} = g\,\sigma(g,\chi)\,\mathrm{d}\hat{\boldsymbol{g}}'\,\mathrm{d}\boldsymbol{g}\,\mathrm{d}\boldsymbol{G}\,, \tag{12b}$$

where $\boldsymbol{x}'$ bears the same relation to $\boldsymbol{c}'$ as $\boldsymbol{x}$ does to $\boldsymbol{c}$. By standard manipulations equation (12a) is converted to the following form, which is the starting point of our calculations:

$$J_{\nu\nu'} = \int \bar{w}(\alpha_0, c_0)\,\bar{w}(\alpha, x)\,\phi^{[\nu']}(\alpha \boldsymbol{x})\,[\phi^{(\nu)}(\alpha \boldsymbol{x}) - \phi^{(\nu)}(\alpha \boldsymbol{x}')]\,\mathrm{d}\mathscr{V}\,. \tag{13}$$

(a) Gas-temperature or $\boldsymbol{c}$ *Basis*

This is the simplest representation, also known as the one-temperature representation (or expansion). We put $\tau = \mathbf{1}$, $W = 0$ and denote the collision matrix by ${}^{\circ}J$. Then

$${}^{\circ}J_{\nu\nu'} = \int \bar{w}(\alpha, c)\,\bar{w}(\alpha_0, c_0)\,\phi^{[\nu']}(\alpha \boldsymbol{c})\,[\phi^{(\nu)}(\alpha \boldsymbol{c}) - \phi^{(\nu)}(\alpha \boldsymbol{c}')]\,\mathrm{d}\mathscr{V}\,. \tag{14}$$

From equations (11b) and (11c), the gaussian in the integrand may be written as

$$\bar{w}(\alpha, c)\,\bar{w}(\alpha_0, c_0) = \bar{w}(\Gamma, G)\,\bar{w}(\gamma, g)\,. \tag{15}$$

To evaluate the integral in equation (14) we transform the rest of the integrand to separate the dependence on $\boldsymbol{G}$, $\boldsymbol{g}$ and $\boldsymbol{g}'$ by using the relation (9). We have the following steps:

$$\phi^{[v']}(\alpha \boldsymbol{c}) = \sum T(\boldsymbol{N}', \boldsymbol{n}' \mid \alpha \mathbf{v}', \alpha_0 \boldsymbol{0})\,\phi^{[N']}(\Gamma \boldsymbol{G})\,\phi^{[n']}(\gamma \boldsymbol{g})\,, \tag{16a}$$

$$[\phi^{(v)}(\alpha \boldsymbol{c}) - \phi^{(v)}(\alpha \boldsymbol{c}')]$$

$$= \sum T(\boldsymbol{N}, \boldsymbol{n} \mid \alpha \mathbf{v}, \alpha_0 \boldsymbol{0})\,\phi^{(N)}(\Gamma \boldsymbol{G})\,[\phi^{(n)}(\gamma \boldsymbol{g}) - \phi^{(n)}(\gamma \boldsymbol{g}')]\,, \tag{16b}$$

$$\int [\phi^{(n)}(\gamma \boldsymbol{g}) - \phi^{(n)}(\gamma \boldsymbol{g}')]\, g\,\sigma(g, \chi)\,\mathrm{d}\hat{\boldsymbol{g}}' = \phi^{(n)}(\gamma \boldsymbol{g})\, g\,\sigma^{(l)}(g)\,, \tag{16c}$$

$$\sigma^{(l)}(g) = 2\pi \int \sigma(g, \chi)\,\{1 - \mathrm{P}_l(\cos\chi)\}\,\mathrm{d}(\cos\chi)\,. \tag{16d}$$

The integration over $\mathrm{d}\boldsymbol{G}$ gives $\delta_{NN'}$ and we arrive at the formula

$${}^{\circ}J_{\mathbf{v}\mathbf{v}'} = \sum_{\boldsymbol{N}\boldsymbol{n}\boldsymbol{n}'} T(\boldsymbol{N}, \boldsymbol{n} \mid \alpha \mathbf{v}, \alpha_0 \boldsymbol{0})\, T(\boldsymbol{N}, \boldsymbol{n}' \mid \alpha \mathbf{v}', \alpha_0 \boldsymbol{0})\, V^{l}_{\boldsymbol{n}\boldsymbol{n}'}\,, \tag{17a}$$

with

$$V^{l}_{\boldsymbol{n}\boldsymbol{n}'} = \int \bar{w}(\gamma, g)\,\phi^{[n']}(\gamma \boldsymbol{g})\,\phi^{(n)}(\gamma \boldsymbol{g})\, g\,\sigma^{(l)}(g)\,\mathrm{d}\boldsymbol{g}\,. \tag{17b}$$

The integration over $\mathrm{d}\hat{\boldsymbol{g}}$ results in the simplifications

$$V^{l}_{\boldsymbol{n}\boldsymbol{n}'} = V^{l}_{nn'}(\gamma)\,\delta_{ll'}\,\delta_{mm'}\,, \tag{18a}$$

$$V^{l}_{nn'}(\gamma) = \int \bar{w}(\gamma, g)\, R_{nl}(\gamma g)\, R_{n'l}(\gamma g)\, g^3\,\sigma^{(l)}(g)\,\mathrm{d}g\,, \tag{18b}$$

$${}^{\circ}J_{\mathbf{v}\mathbf{v}'} = {}^{\circ}J^{l}_{vv'}\,\delta_{ll'}\,\delta_{mm'}\,. \tag{18c}$$

The quantities V are called the interaction integrals. From equation (18b) it is seen that only a one-dimensional integral over the cross section is needed in this case. Equations (18a) and (18c) exhibit the rotational invariance of the quantities.

We now note some characteristics of this derivation for future reference. A crucial step in the derivation is equation (16c) where the integration over $\mathrm{d}\hat{\boldsymbol{g}}'$ and cross section $\sigma(g, \chi)$ is carried out to isolate the χ dependence via equation (16d). There are two aspects to be noted. Firstly, the calculation of $\sigma^{(l)}(g)$ from a given potential is a complicated process. Thus equations (16d) and (18b) account for most of the computational time and any alteration in these quantities can make a big difference in the amount of calculation needed. Secondly, the necessity of being able to integrate over $\mathrm{d}\hat{\boldsymbol{g}}'$ requires that the dependence on $\hat{\boldsymbol{g}}'$ should be made explicit at some point. The variable transformations (16a) and (16b) are designed to serve this need. For calculations in the general bases we have to devise other transformations to put the $\hat{\boldsymbol{g}}'$ dependence in a suitable form. Much of the complication of the subsequent formulae comes from this source.

(b) Diagram Representation

The derivation above and the resulting formula (17a) are summarized in Fig. 1. Similar diagrams will be used for other formulae.

In any diagram the boxes represent the coefficients in the summand. The symbol inside the box indicates the particular coefficient and its dependence on the parameters of the weight function. The lines joining a box are labelled by the indices on which the coefficient depends. In each diagram the indices $\mathbf{v}$ and $\mathbf{v}'$ have given fixed values. The indices $\mathbf{0}$, occurring at the top of the diagram stand for $v = l = m = 0$ and are to be thought of as arising from the dependence on neutral velocities.

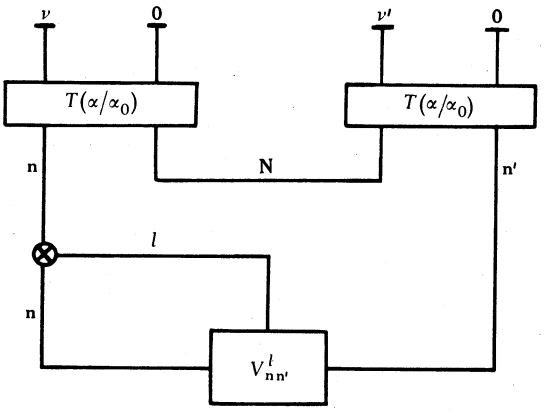

Fig. 1. Matrix element of the Boltzmann collision operator in the c basis (equations 17). The conventions for reading this diagram and the following Figs 2–5 are explained in Section 2*b* of the text.

To obtain the formula corresponding to the particular diagram, write the product of all the boxed coefficients with labels from lines joining the box and sum over all indices (except, of course, $\mathbf{v}$ and $\mathbf{v}'$). The values taken by these indices are restricted by the properties of the coefficients. Single lines indicate that the corresponding index takes on a finite number of values. Double lines indicate that the sum in general consists of an infinite number of nonvanishing terms, or briefly is an infinite sum.

The diagram also provides a summary of the derivation as follows. Each line represents a Burnett function and each box represents a variable transformation. The symbol $\otimes$ represents the $d\hat{\boldsymbol{g}}'$ integration. Starting from the top with given $\mathbf{v}$ and $\mathbf{v}'$, each box represents a step in the derivation, and horizontal joining lines represent integrations.

3. Similarity Transformation

It is known that a change of basis results in a similarity transformation of the matrix. This is verified in the present case by using both equations (6) in the formula (13) and comparing the result with (14). The matrix element in the x basis is then given by

$$J_{\mathbf{v}\mathbf{v}'} = \sum_{\mathbf{v}_1\mathbf{v}_1'} A^{\mathbf{v}\mathbf{v}_1} \circ J_{\mathbf{v}_1\mathbf{v}_1'} [A^{-1}]^{\mathbf{v}_1'\mathbf{v}'}. \tag{19}$$

The transformation matrix $A \equiv A(\tau, \alpha W)$ carries the dependence on the parameters τ and W of the weight function. From the block lower triangular property of A (Paper III) it follows that the sum over ν_1 is finite but that over ν_1' is infinite. The corresponding diagram is Fig. 2.

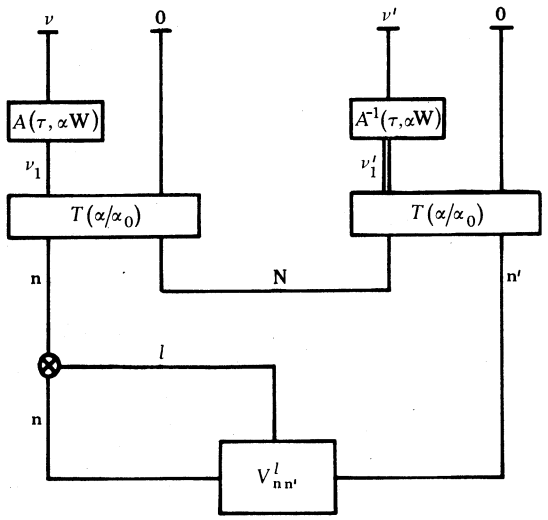

Fig. 2. Matrix element in the x basis, from a similarity transformation (equation 19).

In applications, the formulae will work only if the infinite summation converges rapidly and can be represented by a reasonably small number of terms. It is known that, in most cases, the off-diagonal elements of ${}^{\circ}J^{l}_{\nu\nu'}$ (equation 18c) decrease rapidly with $|\nu - \nu'|$. One can then use those parameters τ and W for which the off-diagonal elements of A^{-1} do not increase fast enough to compensate for the decrease of ${}^{\circ}J^{l}_{\nu\nu'}$. This question has to be examined in each particular case. In general, for a given cross section and other intrinsic parameters, this formula will work only for a limited set of parameters τ and W.

The situation is quite favourable for the case $\tau = \tau \mathbf{1}$, $W = 0$. This corresponds to the two-temperature expansion of Viehland and Mason (1975, 1978). From equation (43a) of Paper III we have

$$[A^{-1}(\tau, 0)]^{\nu_1'\nu'} = [A_{l_1'}(\tau^{-1})]^{\nu_1'\nu'} \delta_{l_1'l'} \delta_{m_1'm'}, \tag{20}$$

$$[A_{l_1'}(\tau^{-1})]^{\nu_1'\nu'} = \{(\nu_1' - \nu')!\}^{-1} \{(\nu_1'! \Gamma(\nu_1' + l_1' + \tfrac{3}{2}))/(\nu'! \Gamma(\nu' + l_1' + \tfrac{3}{2}))\}^{\frac{1}{2}}$$

$$\times \tau^{-(2\nu' + l_1')} (1 - \tau^{-2})^{\nu_1' - \nu'}, \quad \text{for } \nu_1' \geqslant \nu', \tag{21a}$$

$$= 0, \quad \text{for } \nu_1' < \nu'. \tag{21b}$$

This shows that for any $\tau > 1$ there is a moderate decrease with $(\nu_1' - \nu')$ at least for large $(\nu_1' - \nu')$. Coupled with the decrease in ${}^{\circ}J^{l}_{\nu\nu'}$, which is usually quite rapid, this shows that there is a good chance of success. Nevertheless, the matter can be decided only by actual numerical work for specific cases, since something more than mere convergence in principle is required.

The dependence on W is of a different nature. Consider the case of pure drift, that is, $\tau = \mathbf{1}$, $W \neq 0$. The formula for A is now more complicated (equation 52a of Paper III). It is seen, however, that the relevant matrix element has a leading term $\sim(\alpha W)^{\nu_1'-\nu'}$. This now grows with W, so that no matter how fast the ${}^{0}J^{l}_{\nu\nu'}$ decreases there will be some value of W for which the method will fail. Again, numerical work is needed to find the practically useful range of W for a given set of intrinsic parameters.

The main point about the use of this method of calculation is that although there is an infinite sum involved, to some given accuracy, the fast decrease in the non-diagonal elements of ${}^{0}J^{l}_{\nu\nu'}$ can compensate for the increase in corresponding elements of A^{-1}, for a certain range of the parameters τ and W. This range is to be found by actual numerical work in specific cases.

4. Expansion of Neutral Distribution in x_0 Basis

This method was used by Lin *et al.* (1979*a*) and by Forsth (1979) for electrons in a two-temperature expansion, that is, with $\tau = \tau\mathbf{1}$ and $W = 0$. Applying equation (6b) to the neutral distribution, we have

$$\bar{w}(\alpha_0, c_0) = \sum_{\nu_1} \bar{w}(\alpha_0, x_0)\, \phi^{[\nu_1]}(\alpha_0 x_0)\, [A^{-1}(\tau, \alpha_0 W)]^{\nu_1 0}. \tag{22}$$

Substitution into equation (13) then yields

$$J_{\nu\nu'} = \sum_{\nu_1} (\nu \mid J \mid \nu_1, \nu')\, [A^{-1}(\tau, \alpha_0 W)]^{\nu_1 0}, \tag{23a}$$

$$(\nu \mid J \mid \nu_1, \nu') = \int \bar{w}(\alpha, x)\, \bar{w}(\alpha_0, x_0)\, \phi^{[\nu']}(\alpha x)\, \phi^{[\nu_1]}(\alpha_0 x_0) \times [\phi^{(\nu)}(\alpha x) - \phi^{(\nu)}(\alpha x')]\, \mathrm{d}\mathscr{V}. \tag{23b}$$

To evaluate this integral, introduce the variables $\boldsymbol{G}_1$ and $\boldsymbol{g}_1$ by

$$\Gamma^2 \boldsymbol{G}_1 = \alpha^2 \boldsymbol{x} + \alpha_0^2 \boldsymbol{x}_0 = \Gamma^2 \tau (\boldsymbol{G} - \boldsymbol{W}), \tag{24a}$$

$$\boldsymbol{g}_1 = \boldsymbol{x} - \boldsymbol{x}_0 = \tau \boldsymbol{g}, \tag{24b}$$

$$\boldsymbol{g} = \tau^{-1} \boldsymbol{g}_1, \qquad \boldsymbol{G} = \tau^{-1} \boldsymbol{G}_1 + \boldsymbol{W}. \tag{24c}$$

It follows that

$$\alpha^2 x^2 + \alpha_0^2 x_0^2 = \Gamma^2 G_1^2 + \gamma^2 g_1^2, \tag{25a}$$

$$\bar{w}(\alpha, x)\, \bar{w}(\alpha_0, x_0)\, \mathrm{d}\boldsymbol{G}\, \mathrm{d}\boldsymbol{g} = \bar{w}(\Gamma, G_1)\, \bar{w}(\gamma, g_1)\, \mathrm{d}\boldsymbol{G}_1\, \mathrm{d}\boldsymbol{g}_1. \tag{25b}$$

Applying the relation (9) to the product $\phi^{[\nu']}\phi^{[\nu_1]}$ and the difference of ϕ's in square brackets in equation (23b) one gets two ϕ's with the argument $\boldsymbol{G}_1$. From equation (25b), the integration over $\mathrm{d}\boldsymbol{G}_1$ gives a delta function by orthogonality of ϕ's and we have

$$(\nu \mid J \mid \nu_1 \nu') = \sum T(\boldsymbol{N}, \boldsymbol{n}' \mid \alpha \nu', \alpha_0 \nu_1)\, T(\boldsymbol{N}, \boldsymbol{n} \mid \alpha \nu, \alpha_0 \boldsymbol{0}) \times \int \bar{w}(\gamma, g_1)\, \phi^{[n']}(\gamma \boldsymbol{g}_1) \left\{ \int [\phi^{(n)}(\gamma \boldsymbol{g}_1) - \phi^{(n)}(\gamma \boldsymbol{g}_1')]\, g\, \sigma(g, \chi)\, \mathrm{d}\hat{\boldsymbol{g}}' \right\} \mathrm{d}\boldsymbol{g}. \tag{26}$$

To perform the integration over $\mathrm{d}\hat{\boldsymbol{g}}'$ enclosed in braces here, equations (24b) and (6a) are used to go back to the variables $\boldsymbol{g}$ and $\boldsymbol{g}'$. Then equation (16c) is applied with the result

$$\left\{\int [\phi^{(n)}(\gamma \boldsymbol{g}_1) - \phi^{(n)}(\gamma \boldsymbol{g}_1')]\, g\, \sigma(g,\chi)\, \mathrm{d}\hat{\boldsymbol{g}}'\right\} = \sum [A(\tau,0)]^{nn_1}\, \phi^{(n_1)}(\gamma \boldsymbol{g})\, g\, \sigma^{(l_1)}(g)\,. \tag{27}$$

Returning to the variable $\boldsymbol{g}_1$ in the Burnett function by the inverse transformation and introducing the interaction integral

$$V^{l_1}_{nn'}(\tau) = \int \bar{w}(\gamma, g_1)\, \phi^{(n)}(\gamma \boldsymbol{g}_1)\, \phi^{[n']}(\gamma \boldsymbol{g}_1)\, g\, \sigma^{(l_1)}(g)\, \mathrm{d}\boldsymbol{g}_1\,, \tag{28}$$

with $g = \{(\tau^{-1}\boldsymbol{g}_1)^2\}^{\frac{1}{2}}$, we find that equations (26) and (23b) are reduced to the form

$$\begin{aligned}(\mathbf{v} \mid J \mid \mathbf{v}_1 \mathbf{v}') = \sum T(N, \boldsymbol{n}' \mid \alpha \mathbf{v}', \alpha_0 \mathbf{v}_1)\, T(N, \boldsymbol{n} \mid \alpha \mathbf{v}, \alpha_0 \boldsymbol{0}) \\ \times [A(\tau,0)]^{nn_1}\, [A^{-1}(\tau,0)]^{n_1 n_2}\, V^{l_1}_{n_2 n'}(\tau)\,.\end{aligned} \tag{29}$$

The summation is over N, $\boldsymbol{n}$, $\boldsymbol{n}'$, $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$. From the properties of the T's and A's these are all finite sums. Note that the sum over $\boldsymbol{n}_1$ ($\equiv n_1, l_1, m_1$) does not, in general, produce the unit matrix from the A's because l_1 also occurs in the V's.

The matrix element in the $\boldsymbol{x}$ basis is now given by equations (23) and (29) and its diagram representation is given in Fig. 3*a*. The infinite sum in this case is over the index $\mathbf{v}_1$ in equation (23a) and the problems of handling this are the same as in the previous section. Note that in equation (23a) the W dependence occurs only in the A^{-1} term, while the τ dependence is present in all the A's and in the interaction integrals V.

Considerable simplification occurs in the case $\tau = \tau \mathbf{1}$, $W = 0$. Firstly, the A's in equation (29) become diagonal in the l and m indices so that the sum over n_1 can now be carried out giving $l' = l_1 = l_2$, $m' = m_1 = m_2$ and $n' = n_1 = n_2$. Secondly, from equation (28)

$$V^{l}_{nn'}(\tau \mathbf{1}) = V^{l}_{nn'}(\gamma\tau)\, \delta_{ll'}\, \delta_{mm'}\,, \tag{30}$$

where $V^{l}_{nn'}$ was defined by equation (18b). The diagram for the simplified formula for this case is given by Fig. 3*b*.

For the case of electrons, this approach to calculating the matrix elements has been successfully used by Lin *et al.* (1979*a*). Their work shows that the infinite sum of this formula does not present a practical problem, at least for $\tau = \tau \mathbf{1}$ and $W = 0$, and when only the first-order terms in the mass ratio m/m_0 are retained. The method is yet to be tested for the case of ions, and for ions and electrons when $W \neq 0$.

5. Matrix Elements as Finite Sums

The infinite sums of the previous sections arose from the use of equation (6b). This use was motivated by the need to bring the gaussian factors in the integrand of equation (13) to a form where separation of variables may be conveniently performed. The use of equation (6b) can be avoided by introducing a linear change of variables, which converts the product $\bar{w}(\alpha, x)\, \bar{w}(\alpha_0, c_0)$ in equation (13) into another product of gaussians, and always using equation (6a) to convert the Burnett functions. The latter equation always leads to finite sums.

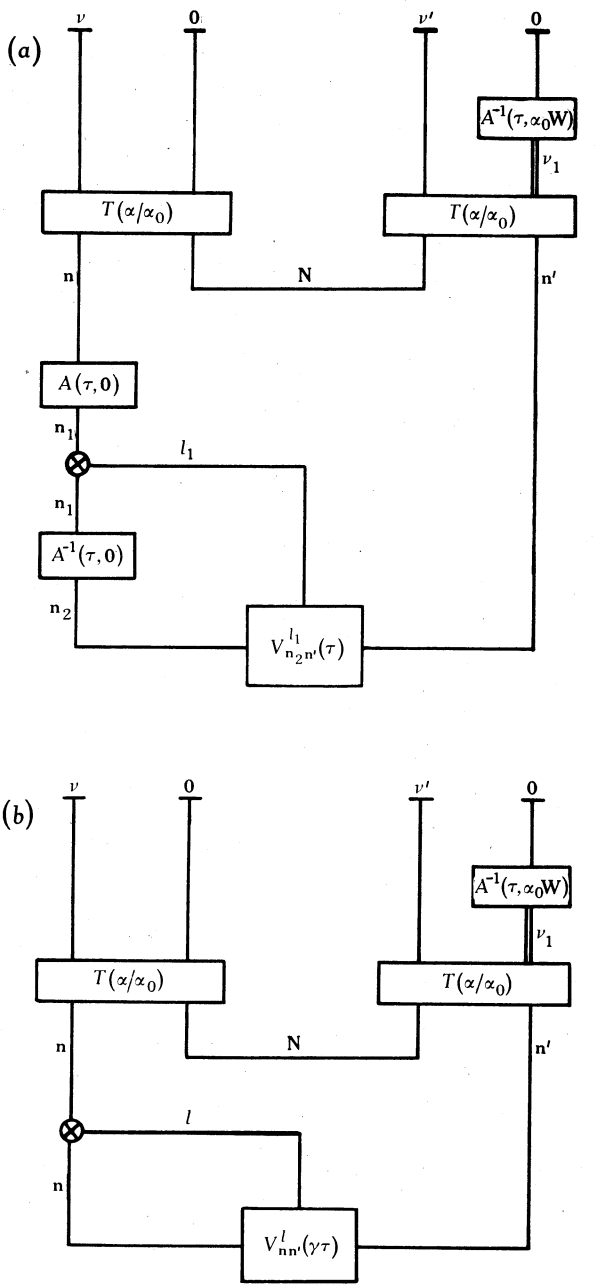

Fig. 3. Diagrams showing:

(*a*) the matrix element in the x basis, from expansion of the neutral distribution (equations 23a and 29);

(*b*) the simplification of (*a*) when τ is a multiple of the unit tensor.

The advantage of finite sums is that all questions of convergence are avoided. In fact, one has a proof that the matrix elements exist. At the computational level the advantage is not so clear: the interaction integrals now involve both τ and W and are more difficult to calculate; at the same time there are more indices to be summed over and the time required will rise rapidly with the magnitude of the indices.

This way of handling the gaussian factors was introduced by Suchy (1964) and has been used by Viehland and Mason (1975, 1978) and by Forsth (1979) in calculations for the two-temperature expansion in a Burnett-function basis. Lin *et al.* (1979*b*) have used the same device for calculating the matrix elements in a Hermite polynomial basis, in the case of cylindrically symmetric anisotropic weight functions with drift.

To begin with, one finds the variables $\boldsymbol{G}_2$ and $\boldsymbol{g}_2$, linearly related to $\boldsymbol{x}$ and $\boldsymbol{c}_0$, such that

$$\alpha^2 x^2 + \alpha_0^2 x_0^2 = \Gamma^2 G_2^2 + \gamma^2 g_2^2 . \tag{31}$$

In terms of the quantities

$$\mu = \alpha^2/\Gamma^2 , \qquad \mu_0 = \alpha_0^2/\Gamma^2 = 1-\mu , \tag{32}$$

and the tensors $\boldsymbol{\tau}_i$, $i = 1,2,3$, and $\boldsymbol{\beta}_j$, $j = 1,2,3,4$, defined by*

$$\boldsymbol{\tau}_1^2 = \mu\boldsymbol{\tau}^2 + \mu_0 \mathbf{1} , \qquad \boldsymbol{\tau}_2 = \boldsymbol{\tau}_1^{-1}\boldsymbol{\tau}^2 , \qquad \boldsymbol{\tau}_3 = \boldsymbol{\tau}_1^{-1}\boldsymbol{\tau} , \tag{33a}$$

$$\boldsymbol{\beta}_1 = \boldsymbol{\tau}_3 , \quad \boldsymbol{\beta}_2 = \mu\boldsymbol{\tau}_1^{-1}(\mathbf{1}-\boldsymbol{\tau}^2) , \quad \boldsymbol{\beta}_3 = \boldsymbol{\tau}_1 , \quad \boldsymbol{\beta}_4 = \boldsymbol{\beta}_2 + \boldsymbol{\beta}_3 = \boldsymbol{\tau}_1^{-1} , \tag{33b}$$

with $\mathbf{1}$ the unit tensor, we have

$$\boldsymbol{G}_2 = \boldsymbol{\tau}_1 \boldsymbol{c}_0 + \mu\boldsymbol{\tau}_2(\boldsymbol{g}-\boldsymbol{W}) = \boldsymbol{\tau}_1 \boldsymbol{G} - \mu\boldsymbol{\tau}_1 \boldsymbol{g} + \mu\boldsymbol{\tau}_2(\boldsymbol{g}-\boldsymbol{W}) , \tag{34a}$$

$$\boldsymbol{g}_2 = \boldsymbol{\tau}_3(\boldsymbol{g}-\boldsymbol{W}) , \qquad \boldsymbol{g} = \boldsymbol{\tau}_3^{-1}\boldsymbol{g}_2 + \boldsymbol{W} , \tag{34b}$$

$$\boldsymbol{c}_0 = \boldsymbol{\tau}_1^{-1}\boldsymbol{G}_2 - \mu\boldsymbol{\tau}_3 \boldsymbol{g}_2 , \tag{34c}$$

$$\boldsymbol{x} = \boldsymbol{\tau}(\boldsymbol{c}-\boldsymbol{W}) = \boldsymbol{\beta}_1 \boldsymbol{G}_2 + \mu_0 \boldsymbol{\beta}_2 \boldsymbol{g}_2 + \mu_0 \boldsymbol{\beta}_3 \boldsymbol{g}_2 , \tag{34d}$$

$$\boldsymbol{x}' = \boldsymbol{\tau}(\boldsymbol{c}'-\boldsymbol{W}) = \boldsymbol{\beta}_1 \boldsymbol{G}_2 + \mu_0 \boldsymbol{\beta}_2 \boldsymbol{g}_2 + \mu_0 \boldsymbol{\beta}_3 \boldsymbol{g}_2' , \tag{34e}$$

$$\bar{w}(\alpha, x_0)\, \bar{w}(\alpha_0, c_0)\, \mathrm{d}\boldsymbol{G}\, \mathrm{d}\boldsymbol{g} = \bar{w}(\Gamma, G_2)\, \bar{w}(\gamma, g_2)\, \mathrm{d}\boldsymbol{G}_2\, \mathrm{d}\boldsymbol{g}_2 . \tag{34f}$$

All the $\boldsymbol{\tau}_i$ and $\boldsymbol{\beta}_j$ are real and symmetric if $\boldsymbol{\tau}^2$ is, they all commute with each other, and $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_3$ and $\boldsymbol{\tau}$ are related by

$$\boldsymbol{\tau}\,\boldsymbol{\tau}_1^{-1}\,\boldsymbol{\tau}_3^{-1} \equiv \mathbf{1} . \tag{35}$$

The definitions are so arranged that when $\boldsymbol{\tau} = \mathbf{1}$ and $\boldsymbol{W} = 0$ one recovers the usual transformation to the centre of mass and relative velocities (equations 11b and 11c). For $\boldsymbol{\tau} = \mathbf{1}$, one has

$$\boldsymbol{\tau}_i = \boldsymbol{\beta}_j = \mathbf{1} \quad (i = 1,2,3, \quad j = 1,3,4) , \qquad \boldsymbol{\beta}_2 = 0 . \tag{36}$$

* The equations (33a) are also applicable for any real nonsingular $\boldsymbol{\tau}$, if $\boldsymbol{\tau}^2$ above is replaced by $\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}$ (the superscript T denoting the transpose). Since this is real, symmetric and positive definite, the tensors $\boldsymbol{\tau}_i$ and $\boldsymbol{\beta}_j$ can be defined and they all commute with each other and with $\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}$. The replacement comes about from the fact that we have to use $x^2 \equiv \boldsymbol{x}^{\mathrm{T}}.\boldsymbol{x} = (\boldsymbol{c}^{\mathrm{T}} - \boldsymbol{W}^{\mathrm{T}})\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}(\boldsymbol{c}-\boldsymbol{W})$ in the quadratic form.

Using equation (34f) in the formula (13), we have

$$J_{\nu\nu'} = \int \bar{w}(\Gamma, G_2)\, \bar{w}(\gamma, g_2)\, \phi^{[\nu']}(\alpha x)\, [\phi^{(\nu)}(\alpha x) - \phi^{(\nu)}(\alpha x')] \times g\, \sigma(g, \chi)\, \mathrm{d}\hat{g}'\, \mathrm{d}G_2\, \mathrm{d}g_2 . \tag{37}$$

The calculation proceeds by using equations (34d) and (34e) for x and x' and expressing the ϕ's in equation (37) in terms of the ϕ's of G_2 and g_2 from equations (9) and (6a). One has the following sequence of steps:

$$\phi^{[\nu']}(\alpha x) = \sum T(N', n' \mid \alpha \nu', \alpha_0\, 0)\, \phi^{[N']}(\Gamma \beta_1 G_2)\, \phi^{[n']}(\gamma \beta_4 g_2), \tag{38a}$$

$$[\phi^{(\nu)}(\alpha x) - \phi^{(\nu)}(\alpha x')] = \sum T(N, n \mid \alpha \nu, \alpha_0\, 0)\, \phi^{(N)}(\Gamma \beta_1 G_2)\, [\ldots]_a, \tag{38b}$$

$$[\ldots]_a \equiv [\phi^{(n)}(\gamma(\beta_2 g_2 + \beta_3 g_2)) - \phi^{(n)}(\gamma(\beta_2 g_2 + \beta_3 g_2'))] = \sum T(n, 0 \mid 1\, n_1,\, 1\, n_2)\, \phi^{(n_1)}(\sqrt{2}\, \gamma \beta_2 g_2)\, [\ldots]_b, \tag{38c}$$

$$[\ldots]_b \equiv [\phi^{(n_2)}(\sqrt{2}\, \gamma \beta_3 g_2) - \phi^{(n_2)}(\sqrt{2}\, \gamma \beta_3 g_2')] = \sum [A(\sqrt{2}\, \beta_3, \gamma W)]^{n_2 n_3}\, [\ldots]_c, \tag{38d}$$

$$[\ldots]_c \equiv \phi^{(n_3)}(\gamma g) - \phi^{(n_3)}(\gamma g'). \tag{38e}$$

The integration over $\mathrm{d}\hat{g}'$ in equation (37) is now carried out using the formula (16c). This leaves the following integrations to be done:

$$I_1 = \int \bar{w}(\Gamma, G_2)\, \phi^{[N']}(\Gamma \beta_1 G_2)\, \phi^{(N)}(\Gamma \beta_1 G_2)\, \mathrm{d}G_2, \tag{39a}$$

$$I_2 = \int \bar{w}(\gamma, g_2)\, \phi^{[n']}(\gamma \beta_4 g_2)\, \phi^{(n_1)}(\sqrt{2}\, \gamma \beta_2 g_2)\, \phi^{(n_3)}(\gamma g)\, g\, \sigma^{(l_3)}(g)\, \mathrm{d}g_2, \tag{39b}$$

where g is related to g_2 by equations (34b). In these integrals the tensors occurring in the arguments of the ϕ's are to be adjusted using equation (6a). Then

$$I_1 = \sum_{N_1} [A^*(\beta_1, 0)]^{N' N_1}\, [A(\beta_1, 0)]^{N N_1}, \tag{40a}$$

$$I_2 = \sum\nolimits_{\blacksquare} [A^*(\beta_4, 0)]^{n' n_4} [A(\sqrt{2}\, \beta_2, 0)]^{n_1 n_5}\, [A^{-1}(\beta_3, \gamma W)]^{n_3 n_6}\, I_3, \tag{40b}$$

$$I_3 = \int \bar{w}(\gamma, g_2)\, \phi^{[n_4]}(\gamma g_2)\, \phi^{(n_5)}(\gamma g_2)\, \phi^{(n_6)}(\gamma g_2)\, g\, \sigma^{(l_3)}(g)\, \mathrm{d}g_2 . \tag{40c}$$

The last step above uses the inverse transformation of equation (6a) to convert $\phi(\gamma g)$ to $\phi(\gamma g_2)$, the resulting sum over n_6 still being finite. To reduce the integral I_3 we introduce the coefficient K defined by

$$\phi^{(n_6)}(\gamma g_2)\, \phi^{(n_5)}(\gamma g_2) = \sum_{n_7} K(n_7; n_6\, n_5)\, \phi^{(n_7)}(\gamma g_2), \tag{41a}$$

$$K(n_7; n_6\, n_5) = \int \bar{w}(\gamma, g_2)\, \phi^{[n_7]}(\gamma g_2)\, \phi^{(n_6)}(\gamma g_2)\, \phi^{(n_5)}(\gamma g_2)\, \mathrm{d}g_2, \tag{41b}$$

and the interaction integral

$$V^{l_3}_{n_7 n_4}(\gamma, \tau_3, W) = \int \bar{w}(\gamma, g_2)\, \phi^{(n_7)}(\gamma \boldsymbol{g}_2)\, \phi^{[n_4]}(\gamma \boldsymbol{g}_2)\, g\, \sigma^{(l_3)}(g)\, \mathrm{d}\boldsymbol{g}_2 . \tag{42}$$

Collecting all terms we have the general formula

$$\begin{aligned} J_{\mathbf{v}\mathbf{v}'} = \sum T(\boldsymbol{N}', \boldsymbol{n}' \mid \alpha \mathbf{v}', \alpha_0 0)\, T(\boldsymbol{N}, \boldsymbol{n} \mid \alpha \mathbf{v}, \alpha_0 0)\, T(\boldsymbol{n}, 0 \mid 1\, \boldsymbol{n}_1, 1\, \boldsymbol{n}_2) \\ \times [A(\boldsymbol{\beta}_1, 0)]^{NN_1}\, [A^*(\boldsymbol{\beta}_1, 0)]^{N'N_1}\, [A(\sqrt{2}\, \boldsymbol{\beta}_3, \gamma W)]^{n_2 n_3}\, [A(\sqrt{2}\, \boldsymbol{\beta}_2, 0)]^{n_1 n_5} \\ \times [A^*(\boldsymbol{\beta}_4, 0)]^{n' n_4}\, [A^{-1}(\boldsymbol{\beta}_3, \gamma W)]^{n_3 n_6}\, K(\boldsymbol{n}_7; \boldsymbol{n}_6\, \boldsymbol{n}_5)\, V^{l_3}_{n_7 n_4}(\gamma, \tau_3, W) . \end{aligned} \tag{43}$$

The sum is over the indices $\boldsymbol{N}, \boldsymbol{N}', \boldsymbol{N}_1$, $\boldsymbol{n}, \boldsymbol{n}'$ and $\boldsymbol{n}_1$–$\boldsymbol{n}_7$, there being in general 36 indices. No defence is offered for this large number of indices. The first two T's depend only on α/α_0, that is, on the mass ratio m/m_0, while the third T and the K are pure numbers; for the evaluation of these latter coefficients see Kumar (1966). The dependence on the parameters τ and W of the weight function is contained in the A's and V's, as shown. The diagram corresponding to the formula (43) is given in Fig. 4*a*.

We now consider some special cases.

(*a*) *One-temperature Case*

Here we have

$$\tau = 1, \qquad x = c - W .$$

Then equations (36) hold and the formula (43) simplifies to (see Fig. 4*b*)

$$\begin{aligned} J_{\mathbf{v}\mathbf{v}'} = \sum T(\boldsymbol{N}, \boldsymbol{n}' \mid \alpha \mathbf{v}', \alpha_0 0)\, T(\boldsymbol{N}, \boldsymbol{n} \mid \alpha \mathbf{v}, \alpha_0 0) \\ \times [A(\mathbf{1}, \gamma W)]^{n n_1}\, [A^{-1}(\mathbf{1}, \gamma W)]^{n_1 n_2}\, V^{l_1}_{n_2 n'}(\gamma, \mathbf{1}, W) . \end{aligned} \tag{44}$$

To show this, the following identities are needed:

$$[A(\mathbf{0}, 0)]^{n n'} = \phi^{(n)}(0)\, \delta_{n'0} , \qquad K(\boldsymbol{n}; \boldsymbol{n}' 0) = \delta_{n n'} , \tag{45a,b}$$

$$\sum_{n, n_2} T(\boldsymbol{n}, 0 \mid 1\, \boldsymbol{n}_1, 1\, \boldsymbol{n}_2)\, \phi^{(n_1)}(0)\, [A(\sqrt{2}\, \mathbf{1}, \gamma W)]^{n_2 n_3} = [A(\mathbf{1}, \gamma W)]^{n n_3} . \tag{45c}$$

The identity (45a) follows from the definition of the matrix element given in equation (24) of Paper III, and the identity (45b) follows from equation (41b) and the orthogonality of the ϕ's. The last identity (45c) may be verified by using equation (24) of Paper III in (45c), followed by the inverse of equation (9) and the orthogonality relation, with appropriate choice of variables.

Alternatively, the result (44) may be derived directly from equations (37) and (36). In the expression (42) for the interaction integral, where

$$\boldsymbol{g}_2 = \boldsymbol{g} - \boldsymbol{W} \qquad \text{and} \qquad g^2 = g_2^2 + W^2 + 2 g_2 W \cos\theta ,$$

one can take W along the z axis. Integration over the azimuth then gives

$$V^{l_1}_{n n'} \sim \delta_{m m'} ,$$

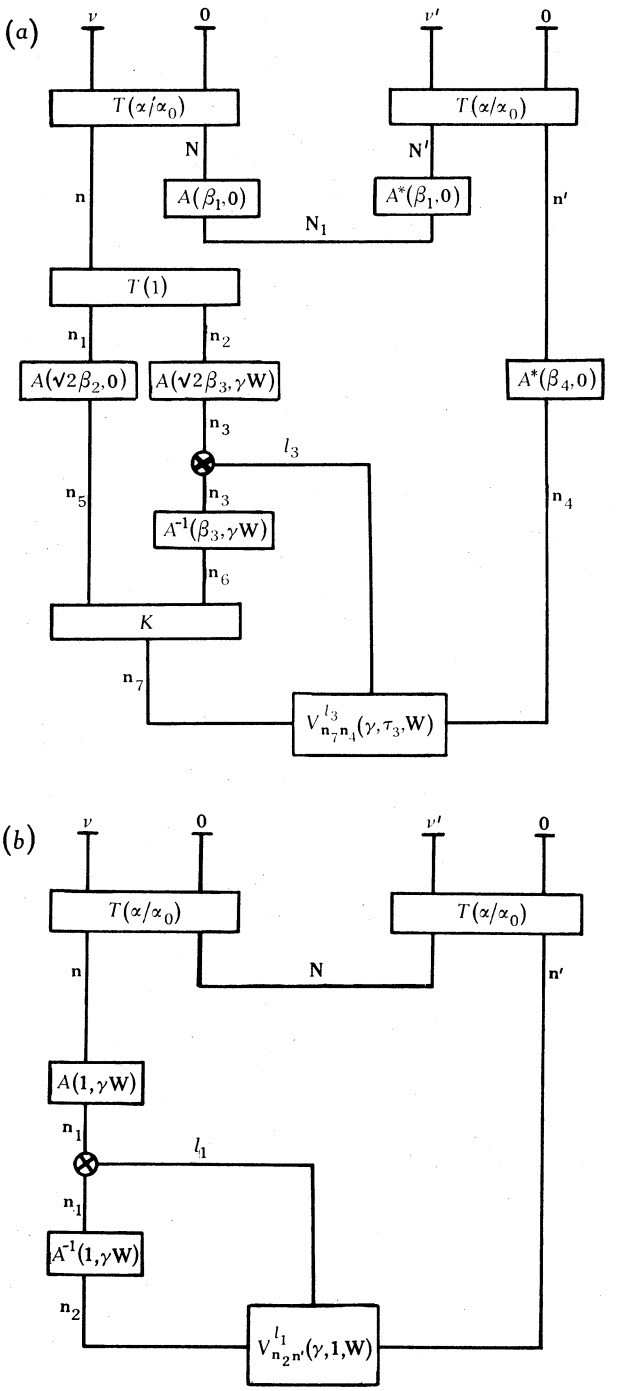

Fig. 4. Diagrams showing:
(*a*) the matrix element in the x basis, as a finite sum (equations 42 and 43);
(*b*) the simplification of (*a*) when $\tau = 1$ (equation 44).

leaving a two-dimensional integration over g_2 and $\cos\theta$, which depends on γ, W and the cross sections.

For $W = 0$, one reverts to the $\boldsymbol{c}$ basis discussed in Section 2*a*.

(*b*) *Two-temperature Case*

Here we have

$$\boldsymbol{\tau} = \tau \mathbf{1}, \qquad \boldsymbol{x} = \tau(\boldsymbol{c} - \boldsymbol{W}).$$

All the tensors $\boldsymbol{\tau}_i$ and $\boldsymbol{\beta}_1$ are multiples of the unit tensor and the corresponding A's are diagonal in the l and m indices (equation 20). There is a considerable reduction in the number of indices to be summed over. However, the appearance of the formula or the corresponding diagram does not change since we have already used an abbreviated notation. Here $\boldsymbol{g}_2 = \tau_3(\boldsymbol{g} - \boldsymbol{W})$ so that again we can take $\boldsymbol{W}$ along the z-axis, with

$$g^2 = \tau_3^{-2} g_2^2 + W^2 + 2\tau_3^{-1} g_2 W \cos\theta .$$

The interaction integral is then again diagonal in the m indices and a two-dimensional integration over g_2 and $\cos\theta$ is to be performed.

For $W = 0$, we have the case studied by Viehland and Mason (1975, 1978) and by Forsth (1979). Our formulae are somewhat different from the formulae given by these authors.

(*c*) *Anisotropic Case with Cylindrical Symmetry: Three-temperature Case*

Here we have

$$\boldsymbol{\tau} = \operatorname{diag}(\tau_\perp, \tau_\perp, \tau_\parallel), \qquad \boldsymbol{W} = (0, 0, W). \tag{46}$$

This case, in a Hermite polynomial basis, was treated by Lin *et al.* (1979*b*). Their velocity vectors are related to ours by $\boldsymbol{\gamma} = \gamma g_2/\sqrt{2}$ and $\boldsymbol{\chi} = \boldsymbol{G}_2/\sqrt{2}$. In terms of the quantities d_r, T_r and T_r^{eff} ($r = \perp, \parallel$) introduced by them, we have

$$\boldsymbol{\tau}^2 = \operatorname{diag}(T_0/T_\perp, T_0/T_\perp, T_0/T_\parallel), \tag{47a}$$

$$\boldsymbol{\tau}_1^2 = \operatorname{diag}(\mu_0/d_\perp, \mu_0/d_\perp, \mu_0/d_\parallel), \tag{47b}$$

$$\boldsymbol{\tau}_3^2 = \operatorname{diag}(T_0/T_\perp^{\mathrm{eff}}, T_0/T_\perp^{\mathrm{eff}}, T_0/T_\parallel^{\mathrm{eff}}). \tag{47c}$$

All tensors $\boldsymbol{\tau}_i$ and $\boldsymbol{\beta}_j$ have this cylindrically symmetric form, that is, they are diagonal and the first two elements are equal. The A matrix for this case is given by equation (48) of Paper III. It is diagonal in the m indices but not diagonal in the l indices. The interaction integral has the same property. We consider this in greater detail:

In equation (42) let $\boldsymbol{n}_7 = \boldsymbol{n}$, $\boldsymbol{n}_4 = \boldsymbol{n}'$, $l_3 = \lambda$ and couple the spherical harmonics of the ϕ functions. Then

$$\phi^{[n']}(\gamma \boldsymbol{g}_2)\, \phi^{(n)}(\gamma \boldsymbol{g}_2) = R_{n'l'}(\gamma g_2) R_{nl}(\gamma g_2) \sum_{l_1 m_1} (lm\, l_1 m_1 \mid l'm')\, \sigma(l\, l_1\, l')\, \mathrm{Y}_{m_1}^{[l_1]}(\hat{\boldsymbol{g}}_2). \tag{48}$$

The angular integration is now

$$I_{l_1 m_1}^{\lambda}(g_2) = \int \mathrm{Y}_{m_1}^{[l_1]}(\hat{\boldsymbol{g}}_2)\, g\, \sigma^{(\lambda)}(g)\, \mathrm{d}\hat{\boldsymbol{g}}_2 , \tag{49a}$$

where from equations (34b)

$$g^2 = \boldsymbol{g}_2 \cdot \boldsymbol{\tau}_3^{-2} \cdot \boldsymbol{g}_2 + 2\boldsymbol{g}_2 \cdot \boldsymbol{\tau}_3^{-1} \cdot \boldsymbol{W} + W^2 . \tag{49b}$$

Taking the z axis along $\boldsymbol{W}$ we see that this is independent of the azimuth so that

$$I^{\lambda}_{l_1 m_1}(g_2) = \delta_{m_1 0} I^{\lambda}_{l_1}(g_2), \tag{50a}$$

$$I^{\lambda}_{l_1}(g_2) = \int_{-1}^{+1} \mathrm{P}_{l_1}(x)\, g\, \sigma^{(\lambda)}(g)\, \mathrm{d}x, \tag{50b}$$

where g is to be expressed in terms of g_2, $\boldsymbol{W}$ and x (the cosine of the angle between $\boldsymbol{g}_2$ and $\boldsymbol{W}$) by equation (49b). Finally we have

$$V^{\lambda}_{nn'} = \delta_{mm'} \sum_{l_1=l-l'}^{l+l'} (l\, m\, l_1\, 0 \,|\, l'\, m)\, \sigma(l\, l_1\, l')\, \hat{V}^{\lambda}_{nl,n'l',l_1}, \tag{51a}$$

$$\hat{V}^{\lambda}_{nl,n'l',l_1} = \int \bar{w}(\gamma, g_2)\, R_{nl}(\gamma g_2)\, R_{n'l'}(\gamma g_2)\, I^{\lambda}_{l_1}(g_2)\, g_2^2\, \mathrm{d}g_2 . \tag{51b}$$

We have here expressed the interaction integral in terms of the two integrals (50b) and (51b)—effectively we have a double integration. In (50b), instead of x we can use g as the integration variable since equation (49b) holds. For numerical work, however, this alteration in the interaction integral could be even more taxing than the increased number of indices brought in by the A matrices.

The matrix elements calculated by Lin *et al.* (1979*b*) are related to the present ones by a unitary transformation.

This completes our treatment of the collision integral in the $\boldsymbol{x}$ basis, for the case where only elastic collisions are considered.

6. Inelastic Collisions: Particles with Internal Structure

The full treatment for particles with internal structure requires the quantum mechanical generalization of the Boltzmann equation, on which there is a considerable literature. From among these, we note the work of Hess (1967) where it is shown that in appropriate circumstances the equations proposed by Waldmann, by Snider and by Wang-Chang and Uhlenbeck are obtained. It has been shown, for instance, in the work of McCourt and Snider (1967, their equation 72) that collision integrals can be obtained in terms of degeneracy-averaged cross sections defined in terms of reaction matrices describing the molecular collisions.

For the purposes of applications contemplated here, it is sufficient to assume that the internal structure is characterized by nondegenerate energy states labelled by $i, i' \ldots$ for charged particles and $j, j' \ldots$ for the neutrals. The corresponding energies are E_i and E^0_j etc. A collision leading to the change of variables

$$(\boldsymbol{G}, \boldsymbol{g}, E_i, E^0_j) \rightarrow (\boldsymbol{G}, \boldsymbol{g}', E_{i'}, E^0_{j'}) \tag{52}$$

is characterized by a degeneracy-averaged cross section $\sigma^{i'j'}_{ij}(g, \chi)$, where χ is the angle between the initial and final relative velocities $\boldsymbol{g}$ and $\boldsymbol{g}'$. The magnitudes of the relative velocities are related by energy conservation:

$$\tfrac{1}{2}(\mu\mu_0)^{\frac{1}{2}} g^2 + E_i + E^0_j = \tfrac{1}{2}(\mu\mu_0)^{\frac{1}{2}} g'^2 + E_{i'} + E^0_{j'},$$

or

$$g'^2 = g^2 - \Delta^{i'j'}_{ij}, \qquad \Delta^{i'j'}_{ij} = 2\{E_{i'} + E^0_{j'} - (E_i + E^0_j)\}/(\mu\mu_0)^{\frac{1}{2}}. \tag{53}$$

The change Δ in the energy can be positive or negative but the cross section must vanish if we have $g'^2 < 0$. Elastic collisions correspond to $\Delta = 0$.

The distribution function for the neutrals, assumed to be in equilibrium, is given by

$$f_0(\boldsymbol{c}_0, j) = n_0 \, \bar{w}(\alpha_0, c_0) \, h_j , \tag{54a}$$

$$h_j = Z_0^{-1} \exp(-E_j^0/kT_0) , \qquad Z_0 = \sum_j \exp(-E_j^0/kT_0) . \tag{54b}$$

The distribution function for the charged particles $f(\boldsymbol{c}, i)$, has the following expansion in the $\boldsymbol{x}$ basis:

$$f(\boldsymbol{c}, i) = n \, \bar{w}(\alpha, x) \sum_{\mathbf{v}} \phi^{[\mathbf{v}]}(\alpha \boldsymbol{x}) \, \mathfrak{F}_i^{(\mathbf{v})} , \tag{55a}$$

$$\mathfrak{F}_i^{(\mathbf{v})} = n^{-1} \int f(\boldsymbol{c}, i) \, \phi^{(\mathbf{v})}(\alpha \boldsymbol{x}) \, \mathrm{d}\boldsymbol{c} . \tag{55b}$$

It is always possible to assume an expansion of this form. The distribution of internal states is contained in the expansion coefficients $\mathfrak{F}_i^{(\mathbf{v})}$.

The collision integral has the form (see Wang-Chang *et al.* 1964)

$$J(f(\boldsymbol{c}, i)) = \sum_{j, i'j'} \int \left(f(\boldsymbol{c}, i) \, f(\boldsymbol{c}_0, j) - f(\boldsymbol{c}', i') \, f_0(\boldsymbol{c}_0', j') \right) g \, \sigma_{ij}^{i'j'}(g, \chi) \, \mathrm{d}\hat{\boldsymbol{g}}' \, \mathrm{d}\boldsymbol{c}_0 . \tag{56}$$

Consequently, one may write

$$\int \phi^{(\mathbf{v})}(\alpha \boldsymbol{x}) \, J(f(\boldsymbol{c}, i)) \, \mathrm{d}\boldsymbol{c} = n n_0 \sum_{\mathbf{v}' i'} J_{\mathbf{v}\mathbf{v}'}(ii') \, \mathfrak{F}_{i'}^{(\mathbf{v}')} . \tag{57}$$

This defines the matrix element $J_{\mathbf{v}\mathbf{v}'}(ii')$ which now operates on the internal states (ii') and the velocity 'states' $(\mathbf{v}\mathbf{v}')$ of the charged particle. Substituting on the left-hand side of equation (57) from (56), (54a) and (55a), and using the change of variables $(\boldsymbol{x}, \boldsymbol{c}_0) \rightarrow (\boldsymbol{x}', \boldsymbol{c}_0')$, along with the microscopic reversibility of the cross sections in a suitable way, one obtains the integral representation of the matrix element as

$$J_{\mathbf{v}\mathbf{v}'}(ii') = \sum_{ji''j''} \int \bar{w}(\alpha, x) \, \bar{w}(\alpha_0, c_0) \, \phi^{[\mathbf{v}']}(\alpha \boldsymbol{x}) \left[\phi^{(\mathbf{v})}(\alpha \boldsymbol{x}) \, h_j \, \delta_{ii'} - \phi^{(\mathbf{v})}(\alpha \boldsymbol{x}') \, h_{j''} \, \delta_{i''i'} \right]$$

$$\times g \, \sigma_{ij}^{i''j''}(g, \chi) \, \mathrm{d}\hat{\boldsymbol{g}}' \, \mathrm{d}\boldsymbol{g} \, \mathrm{d}\boldsymbol{G} . \tag{58}$$

Here $\delta_{ii'}$ is the Kronecker delta. Comparing this expression with the formula (13) for the elastic case one sees that the analysis of the velocity-dependent part can proceed as before up to the point where the integration over $\mathrm{d}\hat{\boldsymbol{g}}'$ is to be carried out. At this point one gets, instead of equation (16c), an expression of the form

$$\sum_{ji''j''} \int \left[\phi^{(n)}(\gamma \boldsymbol{g}) \, h_j \, \delta_{ii'} - \phi^{(n)}(\gamma \boldsymbol{g}') \, h_{j''} \, \delta_{i''i'} \right] g \, \sigma_{ij}^{i''j''}(g, \chi) \, \mathrm{d}\hat{\boldsymbol{g}}' \equiv \phi_m^{(0l)}(\gamma \boldsymbol{g}) \, S^{(nl)}(ii'; g) . \tag{59}$$

The function S defined here effectively replaces the quantity $g \, \sigma^{(l)}(g)$ in the previous work. The interaction integral corresponding to equation (42) is now given by

$$V_{nn'}^{n_1 l_1}(ii') = \int \bar{w}(\gamma, g_2) \, \phi^{(n)}(\gamma \boldsymbol{g}_2) \, \phi^{[n']}(\gamma \boldsymbol{g}_2) \, S^{(n_1 l_1)}(ii'; g) \, \mathrm{d}\boldsymbol{g}_2 . \tag{60}$$

As before, $\boldsymbol{g}_2$ is related to $\boldsymbol{g}$ by equations (34b) and the integral depends on γ, τ_3 and W. Modifications to the previous formulae arise through equations (59) and (60). Before describing these, it is useful to analyse the function S in greater detail. This function carries the summations over internal states and is given by

$$S^{(nl)}(ii';g) = \left(\frac{\Gamma(l+\frac{3}{2})}{2\pi^{3/2}}\right)^{\frac{1}{2}}\left(\frac{\gamma g}{\sqrt{2}}\right) \sum_{j,i''j''} [R_{nl}(\gamma g)\,\sigma_0^*(g) - R_{nl}(\gamma g'_*)\,\sigma_l^*(g)]\,g\,, \tag{61a}$$

$$\sigma_0^*(g) = 2\pi\,\delta_{ii'}\,h_j \int \sigma_{ij}^{i''j''}(g,\chi)\,\mathrm{d}(\cos\chi)\,, \tag{61b}$$

$$\sigma_l^*(g) = 2\pi\,\delta_{i''i'}\,h_{j''} \int \sigma_{ij}^{i''j''}(g,\chi)\,\mathrm{P}_l(\cos\chi)\,\mathrm{d}(\cos\chi)\,. \tag{61c}$$

Here the asterisk is used as an abbreviation for the state indices and g'_* ($\equiv g'$) is given as a function of g and the state labels by equations (53).

When $i = i'$ the first and second terms in equation (61a) are respectively

$$\sim \sum_{j,i''j''} h_j\,\sigma_{ij}^{i''j''} \qquad \text{and} \qquad \sim \sum_{jj''} h_{j''}\,\sigma_{ij}^{ij''}\,. \tag{62}$$

The elastic collisions of the particles in the state i are a subset of the sums (62) with $i = i''$ and $j = j''$. Both terms are then $\sim h_j\,\sigma_{ij}^{ij}$. Thus, the elements diagonal in internal state labels i contain all the elastic effects and some others which represent reaction-like processes. The cross sections for the latter are finite and do not occur in combinations like $(\sigma_0 - \sigma_l)$ as the elastic cross sections do. Only in the classical models of elastic collisions is it necessary to carry this combination together to avoid divergences.

On the other hand, the elements that are nondiagonal in the internal labels ($i \neq i'$) do not contain the first term (61b) at all. They only involve reaction-like processes

$$\sum_{jj''} h_{j''}\,\sigma_{ij}^{i''j''}\,.$$

The above observations can be incorporated into the calculation at the level of calculating σ_0^* and σ_l^* and the S functions. The J operator can then be evaluated for different processes separately. In other words, the equations (61) contain contributions from all processes including the elastic collisions, but in actual calculations it may be more convenient to develop collision operators representing particular processes. This can be done by selecting appropriate parts of the sum (61a) in constructing the S function.

With the appropriate choice of S function, the modifications required to previous calculations are as follows.

(i) *Gas temperature or* $\boldsymbol{c}$ *basis.* Equation (17a) applies here with

$$V_{nn'}^{l} \to V_{nn'}^{l}(ii')\,, \tag{63a}$$

$$V_{nn'}^{l}(ii') = \delta_{mm'}\,\delta_{ll'} \int \bar{w}(\gamma,g)\,R_{n'l}(\gamma g)\,S^{(nl)}(ii';g)\,g^2\,\mathrm{d}g\,. \tag{63b}$$

The modification required to Fig. 1 is shown in Fig. 5*a*.

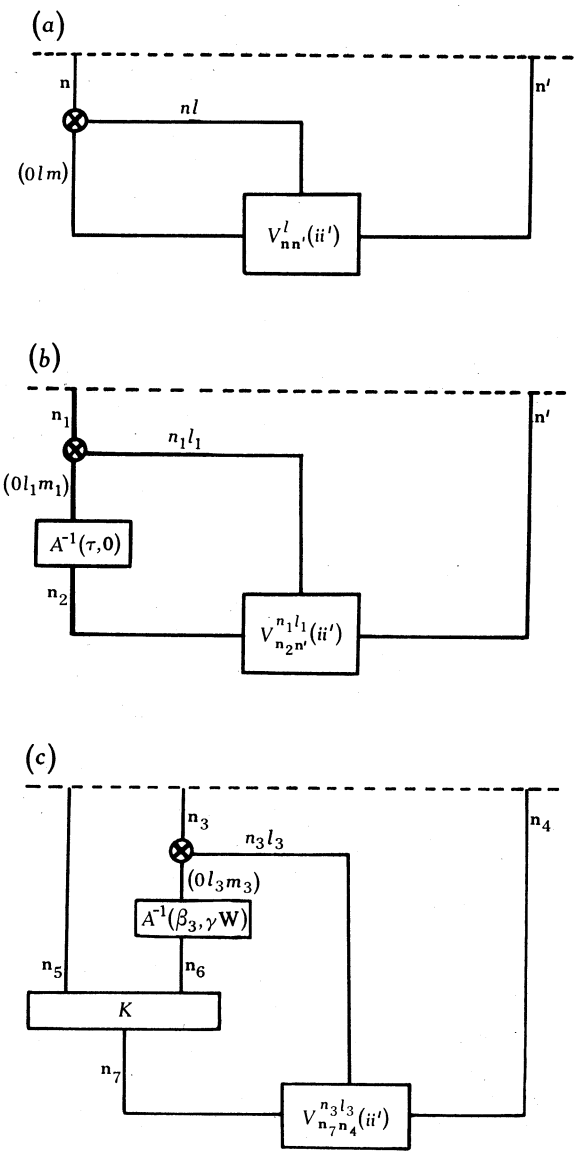

Fig. 5. Modifications required to previous calculations to include inelastic collisions (in each case the earlier diagram remains unaltered above the dashed line):

(*a*) modification to Figs 1 and 2 (see (i) and (ii) in Section 6);

(*b*) modification to Fig. 3*a* (see (iii) in Section 6);

(*c*) modification to Fig. 4*a* (see (iv) in Section 6).

(ii) *Similarity transformation.* Equation (19) applies here with ^{0}J calculated by the amended procedure described above. The modification required to Fig. 2 is shown in Fig. 5*a*.

(iii) *Expansion of neutral distribution in x_0 basis.* Equation (23a) applies here with

$$(\mathbf{v} \mid J \mid \mathbf{v}_1, \mathbf{v}') = \sum T(N, \boldsymbol{n} \mid \alpha \mathbf{v}', \alpha_0 \mathbf{v}_1)\, T(N, \boldsymbol{n}' \mid \alpha \mathbf{v}, \alpha_0 \boldsymbol{0}) \times [A(\tau, 0)]^{n' n_1} [A^{-1}(\tau, 0)]^{0 l_1 m_1, n_2 l_2 m_2}\, V_{n_2 n'}^{n_1 l_1}(ii'), \tag{64a}$$

$$V_{n_2 n'}^{n_1 l_1}(ii') = \int \bar{w}(\gamma, g_1)\, \phi^{(n_2)}(\gamma \boldsymbol{g}_1)\, \phi^{[n']}(\gamma \boldsymbol{g}_1)\, S^{(n_1 l_1)}(ii'; g)\, \mathrm{d}\boldsymbol{g}_1, \tag{64b}$$

with $g = \{(\tau^{-1} \boldsymbol{g}_1)^2\}^{\frac{1}{2}}$. These are modifications of equations (29) and (28) respectively and may be understood with reference to Fig. 5*b*.

(iv) *Matrix elements as finite sums.* Equation (43) applies here, with the replacements

$$[A^{-1}(\boldsymbol{\beta}_3, \gamma \boldsymbol{W})]^{n_3, n_6} \rightarrow [A^{-1}(\boldsymbol{\beta}_3, \gamma \boldsymbol{W})]^{0 l_3 m_3, n_6 l_6 m_6}, \tag{65a}$$

$$V_{n_7 n_4}^{l_3} \rightarrow V_{n_7 n_4}^{n_3 l_3}(ii'), \tag{65b}$$

where the last quantity was defined by equation (60). This modification may be understood by referring to Fig. 5*c*.

Other formulae developed for special cases in previous sections can be similarly adapted for calculations with inelastic collisions.

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