

Approximate Formulas for Ion and Electron Transport Coefficients in Crossed Electric and Magnetic Fields

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Abstract

Momentum-transfer theory is used to derive approximate expressions for transport properties of electrons and ions in a gas in crossed electric and magnetic fields. Included in the formal discussion are the generalised Einstein relations, negative differential conductivity, Tonks' theorem and the equivalent reduced electric field concept. Specific topics dealt with include the ratio D_{\parallel}/D_{\perp} for electrons, which 'flips over' as the magnetic field is increased, the enhancement of negative differential conductivity through increased B/N , and a discussion of anisotropic scattering.

1. Introduction

It was pointed out ten years ago by Blevin and Brennan (1983) that many aspects of electron swarm behaviour in gases in crossed electric and magnetic fields remained unexplored at that time, both theoretically and experimentally, despite a long history (Huxley and Crompton 1974; Heylen 1980) of studies of gas discharges in transverse magnetic fields. Heylen (1980) had previously remarked on the neglect of this topic in standard texts, conjecturing, quite reasonably, that the extra complexity introduced by the magnetic fields had possibly acted as a deterrent to discussion. Since then, Brennan and coworkers (Brennan and Garvie 1990; Garvie and Brennan 1990; Brennan *et al.* 1990), Schmidt and collaborators (Schmidt 1986, 1991, 1992, 1993; Schmidt and Polenz 1988; Kunst 1992; Kunst *et al.* 1993), Ness (1993, 1994), Ikuta and Sugai (1989) and Biagi (1988, 1989) have made significant advances both theoretically and experimentally, but it remains true to say that much work remains to be done to achieve a level of understanding comparable to that attained over the last two decades for transport in electric fields only (Robson and Ness 1986; Ness and Robson 1986; Mason and McDaniel 1988; Viehland 1992). This remark applies especially to transport in the presence of 'reactive', non-particle-conserving collisions (e.g. ionising and attaching collisions), which still generates some debate (Robson 1991), even in the absence of the extra dimension provided by a transverse magnetic field. One of the main motivating forces behind the investigations of the Heidelberg group led by Heintze (1978, 1982) and Schmidt (*loc. cit.*) is the application to multiwire drift tube detection of high-energy particles (Hargrove *et al.* 1984). However, the problem has an intrinsic interest in its own right, and this is the thrust of the present paper.

As a natural progression from previous work for magnetic field-free situations (Robson and Ness 1986; Ness and Robson 1986), Ness (1993, 1994) has developed a 'multi-term' solution of the Boltzmann equation

$$\left(\partial_t + \mathbf{v} \cdot \nabla + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \partial_{\mathbf{v}} + J \right) f = 0$$

for the swarm particle phase-space distribution function $f(\mathbf{r}, \mathbf{v}, t)$. In this approach, one represents f by an expansion like (57) below to whatever order ℓ of spherical harmonics $Y_{\ell m}(\hat{\mathbf{v}})$ that is necessary to meet some accuracy criterion. This generalises the 'two-term' ($\ell \leq 1$) theory which underpinned earlier studies of electron swarms (Huxley and Crompton 1974). Neither is there any restriction to simple collision cross sections (Braglia and Ferrari 1973*a*, 1973*b*). Agreement with experiment is excellent over a wide range of E/N and B/N . However, the associated tensor analysis and algebra, along with the detailed numerical computation, do not readily lend themselves to physical interpretation. There is thus an identifiable need at this time for a straightforward qualitative or semiquantitative analysis which provides the necessary insight. Momentum-transfer theory (Mason and McDaniel 1988; Robson 1984, 1986; Robson and Ness 1988; Ness and Robson 1988) has served this purpose well for the magnetic field-free case and there is every reason to believe that it will do the same for the far more difficult case when $B \neq 0$.

The scope of the present paper is the provision of relatively simple but approximate formulas for transport properties of ion and electron swarms in crossed electric and magnetic fields, in the absence of reactive effects. This latter proviso is made in this initial study in order to keep the complexity of the equations to a minimum. However, it is acknowledged that many important and interesting phenomena occur in gaseous discharges involving ionisation, recombination and attachment, and a follow-up paper is planned specifically for this purpose, along the lines of Robson (1986) and Robson and Ness (1988).

Although we do exclude non-particle-conserving collisions at present, both elastic and inelastic processes are considered and the formulas obtained are valid for both ions and electrons. Specific topics dealt with in Section 2 are:

- (i) calculation of the temperature tensor \mathbf{T} (four independent components);
- (ii) derivation of generalised Einstein relations (GER) linking the five independent components of the diffusion tensor \mathbf{D} with mobilities along \mathbf{E} and $\mathbf{E} \times \mathbf{B}$ respectively;
- (iii) negative differential conductivity (NDC);
- (iv) the equivalent reduced electric field concept; and
- (v) Tonks' theorem.

Section 3 involves further discussion of the formulas, along with some calculations for electron swarms in simple model gases.

2. Theory

(a) Balance Equations

In what follows, we refer to Robson (1984) as I. Balance or 'moment' equations can be derived from Boltzmann's equation in Section 1 by multiplying by

appropriate functions $\phi(\mathbf{v})$ of ion velocity \mathbf{v} and integrating over all \mathbf{v} . Setting $\phi(\mathbf{v}) = 1$, $m\mathbf{v}$ and $\frac{1}{2}m\mathbf{v}^2$ gives, respectively, the equation of continuity

$$\partial_t n + \nabla \cdot n\langle \mathbf{v} \rangle = 0, \tag{1}$$

the momentum balance equation,

$$-k\mathbf{T} \cdot \nabla n + nq(\mathbf{E} + \langle \mathbf{v} \rangle \times \mathbf{B}) = n\mu\nu_m(\langle \epsilon \rangle)\langle \mathbf{v} \rangle, \tag{2}$$

and the energy balance equation

$$-\frac{Q}{n\nu_e} \cdot \nabla n = \langle \epsilon \rangle - \frac{1}{2}M\langle V^2 \rangle - \frac{1}{2}M\langle \mathbf{v} \rangle^2 + \Omega(\langle \epsilon \rangle). \tag{3}$$

Equations (2) and (3) are valid to first order in the density gradient ∇n ; if non-particle-conserving collisions were considered, it would be necessary to go to second order in density gradient (Robson 1986). Equations (2) and (3) are also approximate to the extent that the traditional approximation, e.g. I(9) of momentum-transfer theory has been made. Again, if non-conservative collisions were dealt with, the next highest term in I(8) would need to be included. Such higher-order reactive effects are considered in later work.

In these equations m and M denote the masses of an ion and neutral molecule respectively, while \mathbf{v} and \mathbf{V} denote their velocities. The reduced mass is $\mu = mM/(m+M)$, while the average of the energy ϵ in the centre of mass is

$$\langle \epsilon \rangle = \frac{1}{2}\mu(\langle v^2 \rangle + \langle V^2 \rangle), \tag{4}$$

if $\langle \mathbf{V} \rangle = 0$. Equation (2) is a generalisation of I(10) to the extent that \mathbf{E} is replaced by $\mathbf{E} + \langle \mathbf{v} \rangle \times \mathbf{B}$, but the energy balance (3) is identical with I(11), i.e. the magnetic field does not explicitly modify the energy balance.

In equation (2) $\nu_m(\epsilon)$ denotes the total momentum-transfer collision frequency, accounting for all scattering channels, both elastic and inelastic, while in (3),

$$\nu_e \equiv \frac{2m}{m+M} \nu_m \tag{5}$$

can be thought of as a collision frequency for kinetic energy transfer. Also in (3),

$$\mathbf{Q} = \frac{1}{2}m\langle (\mathbf{v} - \langle \mathbf{v} \rangle)^2 (\mathbf{v} - \langle \mathbf{v} \rangle) \rangle \tag{6}$$

is the heat flux per ion, while as in I(13),

$$\Omega(\langle \epsilon \rangle) \equiv \frac{M}{m+M} \sum_i \epsilon_i^* \{ \langle \vec{v}_i \rangle - \langle \vec{v}_i \rangle \} / \nu_e, \tag{7}$$

the sum being over all inelastic processes i , characterised by threshold energy ϵ_i^* and (total) collision frequencies \vec{v}_i . Superelastic processes are accounted for by the collision frequency \vec{v}_i , for which we have approximately (Ness and Robson 1988):

$$\langle \vec{\nu}_i(\epsilon) \rangle \approx \langle \vec{\nu}_i(\epsilon) \rangle \exp \left[-\epsilon_i^* \left(\frac{1}{kT_g} - \frac{3}{2\langle \epsilon \rangle} \right) \right], \quad (8)$$

where $T_g = M\langle v^2 \rangle / 3k$ is the neutral gas temperature. As noted in I, a reasonable representation of the average inelastic rate is

$$\langle \vec{\nu}_i(\epsilon) \rangle \approx \vec{\nu}_i(\langle \epsilon \rangle) S(3\epsilon_i^* / 2\langle \epsilon \rangle), \quad (9)$$

where

$$S(\xi) \equiv (1 + \xi)e^{-\xi} \quad (10)$$

varies smoothly between 0 and 1 corresponding to energies well below and well above threshold respectively. Equations (8) and (9) are exact for Maxwellian energy distributions. A further discussion of collision frequencies, including explicit formulas and definitions, can be found in Appendix A.

The ion temperature tensor appearing on the left side of (2) is defined by

$$k\mathbf{T} = m\langle (\mathbf{v} - \langle \mathbf{v} \rangle)(\mathbf{v} - \langle \mathbf{v} \rangle) \rangle. \quad (11)$$

Note that it is symmetric. Since this appears with ∇n , we need calculate it only to zero order in density gradient. The balance equation, obtained by taking the moment of the Boltzmann equation in Section 1 w.r.t. $\phi = m\mathbf{c}\mathbf{c}$ plus some algebraic manipulation, is

$$\begin{aligned} r_e(k\mathbf{T} \times \hat{B} - \hat{B} \times k\mathbf{T}) &= \left(1 + \frac{3M\bar{\nu}_v}{4m\nu_m}\right) k\mathbf{T} - \left(1 - \frac{3\bar{\nu}_v}{4\nu_m}\right) M\langle \mathbf{v} \rangle \langle \mathbf{v} \rangle \\ &\quad - \left[\frac{M\bar{\bar{\nu}}_v}{2m\nu_m} \langle \epsilon \rangle + kT_g \left(1 - \frac{3\bar{\nu}_v}{4\nu_m}\right) \right] \mathbf{1}, \end{aligned} \quad (12)$$

where

$$r_e \equiv \frac{qB}{\mu\nu_e}, \quad (13)$$

$$\bar{\nu}_v \equiv \nu_v - \frac{2m\nu_m \Omega(\langle \epsilon \rangle)}{3M\langle \epsilon \rangle}, \quad (14a)$$

$$\bar{\bar{\nu}}_v \equiv \nu_v - \frac{2m\nu_m \Omega(\langle \epsilon \rangle)}{M\langle \epsilon \rangle}. \quad (14b)$$

The (total) collision frequency for the viscosity ν_v is defined in Appendix A.

We can solve (2), (3) and (12) simultaneously for $\langle \mathbf{v} \rangle$, $\langle \epsilon \rangle$ and $k\mathbf{T}$, once the collision frequencies $\nu_m(\epsilon)$, $\nu_v(\epsilon)$ and $\vec{\nu}_i(\epsilon)$ are specified. However, as has always been the philosophy behind momentum-transfer theory, our aim is to derive *relationships* between experimentally measured quantities, rather than trying to evaluate the quantities separately. In particular, we obtain the generalised Einstein relations (GER) below, linking diffusion coefficients and mobilities.

(b) Spatial Homogeneity, Drift Velocity and NDC Criterion

As in I, it is convenient to omit averaging brackets in what follows, i.e.

$$\langle \mathbf{v} \rangle \rightarrow \mathbf{v}, \quad \langle \epsilon \rangle \rightarrow \epsilon. \quad (15)$$

For spatially uniform conditions, (2) and (3) yield

$$q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) = \mu\nu_m(\epsilon)\mathbf{v}, \quad (16)$$

$$\epsilon = \frac{3}{2}kT_g + \frac{1}{2}Mv^2 - \Omega(\epsilon), \quad (17)$$

respectively. Equation (16) can be rearranged to read

$$\mathbf{v} = v_{\parallel} \hat{\mathbf{E}} \cdot (\mathbf{1} - \hat{\mathbf{B}}\hat{\mathbf{B}}) + v_{\perp} \hat{\mathbf{E}} \times \hat{\mathbf{B}} + v_0 \hat{\mathbf{B}}, \quad (18)$$

where

$$v_{\parallel} \equiv KE/[1 + (KB)^2], \quad v_{\perp} \equiv KBv_{\parallel}, \quad (19a, b)$$

$$v_0 \equiv K \mathbf{E} \cdot \hat{\mathbf{B}}, \quad K \equiv q/\nu_m(\epsilon). \quad (19c, d)$$

The quantities v_{\parallel} , v_{\perp} denote drift velocities in a plane perpendicular to \mathbf{B} , in directions parallel and perpendicular to the projection of \mathbf{E} in that plane respectively, while v_0 is the drift velocity along \mathbf{B} . In this work for the greater part we consider \mathbf{E} and \mathbf{B} to be orthogonal, i.e.

$$\hat{\mathbf{E}} \cdot \hat{\mathbf{B}} = 0, \quad v_0 = 0, \quad (20)$$

so that

$$\mathbf{v} = v_{\parallel} \hat{\mathbf{E}} + v_{\perp} \hat{\mathbf{E}} \times \hat{\mathbf{B}}. \quad (18')$$

We shall henceforth assume (20) to be true. In the case of constant collision frequency, equations (19) constitute actual solutions, but otherwise they are merely rearrangements of equation (16), which must be solved simultaneously with the energy balance equation (17).

The ratio

$$r_m = KB = qB/\mu\nu_m \quad (21)$$

represents the ratio of the magnetic gyro frequency (in the centre of mass frame) to the momentum-transfer collision frequency. The so-called Lorentz angle φ is determined by:

$$\tan\varphi \equiv v_{\perp}/v_{\parallel} = KB. \quad (22)$$

On the other hand, the drift speed is given by

$$v = (v_{\parallel}^2 + v_{\perp}^2)^{\frac{1}{2}} = \frac{KE}{(1 + K^2 B^2)^{\frac{1}{2}}} \quad (23)$$

$$= \frac{E}{B} \sin \varphi. \quad (24)$$

Other equivalent expressions for the drift velocity are

$$v_{\parallel} = v \cos \varphi, \quad v_{\perp} = v \sin \varphi. \quad (25)$$

These formulas and their relation to previous work will be further discussed below.

The following differential identities are obtained from (B16) and (B17) in Appendix B:

$$\frac{\partial v_{\parallel}}{\partial E} = \frac{1 + \Omega' + Mv_{\perp}^2 \nu_m' / \nu_m}{MKE} \frac{\partial \epsilon}{\partial E}, \quad (26a)$$

$$\frac{\partial v_{\perp}}{\partial E} = \frac{B(1 + \Omega' - Mv_{\parallel}^2 \nu_m' / \nu_m)}{ME} \frac{\partial \epsilon}{\partial E}. \quad (26b)$$

Thus, assuming that $\partial \epsilon / \partial E > 0$ always, there is NDC in the direction parallel to \mathbf{E} if

$$1 + \Omega' + Mv_{\perp}^2 \nu_m' / \nu_m < 0, \quad (27)$$

while the NDC criterion transverse to \mathbf{E} is

$$1 + \Omega' - Mv_{\parallel}^2 \nu_m' / \nu_m < 0. \quad (28)$$

Equation (27) reduces to the condition I(19) in the limit as B (and therefore v_{\perp}) $\rightarrow 0$.

Interestingly enough, the field derivative of the drift speed is given by the expression,

$$v \frac{\partial v}{\partial E} = v_{\parallel} \frac{\partial v_{\parallel}}{\partial E} + v_{\perp} \frac{\partial v_{\perp}}{\partial E} = \frac{1 + \Omega'}{M} \frac{\partial \epsilon}{\partial E}, \quad (29)$$

and so NDC occurs in speed if

$$1 + \Omega' < 0. \quad (30)$$

Equations (29) and (30) are identical to equations I(18) and I(19) respectively. The types of elastic/inelastic cross section combinations which satisfy (30) are discussed in I.

Further discussion of these NDC criteria can be found below. Finally, we note another pair of useful identities, also obtained in Appendix B:

$$\frac{M\nu_m'/\nu_m}{1 + \Omega} = \left(\frac{E}{v_{\parallel}} \frac{\partial v_{\parallel}}{\partial E} - 1 \right) / \left(v_{\perp}^2 - Ev_{\parallel} \frac{\partial v_{\parallel}}{\partial E} \right) \tag{31a}$$

$$= KB \left(1 - \frac{E}{v_{\perp}} \frac{\partial v_{\perp}}{\partial E} \right) / \left(v_{\parallel} v_{\perp} + Ev_{\parallel} \frac{\partial v_{\perp}}{\partial E} \right). \tag{31b}$$

These last two formulas are invaluable in formulating the GER. They have a counterpart in I(17) for the zero magnetic field situation.

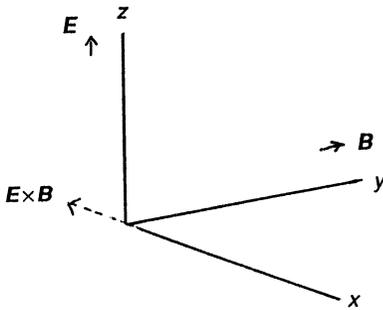


Fig. 1. System of coordinates used in this paper.

We shall defer discussion of the solution of the temperature tensor equation (12) to Appendix C and here merely note that **T** has the following structure,

$$\mathbf{T} = \begin{bmatrix} T_{\perp} & \cdot & T_{\mathcal{H}} \\ \cdot & T_{\perp}' & \cdot \\ T_{\mathcal{H}} & \cdot & T_{\parallel} \end{bmatrix}, \tag{32}$$

for the system of coordinates shown in Fig. 1.

(c) *Spatial Inhomogeneity: Diffusion Tensor, Generalised Einstein Relations*

We now write

$$\langle \mathbf{v} \rangle = \mathbf{v} + \delta \mathbf{v}, \quad \langle \epsilon \rangle = \epsilon + \delta \epsilon, \tag{33}$$

where **v**, ϵ are the spatially homogeneous drift velocity and mean energy of the previous section and $\delta \mathbf{v}$, $\delta \epsilon$ are corrections to these, respectively, of order ∇n . If equations (33) are substituted into (2) and (3) and only terms to first order in small quantities are retained, we obtain

$$k\mathbf{T} \cdot \nabla n - nq \delta \mathbf{v} \times \mathbf{B} = n\mu[\nu_m(\epsilon) \delta \mathbf{v} + \nu_m'(\epsilon) \delta \epsilon \mathbf{v}], \tag{34}$$

$$- \frac{Q}{n\nu_e(\epsilon)} \cdot \nabla n = \delta \epsilon [1 + \Omega'(\epsilon)] - M\mathbf{v} \cdot \delta \mathbf{v}. \tag{35}$$

Elimination of $\delta\epsilon$ between these equations then gives

$$k\bar{\mathbf{T}} \cdot \frac{1}{n} \nabla n - q\delta\mathbf{v} \times \mathbf{B} = -\mu \left(\nu_m \mathbf{1} + \frac{\nu_m'}{1+\Omega'} M\mathbf{v}\mathbf{v} \right) \cdot \delta\mathbf{v}, \quad (36)$$

where

$$k\bar{\mathbf{T}} \equiv k\mathbf{T} - \frac{\mu\nu_m' \mathbf{v}\mathbf{Q}}{(1+\Omega')\nu_e}. \quad (37)$$

Now the diffusion tensor \mathbf{D} is defined by the relation

$$n\delta\mathbf{v} = -\mathbf{D} \cdot \nabla n, \quad (38)$$

and substitution into (36) and equating coefficients of $n^{-1}\nabla n$ therefore gives

$$k\bar{\mathbf{T}} = q\mathbf{B} \times \mathbf{D} + \mu \left(\nu_m \mathbf{D} + \frac{\nu_m'}{1+\Omega'} \mathbf{v}\mathbf{v} \cdot \mathbf{D} \right). \quad (39)$$

On the other hand, the same *form* of equation results if we differentiate (16) w.r.t. \mathbf{E} and contract the result with $k\bar{\mathbf{T}}$:

$$k\bar{\mathbf{T}} = \mathbf{B} \times (\mathbf{K} \cdot k\bar{\mathbf{T}}) + \frac{\mu}{q} \left(\nu_m \mathbf{K} \cdot k\bar{\mathbf{T}} + \frac{\nu_m'}{1+\Omega'} M\mathbf{v}\mathbf{v} \cdot (\mathbf{K} \cdot k\bar{\mathbf{T}}) \right), \quad (40)$$

where \mathbf{K} is the differential mobility tensor

$$K_{ij} \equiv \frac{\partial v_i}{\partial E_j}. \quad (41)$$

Comparison of (40) and (39) shows that

$$\mathbf{D} = \mathbf{K} \cdot \frac{k}{q} \bar{\mathbf{T}} \quad (42)$$

or equivalently, with implied summation on repeated indices,

$$D_{ij} = K_{il} \frac{k}{q} \bar{T}_{lj} = \frac{k}{q} \bar{T}_{lj} \frac{\partial v_i}{\partial E_l}. \quad (43)$$

This is the generalised Einstein relation, through not yet in a particularly useful form.

We can calculate \mathbf{K} explicitly by differentiating (18) w.r.t. \mathbf{E} . Then, assuming the form (32) for the temperature tensor, we find that (42) yields the diffusion tensor

$$\mathbf{D} = \begin{bmatrix} D_{\perp} & \cdot & \bar{D}_{\mathcal{H}} \\ \cdot & D_{\perp}' & \cdot \\ D_{\mathcal{H}} & \cdot & D_{\parallel} \end{bmatrix}, \quad (44)$$

where

$$D_{\perp} = \frac{K_{\parallel}}{q} kT_{\perp} - \frac{kT_{\mathcal{H}}}{q} \frac{\partial v_{\perp}}{\partial E} + \frac{MQ_{\perp} \nu_m' / \nu_m}{2q(1 + \Omega')} \left(\frac{v_{\parallel} v_{\perp}}{E} + v_{\parallel} \frac{\partial v_{\perp}}{\partial E} \right), \quad (45)$$

$$\bar{D}_{\mathcal{H}} = K_{\parallel} \frac{kT_{\mathcal{H}}}{q} - \frac{kT_{\parallel}}{q} \frac{\partial v_{\perp}}{\partial E} + \frac{MQ_{\parallel} \nu_m' / \nu_m}{2q(1 + \Omega')} \left(\frac{v_{\parallel} v_{\perp}}{E} + v_{\parallel} \frac{\partial v_{\perp}}{\partial E} \right), \quad (46)$$

$$D_{\perp}' = K \frac{kT_{\perp}'}{q} \quad (47)$$

$$D_{\mathcal{H}} = K_{\perp} \frac{kT_{\perp}}{q} + \frac{\partial v_{\parallel}}{\partial E} \frac{kT_{\mathcal{H}}}{q} + \frac{M\nu_m' / \nu_m Q_{\perp}}{2(1 + \Omega')q} \left(\frac{v_{\perp}^2}{E} - v_{\parallel} \frac{\partial v_{\parallel}}{\partial E} \right), \quad (48)$$

$$D_{\parallel} = K_{\perp} \frac{kT_{\mathcal{H}}}{q} + \frac{\partial v_{\parallel}}{\partial E} \frac{kT_{\parallel}}{q} + \frac{M\nu_m' / \nu_m Q_{\parallel}}{2(1 + \Omega')q} \left(\frac{v_{\perp}^2}{E} - v_{\parallel} \frac{\partial v_{\parallel}}{\partial E} \right), \quad (49)$$

with

$$K_{\parallel} \equiv v_{\parallel} / E, \quad K_{\perp} \equiv v_{\perp} / E. \quad (50a)$$

Notice that Q_{\perp} and Q_{\parallel} are elements of the heat flux vector, defined by

$$\mathbf{Q} = (Q_{\perp}, 0, Q_{\parallel}). \quad (50b)$$

These formulas can be considerably simplified by making use of the identities (31) and by defining the 'correction factors':

$$\Delta_{\parallel} \equiv \frac{Q_{\parallel}}{2kT_{\parallel} v_{\parallel}}, \quad \Delta_{\perp} \equiv \frac{Q_{\perp}}{2kT_{\mathcal{H}} v_{\parallel}}. \quad (51)$$

Thus, we have the generalised Einstein relations

$$D_{\perp} = K_{\parallel} \frac{kT_{\perp}}{q} - K_{\perp} \frac{kT_{\mathcal{H}}}{q} \left(1 + (1 + \Delta_{\perp}) \frac{\partial \ln K_{\perp}}{\partial \ln E} \right), \quad (52)$$

$$\bar{D}_{\mathcal{H}} = K_{\parallel} \frac{kT_{\mathcal{H}}}{q} - K_{\perp} \frac{kT_{\parallel}}{q} \left(1 + (1 + \Delta_{\parallel}) \frac{\partial \ln K_{\perp}}{\partial \ln E} \right), \quad (53)$$

$$D_{\perp}' = K \frac{kT_{\perp}'}{q}, \quad (54)$$

$$D_{\mathcal{H}} = K_{\perp} \frac{kT_{\perp}}{q} + K_{\parallel} \frac{kT_{\mathcal{H}}}{q} \left(1 + (1 + \Delta_{\perp}) \frac{\partial \ln K_{\parallel}}{\partial \ln E} \right), \quad (55)$$

$$D_{\parallel} = K_{\perp} \frac{kT_{\mathcal{H}}}{q} + K_{\parallel} \frac{kT_{\parallel}}{q} \left(1 + (1 + \Delta_{\parallel}) \frac{\partial \ln K_{\parallel}}{\partial \ln E} \right). \quad (56)$$

It can be seen that the GER are considerably more complex than the corresponding relations I(3) and (4), to which they reduce, of course, in the limit as $B \rightarrow 0$.

(d) *Considerations of Anisotropy: Temperature Tensor*

The ion temperature tensor is defined by (11) and explicit expressions for the elements shown in (32) are given in Appendix C. The differences between these elements reflect the degree of anisotropy of the velocity distribution function $f(\mathbf{v})$ in velocity space. Normally one accounts for such anisotropy through a spherical harmonic decomposition,

$$f(\mathbf{v}) \approx f^{(L)}(\mathbf{v}) = \sum_{\ell=0}^L \sum_{m=-\ell}^{\ell} f_{\ell m}(\mathbf{v}) Y_{\ell m}(\hat{\mathbf{v}}), \quad (57)$$

in which the number $L+1$ of spherical harmonics is chosen to satisfy predetermined accuracy criteria for transport properties. For electrons, for which $m \ll M$, the so-called two-term approximation ($L = 1$) dominated transport coefficient theory and computation until the late 1970s, when it became recognised that 'multi-term' analysis ($L \geq 2$) is required, especially when inelastic electron-molecule collisions are important. (See the review by Robson and Ness 1986.) The results of Allis (1956) and Huxley and Crompton (1974) are derived from two-term theory. On the other hand, for ions it has long been recognised that $f(\mathbf{v})$ is generally appreciably anisotropic (see for example Fig. 12 of Wannier 1953), even when collisions are elastic, and that multi-term analysis is almost always required, although this terminology is not commonly used by workers in ion transport (Mason and McDaniel 1988).

In the two-term approximation, with $|f_{1m}| \ll |f_0|$, the temperature tensor (32) reduces to a scalar, i.e.

$$T_{\perp} \approx T_{\perp}' \approx T_{\parallel}, \quad T_{\mathcal{H}} \approx 0, \quad (58a, b)$$

as can be readily verified by evaluating the average (11), $f(\mathbf{v})$ being approximated by (57) with $L = 1$. In what follows, we shall establish the conditions under which equations (58) hold, starting from the general expressions for T_{\perp} , T_{\perp}' , T_{\parallel} and $T_{\mathcal{H}}$ given in Appendix C.

Initially we look at the relatively uncomplicated case where $B = 0$. In the absence of inelastic processes we have $\Omega = 0$ and, by (14a, b),

$$\bar{\nu}_v = \bar{\nu}_v = \nu_v = Ng2\pi \int (1 - \cos^2 \chi) \sigma(g, \chi) \sin \chi \, d\chi. \quad (59)$$

In addition, if $B = 0$, then $r_e = 0$, $v_{\perp} = 0$, $v = v_{\parallel}$ and equations (C23)–(C26) reduce to

$$kT_{\perp}' = kT_{\perp} = kT_g + \left[\frac{(m+M)\nu_v}{4m\nu_m} \right] / \left(1 + \frac{3M\nu_v}{4m\nu_m} \right) Mv^2, \quad (60a)$$

$$kT_{\parallel} = kT_g + \left[\left(1 - \frac{3\nu_v}{4\nu_m} + \frac{(m+M)\nu_v}{4m\nu_m} \right) \right] / \left(1 + \frac{3M\nu_v}{4m\nu_m} \right) Mv^2, \quad (60b)$$

$$kT_{\mathcal{H}} = 0. \quad (60c)$$

These results are exact for the Maxwell model where ν_v and ν_m are constants, independent of energy (Wannier 1953), but are only approximations in other cases, where ν_v and ν_m are functions of mean energy $\langle \epsilon \rangle$. It is our intention to use these formulas, and their generalisations which follow, in a qualitative fashion only, for a literal, quantitative application is not always desirable (Skullerud 1973).

For electrons or light ions, $m \ll M$ and the temperature tensor is generally isotropic:

$$kT_{\perp} \approx kT_{\parallel} \approx kT_g + \frac{1}{3}Mv^2, \quad (61)$$

as follows from (60a, b) with

$$M\nu_v/m\nu_m \gg 1. \quad (62)$$

There is an important exception to this, however, for strongly anisotropic, *backward* scattering, for which $\sigma(g, \chi)$ is appreciable only for $\chi \sim \pi$, i.e. $\cos\chi \approx -1$. Then by (59), we have $\nu_v \approx 0$ but the momentum-transfer collision frequency

$$\nu_m = Ng2\pi \int (1 - \cos\chi) \sigma(g, \chi) \sin\chi \, d\chi \quad (63)$$

is not necessarily small. Thus the inequality (62) may not be satisfied and the temperature tensor may not be isotropic for strong backward scattering. The two-term approximation of the velocity distribution function would not be expected to hold in these circumstances and indeed this result has long been known (Lin *et al.* 1981). Notice that strongly *forward* anisotropic scattering ($\chi \approx 0$) does not violate (62), since *both* ν_m and ν_v are then small.

If inelastic as well as elastic collisions are important, then equations (60) no longer hold. Equations (C23)–(C26) then yield for $B = 0$:

$$kT_{\perp}' = kT_{\perp} = ukT_g + A_0 Mv^2 - 2A_0 \Omega, \quad (64a)$$

$$kT_{\parallel} = ukT_g + A_1 Mv^2 - 2A_0 \Omega, \quad (64b)$$

$$kT_{\mathcal{H}} = 0, \quad (64c)$$

where u is defined by (C27) and

$$A_0 \equiv \left[\frac{(m+M)\bar{\nu}_v}{4m\nu_m} \right] / \left(1 + \frac{3M\bar{\nu}_v}{4m\nu_m} \right) Mv^2, \quad (65a)$$

$$A_1 \equiv \left(1 - \frac{3\bar{\nu}_v}{4\nu_m} + \frac{(m+M)\bar{\nu}_v}{4m\nu_m} \right) / \left(1 + \frac{3M\bar{\nu}_v}{4m\nu_m} \right). \quad (65b)$$

If now we take electrons, for which $m \ll M$, and also assume that

$$\frac{M\bar{\nu}_v}{m\nu_m} \gg 1, \quad \frac{M\bar{\nu}_v}{m\nu_m} \gg 1, \quad (66)$$

then

$$A_0 \approx A_1 \approx \frac{1}{3} \bar{\nu}_v / \bar{\nu}_v, \quad u \approx \bar{\nu}_v / \bar{\nu}_v,$$

and (64a, b) then show once more that

$$kT_{\parallel} \approx kT_{\perp} \approx kT_{\perp}' \approx \frac{\bar{\nu}_v}{\bar{\nu}_v} [kT_g + \frac{1}{3}(Mv^2 - 2\Omega)], \quad (67)$$

i.e. the temperature tensor is a scalar.

Either one of the inequalities (66) may be violated, perhaps over a range of mean energies, and the temperature tensor elements consequently unequal, for two different reasons: firstly, if there is strong backward scattering, ν_v (and hence $\bar{\nu}_v$, $\bar{\nu}_v$) may be small compared with ν_m , as discussed previously, but the picture is by no means as clear cut as for the case where only elastic collisions occur. Secondly, even without such anisotropic scattering, $\bar{\nu}_v$ or $\bar{\nu}_v$ could still be small if inelastic collisions dominate. To see this, approximate (14) for electrons ($m \ll M$) by

$$\bar{\nu}_v = \nu_v(1 - \frac{1}{3}\delta), \quad \bar{\nu}_v = \nu_v(1 - \delta), \quad (68)$$

where

$$\delta = \sum_i \frac{\epsilon_i [\langle \bar{\nu}_i(\epsilon) \rangle - \langle \bar{\nu}_i(\epsilon) \rangle]}{\langle \epsilon \rangle \nu_v(\langle \epsilon \rangle)} \quad (69)$$

is a measure of the average inelastic energy exchange in time ν_v^{-1} relative to the mean energy $\langle \epsilon \rangle$ of the electron swarm. If the mean energy is such that δ is near 1 or 3, then $\bar{\nu}_v \sim 0$ or $\bar{\nu}_v \sim 0$ respectively and the isotropy conditions (66) may not hold, leading to a significant difference between kT_{\parallel} and kT_{\perp} . Such a situation occurs in methane, for example, where the elastic scattering cross section has a pronounced Ramsauer minimum for energies in the neighbourhood of the threshold for the first inelastic process (Ness 1985; Ness and Robson 1986). For values of E/N such that the mean energy falls in this critical region, significant anisotropy is observed. For energies well above the Ramsauer

minimum, the parameter becomes very small and the isotropy condition (66) holds. This explains why anisotropy, as reflected in the failure of the two-term approximation, is often found to occur only over a *localised* range of E/N (Ness 1985; Ness and Robson 1986).

We now consider the case where $B > 0$, for which equations (C23)–(C26) give the complete expressions for kT_{\parallel} , kT_{\perp} , kT_{\perp}' and $kT_{\mathcal{H}}$. In the exceptional cases described above (that is, strong backward and/or dominant inelastic scattering), we might expect all these elements to be nonzero and to differ significantly from each other. If, however, inequalities (66) hold then we have (64c) and (67) once again, correct to order m/M . That is, the temperature tensor is effectively a scalar for electron swarms even for $B \neq 0$.

(e) *Tonks' Theorem, Equivalent Field Concept, Magnetic Deflection Coefficient*

Heylen (1980) has reviewed the concept of equivalent electric field E_e (or what is virtually the same, since transport properties scale with E/N , the equivalent density/gas pressure concept), which can be summarised by the statement

$$\epsilon(E, B) = \epsilon(E_e, 0). \quad (70)$$

That is, E_e is the electric field for $B = 0$ required to keep the mean swarm energy at the same value as in the actual situation, where the electric fields are E and B respectively. It can be shown that (70) is consistent with momentum-transfer theory, with

$$E_e = E \cos \varphi. \quad (71)$$

When (70) is extended to include other transport properties, e.g. drift velocity,

$$v(E, B) = v(E_e, 0), \quad (72)$$

it is sometimes called Tonks' theorem (Tonks 1937; Tonks and Allis 1937). At the present level of discussion, based on momentum-transfer theory, it is readily shown that Tonks' theorem holds. The practical application of these ideas is now briefly discussed.

We have from (22) that

$$E_e = E/[1 + (KB)^2]^{\frac{1}{2}}, \quad (73)$$

where $K(\epsilon)$ is defined by (19d), and equation (23) for drift velocity can be written as

$$v = KE_e. \quad (74)$$

Upon substitution of this into (17), we find

$$E_e = \frac{1}{K(\epsilon)} \left(\frac{2}{M} [\epsilon + \Omega(\epsilon) - \frac{3}{2} kT_g] \right)^{\frac{1}{2}}. \quad (75)$$

A scheme of computation based on these formulas is as follows:

- (i) specify the mean energy ϵ ;
- (ii) calculate $K(\epsilon)$ from (19d) and E_e from (75);
- (iii) find the drift velocity from (74);
- (iv) equation (73) then gives the relationship between E and B for this value of E_e ; and
- (v) calculate other transport coefficients.

The magnetic deflection factor ψ was introduced by Frost and Phelps (1962). It is defined by

$$\psi = \frac{(E/B \tan \varphi)}{v}. \quad (76)$$

In the momentum-transfer theory approximation we have from (22) and (23) that

$$\psi = (1 + K^2 B^2)^{\frac{1}{2}}, \quad (77)$$

which for magnetic fields such that $KB = qB/\mu\nu_m < 1$ gives $\psi \approx 1$. This is the expected result for formulas based on the Maxwell model (Huxley and Crompton 1974, Ch. 8).

3. Discussion of Formulae

(a) Calculations of Drift Velocity for Some Simple Models

In the first, most straightforward application of the results of the previous section we take a cold gas ($T_g = 0$), neglect inelastic processes ($\Omega = 0$) and assume a momentum-transfer cross section with a power-law energy dependence

$$Q_m(\epsilon) \sim \epsilon^{\ell/2}, \quad (78)$$

where ℓ is an arbitrary constant. Hence the momentum-transfer collision frequency is

$$\nu_m(\epsilon) = N \left(\frac{2\epsilon}{\mu} \right)^{\frac{1}{2}} Q_m(\epsilon) \sim \epsilon^{(\ell+1)/2} \quad (79)$$

and by (19d)

$$K \sim \epsilon^{-(\ell+1)/2}. \quad (80)$$

Equation (17) reduces to

$$\epsilon = \frac{1}{2} M v^2 \quad (81)$$

for the cold gas-elastic collision model and, together with (80), this yields

$$K \sim v^{-(\ell+1)}. \quad (82)$$

In what follows, we are primarily interested in the way transport properties scale with E and B .

Weak magnetic field. If the magnetic field is weak, then

$$r_m = KB = \frac{qB}{\mu\nu_m} \ll 1, \quad (83)$$

and (19) and (23) reduce to

$$v_{\parallel} \approx v \approx KE, \quad v_{\perp} \approx K^2 EB \approx KBv. \quad (84a, b)$$

Combining (82) and (84a) yields

$$v_{\parallel} \approx v \sim E^{1/(\ell+2)}, \quad (85a)$$

while (82) and (84b) together give

$$v_{\perp} \sim B/v^{\ell} \sim B/E^{\ell/(\ell+2)}. \quad (85b)$$

We note the following derivative for future use:

$$\frac{\partial \ln v_{\parallel}}{\partial \ln E} = \frac{1}{\ell+2}, \quad \frac{\partial \ln v_{\perp}}{\partial \ln E} = -\frac{\ell}{\ell+2}. \quad (86)$$

The Lorentz angle (22) in this case is given by

$$\tan \varphi \sim B/E^{(\ell+1)/(\ell+2)}. \quad (87)$$

Strong magnetic fields. If the inequality (83) is reversed, i.e.

$$KB \gg 1, \quad (88)$$

then (19) and (23) become

$$v_{\perp} \approx v \approx E/B, \quad v_{\parallel} \approx E/KB^2 \approx v/KB. \quad (89a, b)$$

Combining (82) with (89b) gives

$$v_{\parallel} \sim v^{\ell+2}/B$$

and together with (89a) this gives

$$v_{\parallel} \sim E^{\ell+2}/B^{\ell+3}. \quad (90)$$

The strong-field logarithmic derivative are thus

$$\frac{\partial \ln v_{\parallel}}{\partial \ln E} = \ell+2, \quad \frac{\partial \ln v_{\perp}}{\partial \ln E} = 1, \quad (91)$$

while the Lorentz angle (22) is given by

$$\tan\varphi \approx B^{\ell+2}/E^{\ell+1}. \quad (92)$$

(b) *Simple Model Calculations: Electron Diffusion Coefficients*

Although the expressions contained in Section 2 are, for the greater part, applicable to charged particles of arbitrary mass, we choose to perform actual computations at present for electrons, for which $m \ll M$. In that case, we have already established in Section 2d that the temperature tensor is effectively isotropic, i.e.

$$\mathbf{T} \approx T \begin{bmatrix} 1 & . & . \\ . & 1 & . \\ . & . & 1 \end{bmatrix}, \quad (93)$$

apart from certain special circumstances. This observation allows us to greatly simplify the generalised Einstein relations (52)–(56) to

$$D_{\perp} \approx K_{\parallel} \frac{kT}{q}, \quad (94a)$$

$$\bar{D}_{\mathcal{H}} \approx -K_{\perp} \frac{kT}{q} \left(1 + (1 + \Delta_{\parallel}) \frac{\partial \ln K_{\perp}}{\partial \ln E} \right), \quad (94b)$$

$$D_{\perp}' \approx K \frac{kT}{q}, \quad (94c)$$

$$D_{\mathcal{H}} \approx K_{\perp} \frac{kT}{q}, \quad (94d)$$

$$D_{\parallel} \approx K_{\parallel} \frac{kT}{q} \left(1 + (1 + \Delta_{\parallel}) \frac{\partial \ln K_{\parallel}}{\partial \ln E} \right). \quad (94e)$$

It is of interest to form the ratios

$$\frac{D_{\parallel}}{D_{\perp}} = 1 + (1 + \Delta_{\parallel}) \frac{\partial \ln K_{\parallel}}{\partial \ln E}, \quad (95a)$$

$$\frac{\bar{D}_{\mathcal{H}}}{D_{\mathcal{H}}} = - \left(1 + (1 + \Delta_{\parallel}) \frac{\partial \ln K_{\perp}}{\partial \ln E} \right), \quad (95b)$$

$$\frac{D_{\perp}}{D'_{\perp}} = \frac{K_{\parallel}}{K} = \frac{1}{1 + K^2 B^2} = \cos^2 \varphi, \quad (95c)$$

the first two of which simplify further if the heat flux term Δ_{\parallel} , defined by (51), is negligible:

$$\frac{D_{\parallel}}{D_{\perp}} \approx \frac{\partial \ln v_{\parallel}}{\partial \ln E}, \quad \frac{\bar{D}_{\mathcal{H}}}{D_{\mathcal{H}}} = - \frac{\partial \ln v_{\perp}}{\partial \ln E}. \tag{96a, b}$$

These equations yield particularly simple results for the model cross section (78) above. Thus (81), (86) and (91) together yield for the cold gas model

$$D_{\parallel}/D_{\perp} = 1/(\ell + 2), \quad \text{weak magnetic field} \tag{97a}$$

$$= \ell + 2, \quad \text{strong magnetic field;} \tag{97b}$$

$$\bar{D}_{\mathcal{H}}/D_{\mathcal{H}} = \ell/(\ell + 2), \quad \text{weak magnetic field} \tag{97c}$$

$$= -1, \quad \text{strong magnetic field.} \tag{97d}$$

These formulas generalise results obtained over twenty years ago for diffusion in electric fields on the basis of nonequilibrium thermodynamics [Robson (1972); equation (17) of that paper is identical to (97a) above]. Many refinements have been developed in the interim [see Mason and McDaniel (1988) for a summary of the generalised Einstein relations and also Uribe and Mason (1989) and Koutsalos and Mason (1991)].

Notice that the ratio D_{\parallel}/D_{\perp} ‘flips over’ in the progression from a weak to a strong magnetic field, as evidenced by equations (97a) and (97b) respectively. For example, for a constant cross section, $\ell = 0$ and equation (97a) gives the famous result $D_{\parallel}/D_{\perp} = 0.5$ at $B = 0$ which becomes $D_{\parallel}/D_{\perp} = 2.0$ for high B/N . These results are confirmed by an accurate multi-term solution of Boltzmann’s equation (Ness and Robson 1994).

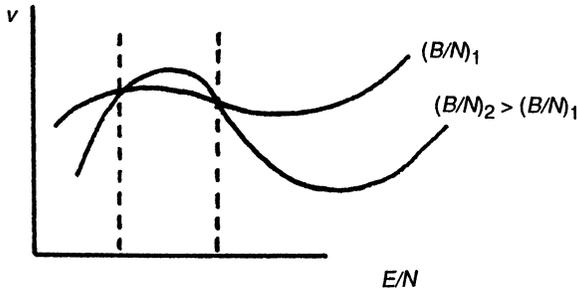


Fig. 2. Schematic diagram showing the B/N dependence in the NDC region. Calculations from the Ness (1994) multi-term code confirm these predictions.

(c) NDC: Variation with B

Ness (1994) also observes another interesting variation with B , specifically, the influence of B/N upon NDC, which we may understand in terms of the formulas developed above.

Upon differentiation of (17) w.r.t. B , we find

$$\frac{\partial \epsilon}{\partial B} = \frac{Mv \partial v / \partial B}{1 + \Omega'} \quad (98)$$

The factor in the denominator also controls the NDC region ($\partial v / \partial E < 0$), as explained in Section 2*b* above. In what follows, it is assumed that ϵ is always a monotonically decreasing function of B , i.e.

$$\partial \epsilon / \partial B < 0, \quad (99)$$

regardless of the type of interaction. Thus, from (30), (98) and (99), it is clear that $\partial v / \partial B > 0$ and v actually *increases* with B inside the NDC region ($1 + \Omega' < 0$). Outside the NDC region ($1 + \Omega' > 0$), however, $\partial v / \partial B < 0$ and v always decreases with B . The crossover point occurs when $1 + \Omega' = 0$, when

$$\frac{\partial v}{\partial E} = 0, \quad \frac{\partial v}{\partial B} = 0. \quad (100)$$

Fig. 2 gives a schematic portrayal of the dual effects of electric and magnetic field variation.

4. Concluding Remarks

We have developed approximate formulas for relationships between the transport properties of ion and electron swarms in a gas in crossed electric and magnetic fields, based upon momentum-transfer theory. Elastic and non-elastic collisions have been considered, but non-particle-conserving collisions, such as ionisation, have been excluded. Proper accounting of these latter effects involves treatment of second-order density gradient terms; this will be done in a subsequent paper. Based upon accurate numerical solution of the Boltzmann equation (Ness and Robson 1994; Ness 1994), we believe our formulas are at least qualitatively correct, but no comprehensive testing has been carried out. However, if the electric field-only formulas are any guide, the expressions obtained in the present paper will have accuracies of around 10%, more or less.

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References

- Allis, W. P. (1956). In 'Handbuch der Physik', Vol. 21 (Springer: Berlin).
- Biagi, S. F. (1988). *Nucl. Instrum. Methods A* **273**, 533.
- Biagi, S. F. (1989). *Nucl. Instrum. Methods A* **283**, 716.
- Blevin, H. A., and Brennan, M. J. (1983). *Aust. J. Phys.* **36**, 859.
- Braglia, G. L., and Ferrari, L. (1973*a*). *Physica* **67**, 249.
- Braglia, G. L., and Ferrari, L. (1973*b*). *Physica* **67**, 274.
- Brennan, M. J., and Garvie, A. M. (1990). *Aust. J. Phys.* **43**, 765.
- Brennan, M. J., Garvie, A. M., and Kelly, L. J. (1990). *Aust. J. Phys.* **43**, 27.

- Frost, L. S., and Phelps, A. V. (1962). *Phys. Rev.* **127**, 1621.
- Garvie, A. M., and Brennan, M. J. (1990). *Aust. J. Phys.* **43**, 779.
- Hargrove, C. K., et al. (1984). *Nucl. Instrum. Methods Phys. Res.* **219**, 461.
- Heylen, A. E. D. (1980). *Proc. IEE* **127**, 221.
- Heintze, J. (1978). *Nucl. Instrum. Methods* **156**, 227.
- Heintze, J. (1982). *Nucl. Instrum. Methods* **196**, 293.
- Huxley, L. G. H., and Crompton, R. W. (1974). 'Diffusion and Drift of Electrons in Gases' (Wiley: New York).
- Ikuta, N., and Sugai, Y. (1989). *J. Phys. Soc. Jpn* **58**, 1228.
- Koutsalos, A. D., and Mason, E. A. (1991). *Chem. Phys.* **153**, 351.
- Kunst, T. (1992). Ph.D. Dissertation, Univ. Heidelberg.
- Kunst, T., Götz, B., and Schmidt, B. (1993). *Nucl. Instrum. Methods A* **324**, 127.
- Lin, S. L., Robson, R. E., and Mason, E. A. (1979). *J. Chem. Phys.* **71**, 3483.
- Lin, S. L., Haddard, G. N., and Robson, R. E. (1981). *Aust. J. Phys.* **34**, 243.
- Mason, E. A., and McDaniel, E. W. (1988). 'Transport Properties of Ions in Gases' (Wiley: New York).
- Ness, K. F. (1985). Ph.D. Thesis, James Cook University.
- Ness, K. F. (1993). *Phys. Rev. E* **47**, 327.
- Ness, K. F. (1994). *J. Phys. D* (submitted).
- Ness, K. F., and Robson, R. E. (1994). *Phys. Scripta* (in press).
- Ness, K. F., and Robson, R. E. (1986). *Phys. Rev. A* **34**, 2185.
- Ness, K. F., and Robson, R. E. (1988). *Phys. Rev. A* **38**, 1446.
- Robson, R. E. (1972). *Aust. J. Phys.* **25**, 685.
- Robson, R. E. (1984). *Aust. J. Phys.* **37**, 35.
- Robson, R. E. (1986). *J. Chem. Phys.* **85**, 4486.
- Robson, R. E. (1991). *Aust. J. Phys.* **44**, 685.
- Robson, R. E., and Ness, K. F. (1986). *Phys. Rev. A* **33**, 2068.
- Robson, R. E., and Ness, K. F. (1988). *J. Chem. Phys.* **89**, 4815.
- Schmidt, B. (1986). *Nucl. Instrum. Methods A* **252**, 579.
- Schmidt, B. (1991). *J. Phys. B* **24**, 4809.
- Schmidt, B. (1992). *Aust. J. Phys.* **45**, 351.
- Schmidt, B. (1993). *Commun. Atom. Mol. Phys.* **28**, 279.
- Schmidt, B., and Polenz, S. (1988). *Nucl. Instrum. Methods A* **273**, 488.
- Skullerud, H. R. (1973). *J. Phys. B* **2**, 696.
- Tonks, L. (1937). *Phys. Rev.* **51**, 744.
- Tonks, L., and Allis, W. P. (1937). *Phys. Rev.* **52**, 710.
- Uribe, F. J., and Mason, E. A. (1989). *Chem. Phys.* **133**, 335.
- Viehland, L. A. (1992). In 'Status and Future Development in Transport Properties' (Ed. W. A. Wakeham), p. 189 (Kluwer: Dordrecht).
- Wannier, G. H. (1953). *Bell Syst. Tech. J.* **32**, 170.

Appendix A: Collision Frequencies and Cross Sections

In what follows, we consider a collision in the centre-of-mass frame whereby the relative velocities before and after a collision are \mathbf{g} and \mathbf{g}' respectively and j , k denote initial and final internal states of the neutral molecule respectively. If $\sigma(jk|g, \chi)$ denotes the differential scattering cross section for a scattering angle, then we define the partial cross sections

$$Q_\ell(jk|g) = 2\pi \int [1 - (g'/g)^\ell \cos^\ell \chi] \sigma(jk|g, \chi) \sin \chi \, d\chi, \quad (\text{A1})$$

where g' is given in terms of g by conservation of energy

$$\frac{1}{2}\mu(g')^2 + \epsilon_k = \frac{1}{2}\mu g^2 + \epsilon_j, \quad (\text{A2})$$

with ϵ_j , ϵ_k denoting the initial and final internal energies respectively of the neutral molecule.

Thus we have the total momentum-transfer collision frequency,

$$\nu_m(g) = \sum_{j,k} N_j g Q_1(jk|g), \quad (\text{A3})$$

where N_j is the population of the neutral molecules in the initial state j (usually taken as a Maxwell-Boltzmann distribution of states at temperature T_g). The total collision frequency for viscosity is defined by

$$\nu_v(g) = \sum_{j,k} N_j g Q_2(jk|g). \quad (\text{A4})$$

In the text, we designated the process $j \rightarrow k$ as the i th *inelastic* process if $j < k$, and the i th *superelastic* process if $j > k$. The corresponding collision frequencies appearing in Section 2a are given by

$$\begin{aligned} N_j g Q_0(jk|g) &= \vec{v}_i(g), \quad j < k \\ &= \overleftarrow{v}_i(g), \quad j > k, \end{aligned} \quad (\text{A5})$$

and the threshold energy is

$$\epsilon_i^* \equiv |\epsilon_j - \epsilon_k|. \quad (\text{A6})$$

We have written collision frequencies above as a function of relative speed g , but in view of the relation

$$\epsilon = \frac{1}{2} \mu g^2, \quad (\text{A7})$$

we can also write them as functions of energy when it is convenient to do so.

Appendix B: Differential Identities

We give below a derivation of equations (26) and (31), which are central to establishing NDC criteria and the GER. With $\mathbf{v} = (-v_\perp, 0, v_\parallel)$, equation (16) can be written in component form:

$$v_\parallel B = \sigma v_\perp, \quad E - v_\perp B = \sigma v_\parallel, \quad (\text{B1a, b})$$

where for convenience we have defined

$$\sigma(\epsilon) = \frac{1}{K} = \mu \nu_m(\epsilon)/q. \quad (\text{B2})$$

In what follows we write

$$\sigma' = d\sigma/d\epsilon.$$

If equations (B1) are differentiated w.r.t. E , we get

$$B \frac{\partial v_{\parallel}}{\partial E} = \sigma' \frac{\partial \epsilon}{\partial E} v_{\perp} + \sigma \frac{\partial v_{\perp}}{\partial E}, \quad (\text{B3a})$$

$$1 - B \frac{\partial v_{\perp}}{\partial E} = \sigma' \frac{\partial \epsilon}{\partial E} v_{\parallel} + \sigma \frac{\partial v_{\parallel}}{\partial E}, \quad (\text{B3b})$$

respectively. On the other hand, differentiation of (17) w.r.t. E gives

$$\frac{\partial \epsilon}{\partial E} = \frac{M}{1 + \Omega'} \left(v_{\parallel} \frac{\partial v_{\parallel}}{\partial E} + v_{\perp} \frac{\partial v_{\perp}}{\partial E} \right). \quad (\text{B4})$$

Equations (B3a, b) and (B4) can be solved simultaneously to give

$$\sigma \frac{\partial v_{\parallel}}{\partial E} = \left(1 + \frac{Mv_{\perp}^2 \sigma' / \sigma}{1 + \Omega'} \right) / \left(1 + \frac{B^2}{\sigma^2} + \frac{Mv^2 \sigma' / \sigma}{1 + \Omega'} \right), \quad (\text{B5})$$

$$\sigma \frac{\partial v_{\perp}}{\partial E} = \frac{B}{\sigma} \left(1 - \frac{Mv_{\parallel}^2 \sigma' / \sigma}{1 + \Omega'} \right) / \left(1 + \frac{B^2}{\sigma^2} + \frac{Mv^2 \sigma' / \sigma}{1 + \Omega'} \right), \quad (\text{B6})$$

$$\sigma^2 \frac{\partial \epsilon}{\partial E} = \frac{ME}{(1 + B^2 / \sigma^2)(1 + \Omega') + Mv^2 \sigma' / \sigma}. \quad (\text{B7})$$

The following interrelations then follow by (B5) and (B7):

$$\frac{\partial v_{\parallel}}{\partial E} = \frac{1 + \Omega' + Mv_{\perp}^2 \sigma' / \sigma}{MKE} \frac{\partial \epsilon}{\partial E}; \quad (\text{B8})$$

from (B6) and (B7),

$$\frac{\partial v_{\perp}}{\partial E} = \frac{B}{ME} (1 + \Omega' - Mv_{\parallel}^2 \sigma' / \sigma) \frac{\partial \epsilon}{\partial E}; \quad (\text{B9})$$

and from (B6) and (B5),

$$\frac{\partial v_{\perp}}{\partial E} = \left[B / \sigma \left(1 - \frac{Mv_{\parallel}^2 \sigma' / \sigma}{1 + \Omega'} \right) / \left(1 + \frac{Mv_{\perp}^2 \sigma' / \sigma}{1 + \Omega'} \right) \right] \frac{\partial v_{\parallel}}{\partial E}. \quad (\text{B10})$$

On the other hand, (B5) can be arranged to give

$$\frac{M\sigma' / \sigma}{1 + \Omega'} = \left[\left(1 + \frac{B^2}{\sigma^2} \right) \sigma \frac{\partial v_{\parallel}}{\partial E} - 1 \right] / \left(v_{\perp}^2 - \sigma v^2 \frac{\partial v_{\parallel}}{\partial E} \right). \quad (\text{B11})$$

By (B2), (19a) and (23), we have

$$\sigma v^2 = \frac{E^2}{\sigma(1 + B^2/\sigma^2)} = \frac{KE^2}{1 + K^2B^2} = Ev_{\parallel}, \quad (\text{B12})$$

$$(1 + B^2/\sigma^2)\sigma = \frac{1 + K^2B^2}{K} = \frac{E}{v_{\parallel}}. \quad (\text{B13})$$

Hence (B11) becomes

$$\frac{M\sigma'/\sigma}{1 + \Omega'} = \left(\frac{E}{v_{\parallel}} \frac{\partial v_{\parallel}}{\partial E} - 1 \right) / \left(v_{\perp}^2 - Ev_{\parallel} \frac{\partial v_{\parallel}}{\partial E} \right). \quad (\text{B14})$$

Similarly, rearrangement of (B6) gives

$$\frac{M\sigma'/\sigma}{1 + \Omega'} = \left[\frac{B}{\sigma} - \sigma \left(1 + \frac{B^2}{\sigma^2} \right) \frac{\partial v_{\perp}}{\partial E} \right] / \left(v_{\parallel}^2 \frac{B}{\sigma} + \sigma v^2 \frac{\partial v_{\perp}}{\partial E} \right), \quad (\text{B15a})$$

which, with (B12) and (B13) reduces to

$$\frac{M\sigma'/\sigma}{1 + \Omega'} = \left(\frac{B}{\sigma} - \frac{E}{v_{\parallel}} \frac{\partial v_{\perp}}{\partial E} \right) / \left(v_{\parallel}^2 \frac{B}{\sigma} + Ev_{\parallel} \frac{\partial v_{\perp}}{\partial E} \right). \quad (\text{B15b})$$

Finally, since by (19b),

$$v_{\perp} = KBv_{\parallel} = \frac{B}{\sigma} v_{\parallel},$$

we have

$$\frac{M\sigma'/\sigma}{1 + \Omega'} = \frac{B}{\sigma} \left(1 - \frac{E}{v_{\perp}} \frac{\partial v_{\perp}}{\partial E} \right) / \left(v_{\parallel} v_{\perp} + Ev_{\parallel} \frac{\partial v_{\perp}}{\partial E} \right). \quad (\text{B16})$$

Equations (B8) and (B9) are identical with (26a, b) if we note that

$$\sigma'/\sigma = \nu_m'/\nu_m \quad (\text{B17})$$

by virtue of equation (B2). In addition, equations (31) follow immediately from (B14) and (B15), again by using (B17).

Appendix C: Temperature Tensor

The temperature tensor T_{ij} is defined by (11) and is obtained by solving the balance equation (12), which we write here as

$$k\mathbf{T} \times \hat{\mathbf{B}} - \hat{\mathbf{B}} \times k\mathbf{T} = \alpha k\mathbf{T} - \beta M\mathbf{v}\mathbf{v} - \gamma \mathbf{1}, \quad (\text{C1})$$

where

$$\alpha \equiv \left(1 + \frac{3M\bar{v}_v}{4M\nu_m}\right)/r_e, \quad (\text{C2})$$

$$\beta \equiv \left(1 - \frac{3\bar{v}_v}{4\nu_m}\right)/r_e, \quad (\text{C3})$$

$$\gamma \equiv \left(\frac{M\bar{v}_v}{2\mu\nu_m}\epsilon + \beta kT_g\right)/r_e. \quad (\text{C4})$$

The notational simplification (15) has been employed for convenience. Upon contraction of tensor indices, (C1) yields (17), as required. The components of (C1) for the coordinate system of Fig. 1 are

xx

$$-kT_{xz} - kT_{zx} = \alpha kT_{xx} - \beta Mv_x^2 - \gamma, \quad (\text{C5})$$

xy

$$-kT_{zy} = \alpha kT_{xy}, \quad (\text{C6})$$

xz

$$kT_{xx} - kT_{zz} = \alpha kT_{xz} - \beta Mv_x v_z, \quad (\text{C7})$$

yx

$$-kT_{yz} = \alpha kT_{yx}, \quad (\text{C8})$$

yy

$$0 = \alpha kT_{yy} - \gamma, \quad (\text{C9})$$

yz

$$kT_{yx} = \alpha kT_{yz}, \quad (\text{C10})$$

zx

$$-kT_{zz} + kT_{xx} = \alpha kT_{zx} - \beta Mv_x v_z, \quad (\text{C11})$$

zy

$$kT_{xy} = \alpha kT_{zy}, \quad (\text{C12})$$

zz

$$kT_{zx} + kT_{xz} = \alpha kT_{zz} - \beta v_z^2 - \gamma. \quad (\text{C13})$$

Notice that T_{ij} is symmetric in the indices, i.e. $T_{xz} = T_{zx}$, etc. Equations (C6), (C8), (C10) and (C12) together imply that

$$T_{xy} = T_{yz} = T_{zy} = T_{yx} = 0. \quad (\text{C14})$$

The remaining four independent elements, i.e.

$$T_{\perp} \equiv T_{xx}, \quad T_{\mathcal{H}} \equiv T_{xz} = T_{zx}, \quad T_{\perp}' \equiv T_{yy}, \quad T_{\parallel} \equiv T_{zz} \quad (\text{C15})$$

are given by solution of (C5), (C7), (C9) and (C13) [note that (C11) is identical with (C7)]. Thus, we have immediately

$$kT_{\perp}' = \gamma/\alpha, \quad (\text{C16})$$

and the remaining three components are obtained as the solutions of

$$\begin{bmatrix} \alpha & 0 & -2 \\ 1 & -1 & \alpha \\ 0 & \alpha & 2 \end{bmatrix} \begin{bmatrix} kT_{\parallel} \\ kT_{\perp} \\ kT_{\mathcal{H}} \end{bmatrix} = \begin{bmatrix} \gamma + \beta M v_{\parallel}^2 \\ -\beta M v_{\parallel} v_{\perp} \\ \gamma + \beta M v_{\perp}^2 \end{bmatrix}. \quad (\text{C17})$$

Solution of (C17) is straightforward and yields

$$kT_{\parallel} = (\gamma + \beta M v_{\parallel}^2)/\alpha + 2kT_{\mathcal{H}}/\alpha, \quad (\text{C19})$$

$$kT_{\perp} = (\gamma + \beta M v_{\perp}^2)/\alpha - 2kT_{\mathcal{H}}/\alpha, \quad (\text{C20})$$

$$kT_{\mathcal{H}} = \frac{\beta M}{\alpha^2 + 4} (v_{\perp}^2 - v_{\parallel}^2 - \alpha v_{\parallel} v_{\perp}). \quad (\text{C21})$$

With (C3) and (17), equation (C4) becomes

$$\begin{aligned} \gamma = & \left[1 + \frac{3}{4\nu_m} \left(\bar{v}_v - \bar{v}_v + \frac{M}{m} \bar{v}_v \right) \right] kT_g \\ & + \frac{(m+M)\bar{v}_v}{4m\nu_m} Mv^2 - \frac{(m+M)\bar{v}_v}{2m\nu_m} \Omega. \end{aligned} \quad (\text{C22})$$

Hence (C16) reduces to

$$kT_{\perp}' = ukT_g + A_0 Mv^2 - 2A_0 \Omega, \quad (\text{C23})$$

while (C19, 20, 21) can be written as

$$kT_{\parallel} = ukT_g + A_1 Mv_{\parallel}^2 + A_2 Mv_{\perp}^2 - CMv_{\parallel} v_{\perp} - 2A_0 \Omega, \quad (\text{C24})$$

$$kT_{\perp} = ukT_g + A_1 Mv_{\perp}^2 + A_2 Mv_{\parallel}^2 + CMv_{\parallel} v_{\perp} - 2A_0 \Omega, \quad (\text{C25})$$

$$kT_{\mathcal{H}} = A_{\mathcal{H}}(Mv_{\perp}^2 - Mv_{\parallel}^2) - C_{\mathcal{H}} Mv_{\parallel} v_{\perp}, \quad (\text{C26})$$

respectively, where

$$u \equiv \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^{-1} \left[1 + \frac{3}{4\nu_m} \left(\frac{M}{m} \bar{v}_v + \bar{v}_v - \bar{v}_v\right)\right], \quad (\text{C27})$$

$$A_0 = \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^{-1} \frac{(m+M)\bar{v}_v}{4m\nu_m}, \quad (\text{C28})$$

$$A_1 = \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^{-1} \left\{1 - \frac{3\bar{v}_v}{4\nu_m} + \frac{(m+M)\bar{v}_v}{4m\nu_m} - 2r_e^2 \left(1 - \frac{3\bar{v}_v}{4\nu_m}\right) \Big/ \left[4r_e^2 + \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^2\right]\right\}, \quad (\text{C29})$$

$$A_2 = \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^{-1} \left\{\frac{(m+M)\bar{v}_v}{4m\nu_m} + 2r_e^2 \left(1 - \frac{3\bar{v}_v}{4\nu_m}\right) \Big/ \left[4r_e^2 + \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^2\right]\right\}, \quad (\text{C30})$$

$$A_{\mathcal{H}} = r_e \left(1 - \frac{3\bar{v}_v}{4\nu_m}\right) \Big/ \left[4r_e^2 + \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^2\right], \quad (\text{C31})$$

$$C_{\mathcal{H}} = \left(1 - \frac{3\bar{v}_v}{4\nu_m}\right) \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right) \Big/ \left[4r_e^2 + \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^2\right], \quad (\text{C32})$$

$$C = 2r_e \left(1 - \frac{3\bar{v}_v}{4\nu_m}\right) \Big/ \left[4r_e^2 + \left(1 + \frac{3M\bar{v}_v}{4m\nu_m}\right)^2\right]. \quad (\text{C33})$$

These are the expressions used in Section 2d in the discussion of anisotropy effects. Notice that the magnetic field appears explicitly in these expressions through the ratio (13), which for light ions ($m \ll M$) becomes

$$r_e = \frac{qB}{m} \Big/ \left(\frac{2m}{M} \nu_m\right). \quad (\text{C34})$$

In contrast, the magnetic field enters the expressions (19) for drift velocity through the ratio

$$r_m = \frac{qB}{m\nu_m} = \frac{2m}{M} r_e \ll r_e, \quad (\text{C35})$$

suggesting that the temperature tensor is influenced by much weaker fields than directed properties, such as drift velocity, at least in the case of light ions.

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