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Comment on FTI Method and Transport Coefficient Definitions for Charged Particle Swarms in Gases

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Abstract

The kinetic theory of charged particle swarms in gases is based upon solution of the space and time dependent Boltzmann's equation for the phase space distribution function $f(\boldsymbol{r}, \boldsymbol{c}, t)$. Hydrodynamic transport coefficients are defined in connection with a density gradient expansion (DGE) of $f(\boldsymbol{r}, \boldsymbol{c}, t)$ and it is believed that these are the quantities measured in experiment. On the other hand, Ikuta and coworkers start with the spatially independent form of the Boltzmann equation, which they solve iteratively as in path-integral methods, and define transport coefficients in terms of the 'starting rate distribution', rather than f itself. Ikuta's procedure has come to be known as the 'flight time integral' (FTI) method and the discrepancies between numerical calculations based upon this and the more commonly known DGE procedure have generated a deal of controversy in recent times. The purpose of this paper is to point out that the respective definitions of the transverse diffusion coefficient D_{T} coincide only for light swarm particles undergoing collisions for which the differential cross section is isotropic, and that the particular technique used for solving Boltzmann's equation, be it a path-integral or a multi-term method, has nothing to do with the numerical discrepancies which are observed when scattering is anisotropic. In particular, it is shown that Ikuta's definition of D_{T} is inconsistent with even the well established result for constant collision frequency.

1. Introduction

The kinetic theory of charged particle swarms (electrons, ions, muons, etc.) in gases in electric fields has been developed substantially over the last forty years or so following the seminal paper of Wannier (1953). The reader is referred to the reviews of Kumar *et al.* (1980) and Viehland (1992) and to the texts of Huxley and Crompton (1974), and Mason and McDaniel (1988) for details. Basically, the problem is to solve Boltzmann's equation

$$(\partial_t + \boldsymbol{c} \,.\, \nabla + \boldsymbol{a} \,.\, \partial_{\boldsymbol{c}} + J)f = 0 \qquad (1)$$

for the phase space distribution function $f(\boldsymbol{r}, \boldsymbol{c}, t)$ of the charged particles, given the field E, the gas number density and temperature, n_0 and T_0 respectively, and the differential cross sections $\sigma(g,\chi)$ describing the various scattering processes. (Note that in swarms interactions between the charged particles may be neglected in view of the fact that their number density $n \ll n_0$.) The collision term in (1) may be written as

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$$J(f) = \int [f(\boldsymbol{c})\, f_0(\boldsymbol{c}_0) - f(\boldsymbol{c}')\, f_0(\boldsymbol{c}')] g\sigma(g,\, \chi)\, \mathrm{d}\hat{\boldsymbol{g}}'\, \mathrm{d}\boldsymbol{c}_0\,, \tag{2}$$

if the swarm particle–neutral gas molecules are elastic, as will be assumed for simplicity throughout this paper. The notation is that $\boldsymbol{c}$, $\boldsymbol{c}_0$ denote the velocities of charged and neutral species respectively, $\boldsymbol{g} = \boldsymbol{c} - \boldsymbol{c}_0$ and $\boldsymbol{g}' = \boldsymbol{c}' - \boldsymbol{c}_0{}'$ denote relative velocities before and after a collision respectively, $\cos\chi \equiv \hat{\boldsymbol{g}} \cdot \hat{\boldsymbol{g}}'$ and $f_0(\boldsymbol{c}_0)$ is the distribution function of the neutrals, assumed to be Maxwellian at temperature T_0. Quantities of physical interest are found by taking averages over f, e.g. for some function $\phi(\boldsymbol{c})$ of swarm particle velocity,

$$\langle \phi(\boldsymbol{c}) \rangle = \frac{1}{n} \int \mathrm{d}\boldsymbol{c}\, \phi(\boldsymbol{c})\, f(\boldsymbol{c})\,, \tag{3}$$

$$n = \int \mathrm{d}\boldsymbol{c}\, f(\boldsymbol{c})\,. \tag{4}$$

Methods for solution of (1) are many and varied (Kumar *et al.* 1980), but most involve decomposition of f in spherical harmonics,

$$f(\boldsymbol{c}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm}(c)\, Y_{lm}(\hat{\boldsymbol{c}})\,, \tag{5}$$

the so-called 'multi-term' representation. In the hydrodynamic regime, a further decomposition in terms of density gradient is generally made (Kumar *et al.* 1980). This procedure, along with appropriate definitions of particular hydrodynamic transport quantities (drift velocity, diffusion, etc.) will be termed the density gradient expansion (DGE) approach in this paper.

On the other hand, the flight-time integral (FTI) method as developed by Ikuta and co-workers (see e.g. Ikuta and Murakami 1987) treats the 'starting rate distribution'

$$\psi_{\mathrm{s}}(f(\boldsymbol{c})) = \int \mathrm{d}\boldsymbol{c}_0 \int d\hat{\boldsymbol{g}}'\, g\,\sigma(g,\chi)\, f(\boldsymbol{c}')\, f_0(\boldsymbol{c}_0{}') \tag{6}$$

as the quantity of principle interest. Moreover, the Boltzmann collision operator (2) is split into two parts, which we write as

$$J(f) = \nu_{\mathrm{T}}\, f - \psi_{\mathrm{s}}(f)\,, \tag{7}$$

where

$$\nu_{\mathrm{T}}(\boldsymbol{c}) \equiv \int \mathrm{d}\boldsymbol{c}_0\, g\sigma_0(g)\, f_0(\boldsymbol{c}_0) \tag{8}$$

and the resulting equation is solved iteratively. The quantities (partial cross sections)

$$\sigma_l(g)=2\pi\int_0^{\pi} P_l(\cos\chi)\,\sigma(g,\,\chi)\sin\chi\;\mathrm{d}\chi \qquad (l=0,\,1,\,2,...) \tag{9}$$

figure prominantly in the kinetic theory of gases.

The FTI method is thus similar in character to the path-integral methods discussed by Skullerud and Kuhn (1983). In addition, Ikuta *et al.* define transport quantities as averages over ψ_{s}, instead of the conventional way as indicated in (3). This is a key point which should be kept in mind when reading this paper.

At the recent Japan–Australia Workshop on Gaseous Electronics and Its Applications (see *Aust. J. Phys.* **48**, 333–569), it was suggested by Ikuta that the standard, multi-term representation (5) somehow fails to describe transport phenomena correctly when scattering is anisotropic, i.e. when $\sigma(g,\chi)$ does in fact have a χ-dependence. In the subsequent discussion two major points for discussion have emerged:

(1) The accuracy of the iterative procedure used in FTI.
(2) The definitions of Ikuta *et al.* for transport coefficients.

In regard to the first point, the observations of Skullerud and Kuhn (1983) are especially relevant. However, it now seems that the second point is the most likely source of discrepancy between Ikuta's results and standard theory, and it is this aspect that we focus on in this paper.

In Section 2 we review the FTI method and in Section 3 we discuss the definition of transport coefficients, in particular, the transverse diffusion coefficient D_{T}. It is shown that Ikuta's definition of D_{T} agrees with the standard DGE definition only for light swarm particles for which the scattering is isotropic [i.e. $\sigma(g,\chi)$ is independent of χ]. The discrepancy for anisotropic scattering is highlighted by appealing to the constant collision frequency model, for which $g\sigma(g,\chi)$ is independent of g, facilitating exact analytic expressions for transport coefficients, which have long been known (Wannier 1953).

2. FTI versus Standard Kinetic Theory

(2a) Hierarchy of Kinetic Equations and Hydrodynamic Transport Coefficients

In the hydrodynamic regime (Kumar *et al.* 1980) a density gradient expansion

$$f(\boldsymbol{r},\boldsymbol{c},t)=n(\boldsymbol{r},t)\,f^{(0)}(\boldsymbol{c},t)\;-\boldsymbol{f}^{(1)}(\boldsymbol{c},t)\,.\,\nabla n(\boldsymbol{r},t)+\,... \tag{10}$$

is usually made to account for (assumed weak) space–time variation. From (10) it follows that the particle flux is given by

$$\boldsymbol{\Gamma}=\int \mathrm{d}\boldsymbol{c}\;\boldsymbol{c}f_{\infty}(\boldsymbol{r},\boldsymbol{c},t)=n\boldsymbol{W}-\boldsymbol{D}\,.\,\nabla n+\,... \tag{11}$$

in the limit as $t\to\infty$, where

$$\boldsymbol{W}\equiv\int \mathrm{d}\boldsymbol{c}\;\boldsymbol{c}\,f_{\infty}^{(0)}(\boldsymbol{c})\,, \tag{12}$$

$$\boldsymbol{D}\equiv\int \mathrm{d}\boldsymbol{c}\;\boldsymbol{c}\,\boldsymbol{f}_{\infty}^{(1)}(\boldsymbol{c}) \tag{13}$$

denote the drift velocity and diffusion tensor respectively and

$$f_{\infty}^{(j)}(\boldsymbol{c}) \equiv \lim_{t\to\infty} f^{(j)}(\boldsymbol{c},t), \qquad j=0,\,1\,.$$

The equations for $f^{(0)}$ and $\boldsymbol{f}^{(1)}$ can be found by substitution of (10) into (1) and equating coefficients of respective orders of ∇n. We write these equations in the form

$$(\partial_t + \boldsymbol{a}\,.\,\partial_{\boldsymbol{c}} + \nu_{\mathrm{T}})f^{(0)} = \psi_{\mathrm{s}}(f^{(0)})\,, \tag{14a}$$

$$(\partial_t + \boldsymbol{a}\,.\,\partial_{\boldsymbol{c}} + \nu_{\mathrm{T}})\boldsymbol{f}^{(1)} = (\boldsymbol{c}-\boldsymbol{W})f^{(0)} + \psi_{\mathrm{s}}(\boldsymbol{f}^{(1)})\,, \tag{14b}$$

where $\psi_{\mathrm{s}}(f^{(0)})$ and $\psi_{\mathrm{s}}(\boldsymbol{f}^{(1)})$ can be found by substituting $f^{(0)}$ and $\boldsymbol{f}^{(1)}$ for f in the right side of (6) respectively.

It is to be emphasised that the above represents a simplification to nonreacting swarms. If reactions occur, and particle number is not conserved in collisions, terms to second order in the density gradient must be retained and definitions of transport coefficients modified (Kumar *et al.* 1980). Finally, note the normalisation

$$\int \mathrm{d}\boldsymbol{c}\; f^{(j)}(\boldsymbol{c})\;\mathrm{d}\boldsymbol{c} = \delta_{j0} \qquad (j=0,\,1,\,\ldots)\,. \tag{15}$$

(2b) Solution of Prototype Equation

Both equations (14a) and (14b) can be written in the form

$$(\partial_t + \boldsymbol{a}\,.\,\partial_{\boldsymbol{c}} + \nu_{\mathrm{T}})f = \rho(\boldsymbol{c},t)\,, \tag{16}$$

with appropriate definitions for $\rho(\boldsymbol{c},t)$. It can be shown that (16) has the solution

$$\begin{aligned} f(\boldsymbol{c},t) &= f(\boldsymbol{c},0)\,\mathrm{e}^{-\int_0^t \nu_{\mathrm{T}}(\boldsymbol{c}-\boldsymbol{a}\tau)\mathrm{d}\tau} \\ &\quad + \int_0^t \mathrm{d}\tau\; e^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}-\boldsymbol{a}\tau')\mathrm{d}\tau'}\rho(\boldsymbol{c}-\boldsymbol{a}\tau,\,t-\tau)\,, \end{aligned} \tag{17}$$

and that in the limit $t\to\infty$ we have the asymptotic solution

$$f_{\infty}(\boldsymbol{c},t) = \int_0^{\infty} \mathrm{d}\tau\;\mathrm{e}^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}-\boldsymbol{a}\tau')\mathrm{d}\tau'}\rho_{\infty}(\boldsymbol{c}-\boldsymbol{a}\tau,\,t-\tau)\,. \tag{18}$$

If $\rho_{\infty} = \rho_{\infty}(\boldsymbol{c})$ is independent of time, then clearly so is f_{∞}, i.e.

$$f_{\infty} = f_{\infty}(\boldsymbol{c})\,. \tag{19}$$

(2c) Averaging, FTI Procedure

Using (18) with

$$\rho_\infty(\boldsymbol{c}) = \psi_\infty(f_\mathrm{s}^{(0)}(\boldsymbol{c}))\,, \tag{20}$$

we obtain the asymptotic solution of (14a) in the form

$$f_\infty^{(0)}(\boldsymbol{c}) = \int_0^\infty \mathrm{d}\tau\; \mathrm{e}^{-\int_0^\tau \nu_\mathrm{T}(\boldsymbol{c}-\boldsymbol{a}\tau')\mathrm{d}\tau'}\psi_\mathrm{s}(f_\infty^{(0)}(\boldsymbol{c}-\boldsymbol{a}\tau))\,. \tag{21}$$

This equation may then be solved iteratively for either $f_\infty^{(0)}$ or $\psi_\mathrm{s}(f_\infty^{(0)})$: for example, using (6) we can recast (21) in the form

$$\psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) = \int_0^\infty \mathrm{d}\tau \int \mathrm{d}\boldsymbol{c}_0 \int \mathrm{d}\hat{\boldsymbol{g}}'\; f_0(\boldsymbol{c}_0')\mathrm{e}^{-\int_0^\tau \nu_\mathrm{T}(\boldsymbol{c}'-\boldsymbol{a}\tau')\mathrm{d}\tau'}$$

$$\times\, \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}'-\boldsymbol{a}\tau)\, g\sigma(g,\chi)\,, \tag{22}$$

where we have written

$$\psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) \equiv \psi_\mathrm{s}(f_\infty^{(0)}(\boldsymbol{c})) \tag{23}$$

for convenience, and calculate a new value of $\psi_{\mathrm{s},\infty}^{(0)}$, after inserting an initial estimate in the right-hand side, and repeat until some convergence criterion is satisfied. This is the essence of the FTI procedure.

At present, however, our attention is focussed on definitions of transport coefficients, rather than calculation of f or ψ_s *per se*. The connection between averages over these properties is readily established. Let $\phi(\boldsymbol{c})$ be some function of swarm particle velocity $\boldsymbol{c}$. The the standard averaging process (3) for the spatially homogeneous state and asymptotic limit gives

$$\begin{aligned}
\langle\phi(\boldsymbol{c})\rangle_\infty^{(0)} &= \int \mathrm{d}\boldsymbol{c}\,\phi(\boldsymbol{c})\,f_\infty^{(0)}(\boldsymbol{c})\\
&= \int_0^\infty \mathrm{d}\tau \int \mathrm{d}\boldsymbol{c}\; \mathrm{e}^{-\int_0^\tau \nu_\mathrm{T}(\boldsymbol{c}-\boldsymbol{a}\tau')\mathrm{d}\tau'}\psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}-\boldsymbol{a}\tau)\,\phi(\boldsymbol{c})\\
&= \int_0^\infty \mathrm{d}\tau \int \mathrm{d}\boldsymbol{c}\; \mathrm{e}^{-\int_0^\tau \nu_\mathrm{T}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'}\psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c})\,\phi(\boldsymbol{c}+\boldsymbol{a}\tau)\\
&= [G_\mathrm{f}\,\phi(\boldsymbol{c})]_\infty^{(0)}\,,
\end{aligned} \tag{24}$$

where

$$G_\mathrm{f}\,\phi(\boldsymbol{c}) \equiv \int_0^\infty \mathrm{d}\tau\; \mathrm{e}^{-\int_0^\tau \nu_\mathrm{T}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'}\phi(\boldsymbol{c}+\boldsymbol{a}\tau)\,, \tag{25}$$

$$[\ldots]_\infty^{(0)} \equiv \int \ldots\, \psi_{s,\infty}^{(0)}(\boldsymbol{c})\,\mathrm{d}\boldsymbol{c} \tag{26}$$

is essentially an average over $\psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c})$. Equation (24) expresses the connection between the standard and FTI methods of averaging.

Before applying these formulas to calculation of transport quantities, we digress briefly to establish an important result for isotropic scattering.

(2d) Isotropic Scattering

If the scattering is isotropic, i.e.

$$\sigma(g,\chi)=\sigma(g)\,, \tag{27}$$

then certain averages can be shown to vanish identically and simplifications follow. If (27) holds, then by equation (9) all partial cross sections vanish for $l\geq 1$, i.e.

$$\sigma_l(g)=\sigma_0(g)\,\delta_{l0}\,. \tag{28}$$

Consider now some tensor function $\Phi(\boldsymbol{c})$ of rank l,

$$\Phi(\boldsymbol{c})=\phi(c)\,Y_{lm}(\hat{\boldsymbol{c}}) \tag{29}$$

and its integral with $\psi_{\mathrm{s}}(f(\boldsymbol{c}))$, where $f(\boldsymbol{c})$ is *any* distribution function: Using similar notation to (26), we have

$$\begin{aligned}[\Phi(\boldsymbol{c})] &\equiv \int \mathrm{d}\boldsymbol{c}\,\Phi(\boldsymbol{c})\,\psi_{\mathrm{s}}(f(\boldsymbol{c}))\\ &\equiv \int \mathrm{d}\boldsymbol{c}\int \mathrm{d}\boldsymbol{c}_0\int \mathrm{d}\hat{\boldsymbol{g}}'\;\Phi(\boldsymbol{c})\,f(\boldsymbol{c}')\,f_0(\boldsymbol{c}_0{}')\,g\sigma(g,\chi)\\ &= \int \mathrm{d}\boldsymbol{c}\int \mathrm{d}\boldsymbol{c}_0\;f(\boldsymbol{c})\,f_0(\boldsymbol{c}_0)\int \mathrm{d}\hat{\boldsymbol{g}}'\;\Phi(\boldsymbol{c}')\,g\sigma(g,\chi)\,,\end{aligned} \tag{30}$$

where a standard transformation between pre- and post-collisional velocities has been applied, and a general, anisotropic differential cross section retained for the moment. To obtain the desired result, we take a cold gas

$$f_0(\boldsymbol{c}_0)=n_0\,\delta(\boldsymbol{c}_0) \tag{31}$$

and assume light swarm particles, $m\ll m_0$. Then we get

$$\boldsymbol{g}\approx\boldsymbol{c},\qquad \boldsymbol{g}'\approx\boldsymbol{c}'\quad\text{and}\quad\cos\chi\approx\hat{\boldsymbol{c}}\,.\,\hat{\boldsymbol{c}}'\,. \tag{32}$$

Thus (30) becomes approximately

$$\begin{aligned}[\Phi(\boldsymbol{c})] &= n_0\int \mathrm{d}\boldsymbol{c}\;f(\boldsymbol{c})\int \mathrm{d}\hat{\boldsymbol{c}}'\;\Phi(\boldsymbol{c}')\,c\sigma(c,\,\hat{\boldsymbol{c}}\,.\,\hat{\boldsymbol{c}}')\\ &= n_0\int \mathrm{d}\boldsymbol{c}\;f(\boldsymbol{c})\,\phi(c)\,c\sigma_l(c)\,.\end{aligned} \tag{33}$$

Clearly, for isotropic scattering (IS) the right side vanishes for $l\geq 1$ by virtue of (28), and we may write

$$[\Phi(\boldsymbol{c})]_{\mathrm{IS}}=0 \tag{34}$$

for all functions $\Phi(\boldsymbol{c})$ of velocity which do not have a scalar ($l = 0$) contribution. In particular if $\Phi(\boldsymbol{c}) = \boldsymbol{c}$, we must have

$$[\boldsymbol{c}]_{\mathrm{IS}} = 0\,. \tag{35}$$

This result is of crucial importance in establishing the convergence of Ikuta's definition of D_{T} with the DGE definition (13) when scattering is isotropic.

(2e) Drift Velocity

We now return to (24) and set $\phi(\boldsymbol{c}) = \boldsymbol{c}$. Thus

$$\boldsymbol{W} = \langle \boldsymbol{c}\rangle_{\infty}^{(0)} = [G_{\mathrm{f}}\, \boldsymbol{c}]_{\infty}^{(0)}\,, \tag{36}$$

$$\begin{aligned} G_{\mathrm{f}}\, \boldsymbol{c} &= \int_0^{\infty} \mathrm{d}\tau\; \mathrm{e}^{-\int_0^{\tau} \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'}(\boldsymbol{c}+\boldsymbol{a}\tau) \\ &= \int_0^{\infty} \mathrm{d}\tau\; \boldsymbol{r}_{\boldsymbol{c}}(\tau)\, \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau)\, \mathrm{e}^{-\int_0^{\tau} \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'}\,, \end{aligned} \tag{37}$$

where an integration by parts has been performed and

$$\boldsymbol{r}_{\boldsymbol{c}}(\tau) \equiv \boldsymbol{c}\tau + \boldsymbol{a}\tau^2/2 \tag{38}$$

is the position of a particle, initially located at the origin and moving with velocity $\boldsymbol{c}$, after time τ. It is then convenient to define

$$G\boldsymbol{r}_{\boldsymbol{c}} = \int_0^{\infty} \mathrm{d}\tau\; \boldsymbol{r}_{\boldsymbol{c}}(\tau)\, \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau)\, e^{-\int_0^{\tau} \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'}\,, \tag{39}$$

so that by (36) and (37)

$$\boldsymbol{W} = [G_{\mathrm{f}}\, \boldsymbol{c}]_{\infty}^{(0)} = [G\boldsymbol{r}_{\boldsymbol{c}}]_{\infty}^{(0)}\,. \tag{40}$$

Notice also that by virtue of the normalisation (15) we have from (24) with $\phi = 1$,

$$1 = [G_{\mathrm{f}}\, 1]_{\infty}^{(0)} = [G\tau]_{\infty}^{(0)}\,, \tag{41}$$

where $G\tau$ is defined in a similar fashion to (39). Thus, from (40) and (41), we have

$$\boldsymbol{W} = [G\boldsymbol{r}_{\boldsymbol{c}}]_{\infty}^{(0)}/[G\tau]_{\infty}^{(0)}\,, \tag{42}$$

which is consistent with Ikuta and Murakami's (1987) expression (36) for drift velocity. That is, we have shown that the DGE and FTI definitions of drift velocity agree in general, without any restrictive assumptions.

Before proceeding to the definition of the diffusion coefficient, it is of interest to investigate the simple, constant collision frequency model in the context of the present discussion. Thus we consider the special case where

$$g\sigma(g,\chi) = \pi(\chi)\,, \tag{43}$$

and note that in this case the quantities

$$g\sigma_l(g) = \int P_l(\cos\chi)\,\pi(\chi)\sin\chi\,\mathrm{d}\chi \equiv \pi_l \tag{44}$$

are all independent of relative speed g. Notice also that by (8), the collision frequency

$$\nu_\mathrm{T} = \int \mathrm{d}\boldsymbol{c}_0\, f_0(\boldsymbol{c}_0)\pi_0 = n_0\,\pi_0 \equiv \nu_0 \tag{45}$$

is independent of $\boldsymbol{c}$ in this case. Thus by (37), we have

$$G_\mathrm{f}\,\boldsymbol{c} = \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-\nu_0\tau}(\boldsymbol{c}+\boldsymbol{a}\tau) = \frac{1}{\nu_0}(\boldsymbol{c}+\boldsymbol{a}/\nu_0)$$

and by (36) it follows that

$$\begin{aligned} \boldsymbol{W} = [G_\mathrm{f}\,\boldsymbol{c}]_\infty^{(0)} &= \frac{1}{\nu_0}[\boldsymbol{c}+\boldsymbol{a}/\nu_0]_\infty^{(0)} \\ &= \frac{1}{\nu_0}[\boldsymbol{c}]_\infty^{(0)} + \boldsymbol{a}/\nu_0^2[1]_\infty^{(0)}\,. \end{aligned} \tag{46}$$

The second term on the right-hand side is readily calculated:

$$\begin{aligned} [1]_\infty^{(0)} &= \int \mathrm{d}\boldsymbol{c} \int \mathrm{d}\boldsymbol{c}_0\, f_\infty^{(0)}(\boldsymbol{c}')\, f_0(\boldsymbol{c}_0')\, g\sigma(g,\chi)\, \mathrm{d}\hat{\boldsymbol{g}}' \\ &= \int \mathrm{d}\boldsymbol{c} \int \mathrm{d}\boldsymbol{c}_0\, f_\infty^{(0)}(\boldsymbol{c})\, f_0(\boldsymbol{c}_0)\, \pi(\chi)\, \mathrm{d}\hat{\boldsymbol{g}}' \\ &= \nu_0\,. \end{aligned} \tag{47}$$

The first term on the right vanishes for light swarm particles undergoing isotropic scattering, according to equation (35), and then (46) and (47) together yield

$$\boldsymbol{W} = \boldsymbol{a}/\nu_0 = e\boldsymbol{E}/m\nu_0\,. \tag{48}$$

In general, however, for particles of arbitrary mass undergoing anisotropic scattering, it can be shown that

$$\begin{aligned} [\boldsymbol{c}]_\infty^{(0)} &= \int \mathrm{d}\boldsymbol{c} \int \mathrm{d}\boldsymbol{c}_0\, f_\infty^{(0)}(\boldsymbol{c})\, f_0(\boldsymbol{c}_0)\, \pi(\chi)\, \boldsymbol{c}'\, d\hat{\boldsymbol{g}}' \\ &= \boldsymbol{W}(m\nu_0 + m_0\,\nu_1)/(m+m_0)\,, \end{aligned} \tag{49}$$

where

$$\nu_1 = n_0\, \pi_1\,. \tag{50}$$

Combining (46), (47) and (49) then gives

$$\boldsymbol{W} = e\boldsymbol{E}/\mu\nu_{\rm m}\,, \tag{51}$$

where $\mu \equiv mm_0/(m+m_0)$ is the reduced mass and

$$\nu_{\rm m} = \nu_0 - \nu_1 = 2\pi \int (1-\cos\chi) g\, \sigma(g,\chi) \sin\chi \, {\rm d}\chi \tag{52}$$

is the momentum transfer collision frequency.

Equation (51) is an exact and very well known result which can be obtained far more simply and directly by taking the velocity moment of (1) under spatially uniform and static conditions. However, it is useful to see its derivation in the context of the FTI formalism and to note in particular the origin of the total and momentum transfer collision frequencies, ν_0 and $\nu_{\rm m}$ respectively, in equations (48) and (51). We shall do the same thing for $D_{\rm T}$ in the following section to highlight the origin of the discrepancy between DGE and FTI definitions.

(2f) Transverse Diffusion Coefficient

We now turn to the second member of the hierarchy of kinetic equations (14b), which again is of the same form as the prototype equation (16), but with

$$\rho_\infty(\boldsymbol{c}) = (\boldsymbol{c}-\boldsymbol{W}) f_\infty^{(0)}(\boldsymbol{c}) + \psi_{\rm s}(f_\infty^{(1)}(\boldsymbol{c}))\,. \tag{53}$$

Thus, by virtue of (18), the solution of (14b) can be obtained (e.g. by an iterative procedure) from

$$\begin{aligned} \boldsymbol{f}_\infty^{(1)}(\boldsymbol{c}) = \int_0^\infty {\rm d}\tau\, {\rm e}^{-\int_0^\tau \nu_{\rm T}(\boldsymbol{c}-\boldsymbol{a}\tau'){\rm d}\tau'} \{ (\boldsymbol{c}-\boldsymbol{a}\tau-\boldsymbol{W}) f_\infty^{(0)}(\boldsymbol{c}-\boldsymbol{a}\tau) \\ + \psi_{\rm s}(\boldsymbol{f}_\infty^{(1)})(\boldsymbol{c}-\boldsymbol{a}\tau))\}\,. \end{aligned} \tag{54}$$

It then follows with (13) that the diffusion tensor is given by

$$\begin{aligned} \mathbf{D} = \int {\rm d}\boldsymbol{c} \int_0^\infty {\rm d}\tau\, {\rm e}^{-\int_0^\tau \nu_{\rm T}(\boldsymbol{c}+\boldsymbol{a}\tau'){\rm d}\tau'} (\boldsymbol{c}+\boldsymbol{a}\tau)\{ (\boldsymbol{c}-\boldsymbol{W}) f_\infty^{(0)}(\boldsymbol{c}) \\ + \psi_{\rm s}(\boldsymbol{f}_\infty^{(1)}(\boldsymbol{c}))\}\,. \end{aligned} \tag{55}$$

It is emphasised that *both* $f_\infty^{(0)}$ and $\boldsymbol{f}_\infty^{(1)}$ are required *in general* to determine $\mathbf{D}$. We now focus on the transverse diffusion coefficient $D_{\rm T}$ and, to facilitate the calculation, we take a coordinate system in which the z-axis is defined by the direction of $\boldsymbol{a}$ and x is a transverse coordinate. Thus by (55)

$$
\begin{aligned}
D_{\mathrm{T}} &= D_{xx} \\
&= \int \mathrm{d}\boldsymbol{c} \int_0^\infty \mathrm{d}\tau \, \mathrm{e}^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'} \{c_x^2 \, f_\infty^{(0)}(\boldsymbol{c}) \\
&\qquad + c_x \, \psi_{\mathrm{s}}(f_{x,\infty}^{(1)}(\boldsymbol{c}))\} \, . \qquad (56)
\end{aligned}
$$

Now follows the key argument: In reality $\nu_{\mathrm{T}}(\boldsymbol{c}) = \nu_{\mathrm{T}}(c)$ depends on the magnitude of the velocity alone. This in turn implies that $\nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')$, which occurs in the argument of the exponential, is a function of c, τ' and c_z, but not c_x. Thus we have

$$
\Phi(\boldsymbol{c}) = c_x \int_0^\infty \mathrm{d}\tau \, \mathrm{e}^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'} = c_x \, h(c, \, c_z) \, , \qquad (57)
$$

where $h(c, c_z)$ is a function of c and c_z, but not c_x. Clearly then the function (57) has vector and higher order tensor contributions, *but no scalar part*. Hence, for light swarm particles in a cold gas undergoing isotropic scattering

$$
\begin{aligned}
[\Phi(\boldsymbol{c})]_{x,\infty}^{(1)} &\equiv \int \mathrm{d}\boldsymbol{c} \int_0^\infty \mathrm{d}\tau \, \mathrm{e}^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'} c_x \, \psi_{\mathrm{s}}(f_{x,\infty}^{(1)}(\boldsymbol{c})) \\
&= 0 \, , \qquad (58)
\end{aligned}
$$

by virtue of the theorem expressed by (34), and hence (56) gives

$$
D_{\mathrm{T}} = \int \mathrm{d}\boldsymbol{c} \int_0^\infty \mathrm{d}\tau \, \mathrm{e}^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'} c_x^2 \, f_\infty^{(0)}(\boldsymbol{c}) \, . \qquad (59)
$$

That is, for $m/m_0 \ll 1$ and $\sigma(g,\chi)$ independent of χ, D_{T} can be found entirely in terms of $f_\infty^{(0)}(\boldsymbol{c})$, according to (59). We show below that the definition of Ikuta matches (59), that is, that the DGE and FTI definitions are in agreement for light particles in a cold gas undergoing isotropic scattering. However, in general, calculations of D_{T} from the standard DGE definition requires $f_{x,\infty}^{(1)}$ as well as $f_\infty^{(0)}$, in contrast to Ikuta's definition. More specifically, the second term in curly brackets in (56) is responsible for the difference between the standard D_{T} (DGE) and D_{T} (FTI).

We now show that we can formulate the expression for D_{T} entirely in terms of $\psi_{s,\infty}^{(0)}$ for isotropic scattering. Thus, if we substitute for $f_\infty^{(0)}$ in (59) from equation (21) we obtain

$$
D_{\mathrm{T}} = \int \mathrm{d}\boldsymbol{c} \int_0^\infty \mathrm{d}\tau \, \mathrm{e}^{-\int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c}+\boldsymbol{a}\tau')\mathrm{d}\tau'} c_x^2 \int_0^\infty \mathrm{d}\bar{\tau} \, \mathrm{e}^{-\int_0^{\bar{\tau}} \nu_{\mathrm{T}}(\boldsymbol{c}-\boldsymbol{a}\tau')\mathrm{d}\tau'} \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}-\boldsymbol{a}\bar{\tau})
$$

$$= \int \mathrm{d}\boldsymbol{c}\, c_x^2\, \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) \int_0^\infty \mathrm{d}\tau \int_0^\infty \mathrm{d}\bar{\tau}$$

$$\times \exp\Big(- \int_0^\tau \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}(\bar{\tau} + \tau'))\mathrm{d}\tau' - \int_0^{\bar{\tau}} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' \Big)$$

$$= \int \mathrm{d}\boldsymbol{c}\, c_x^2\, \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) \int_0^\infty \mathrm{d}\tau \int_0^\infty \mathrm{d}\bar{\tau}$$

$$\times \exp\Big(- \int_{\bar{\tau}}^{\tau+\bar{\tau}} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' - \int_0^{\bar{\tau}} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' \Big)$$

$$= \int \mathrm{d}\boldsymbol{c}\, c_x^2\, \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) \int_0^\infty \mathrm{d}\tau \int_0^\infty \mathrm{d}\bar{\tau} \exp\Big(- \int_0^{\tau+\bar{\tau}} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' \Big)$$

$$= \int \mathrm{d}\boldsymbol{c}\, c_x^2\, \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) \int_0^\infty \mathrm{d}\tau \int_t^\infty \mathrm{d}t' \exp\Big(- \int_0^{t'} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' \Big)$$

$$= \int \mathrm{d}\boldsymbol{c}\, c_x^2\, \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c}) \int_0^\infty \mathrm{d}t\, t \exp\Big(- \int_0^{t} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' \Big)$$

$$= \int \mathrm{d}\boldsymbol{c} \int_0^\infty \mathrm{d}t\, \frac{(c_x\, t)^2}{2} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}t) \exp\Big(- \int_0^{t} \nu_{\mathrm{T}}(\boldsymbol{c} + \boldsymbol{a}\tau')\mathrm{d}\tau' \Big) \psi_{\mathrm{s},\infty}^{(0)}(\boldsymbol{c})$$

$$= \tfrac{1}{2}[Gx_{\boldsymbol{c}}^2]_\infty^{(0)}\,, \tag{60}$$

where $x_{\boldsymbol{c}}(\mathrm{t}) = c_x\, t$ is the x-component of the position vector (38) after time t. Given the normalisation (41), we can also write (60) in the form

$$D_{\mathrm{T}} = [Gx_{\boldsymbol{c}}^2]_\infty^{(0)} / 2[Gt]_\infty^{(0)}\,, \tag{61}$$

which is similar in appearance to equation (37) of Ikuta and Murakami (1987). The main point to note is that Ikuta *et al.* use (61) to calculate D_{T} for *all types* of scattering, whereas the standard DGE definition of D_{T} leads to (61) *only* for *isotropic scattering* of light swarm particles.

We again revert to the 'benchmark', constant collision frequency model to reinforce the above comments. In the case where (27) holds the standard DGE expression (55) for diffusion tensor reduces to

$$\mathbf{D} = \frac{1}{\nu_0} \int \mathrm{d}\boldsymbol{c}(\boldsymbol{c} + \boldsymbol{a}/\nu_0)\{(\boldsymbol{c} - \boldsymbol{W}) f_\infty^{(0)}(\boldsymbol{c}) + \psi_{\mathrm{s}}(f_\infty^{(1)}(\boldsymbol{c}))\}\,. \tag{62}$$

After some algebra and rearrangement this becomes

$$\mathbf{D} = \frac{1}{\nu_0} \int \mathrm{d}\boldsymbol{c}(\boldsymbol{c} - \boldsymbol{W})(\boldsymbol{c} - \boldsymbol{W}) f_\infty^{(0)}(\boldsymbol{c}) + \frac{1}{\nu_0} [\boldsymbol{c}]_\infty^{(1)}\,, \tag{63}$$

where we have used the normalisation requirement (15) and the bracket quantity is defined in a similar way to (26) for $\psi_{\mathrm{s}}(\boldsymbol{f}_\infty^{(1)})$. The latter, by virtue of the theorem represented by (35), vanishes for light particles undergoing isotropic scattering and in that case (and *only* that case)

$$\mathbf{D} = k\mathbf{T}/m\nu_0\,, \tag{64}$$

where the temperature tensor is defined by

$$\begin{aligned} k\mathbf{T} &= m\int \mathrm{d}\boldsymbol{c}(\boldsymbol{c}-\boldsymbol{W})(\boldsymbol{c}-\boldsymbol{W})f_\infty^{(0)}(\boldsymbol{c}) \\ &\equiv m\langle(\boldsymbol{c}-\boldsymbol{W})(\boldsymbol{c}-\boldsymbol{W})\rangle_\infty^{(0)}\,. \end{aligned} \tag{65}$$

However, the bracket quantity can be evaluated *exactly* for the constant collision frequency model, for arbitrary mass ratio and anisotropic scattering:

$$[\boldsymbol{c}]_\infty^{(1)} = (m\nu_0 + m_0\,\nu_1)\mathbf{D}/(m+m_0)\,. \tag{66}$$

Substitution of (66) into the right-hand side of (63) and solving for $\mathbf{D}$ gives the expression

$$\mathbf{D} = k\mathbf{T}/\mu\nu_{\mathrm{m}}\,, \tag{67}$$

well known in the kinetic theory of swarms (Wannier 1953).

As we have already pointed out, Ikuta's definition of the diffusion coefficient is tantamount to neglecting the second term on the right of (63), which leads (for $m \ll m_0$) to (64), where the *total* collision frequency ν_0 appears in the denominator. However, this is consistent with the standard DGE definition for isotropic scattering only. For anisotropic scattering, it is the collision frequency for the *momentum-transfer* collision frequency ν_{m} which occurs naturally, as can be seen from equation (67).

Finally, we note again that the constant collision frequency analysis for diffusion proceeds most simply directly from equation (1). The analysis given in this section serves mainly to highlight precisely where the point of departure is between standard DGE and Ikuta definitions of diffusion coefficient, viz. Ikuta *et al.* effectively neglect the second term in curly brackets in (56), which involves $\boldsymbol{f}_\infty^{(1)}$.

3. Discussion

In this paper we have briefly outlined the standard DGE and FTI approaches to the analysis of swarm transport parameters, and have discussed the respective definitions of drift velocity and transverse diffusion coefficient. It was shown that while the Ikuta/FTI definition of drift velocity matches that of standard DGE kinetic theory, his definition of D_{T} is consistent with the DGE expression only for isotropic scattering and light swarm particles. Numerical studies (not presented in this paper) have produced results which are consistent with this observation. We have used a simple constant collision frequency model to illustrate precisely where the Ikuta definition of D_{T} leads to an expression which differs from the well known DGE result.

Our conclusions are these:

(1) Because of their different definition of D_{T}, Ikuta *et al.* are calculating a *different transport quantity* from the generally accepted one, which is the quantity measured by experiment.

(2) Only for light swarm particles and isotropic scattering do the two definitions agree and only then should there be any expectation of agreement between respective numerical calculations.
(3) The FTI and multi-term expansion techniques are effectively merely different methods for solving the Boltzmann equation and any major discrepancy which exists between numerical calculations of D_T is due to the difference in definitions, rather than the difference of numerical techniques.
(4) However, it does seem that Ikuta (personal communication) may be suggesting that not only the *integral* (56) of $\psi_s(f_x^{(1)})$ vanishes, but that this term itself is zero, in which case the implication is that the Boltzmann collision term (7) should be replaced by

$$J_{\mathrm{Ikuta}}(f) = \nu_T f - \psi_s(f^{(0)}) , \tag{68}$$

The FTI literature should be viewed in that light.

Note added in proof: Professor L. A. Viehland has advised that he reached similar conclusions to those outlined above through an independent though unpublished analysis.

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