Fundamental issues in fluid modeling: Direct substitution and aliasing methods

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It is shown how the accuracy of fluid models of charged particles in gases can be improved significantly by direct substitution of swarm transport coefficient data, rather than cross sections, into the average collision terms. This direct substitution method emerges in a natural way for fluid formulations in which the role of the mean energy is transparent, whatever the mass of the charged particles in equation (ions or electrons), and requires no further approximations. The procedure is illustrated by numerical examples for electrons, including the operational window of *E*/*N* for an idealized Franck-Hertz experiment. Using the same fluid formulation, we develop an aliasing method to estimate otherwise unknown mobility data for one type of particle, from known mobility data for another type of particle. The method is illustrated for muons in hydrogen, using tabulated data for protons in the same gas. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4768421]

I. INTRODUCTION

Experiments measuring the properties of charged particles in gases in drift tubes in the 19th and early 20th centuries helped lay the foundations for the modern era of physics,[1] and swarm experiments[1–6] continue to provide useful information for such diverse areas as low energy atomic and molecular physics,[7] low temperature plasma technology,[8] and detectors used in nuclear and high energy physics experiments.[9] Fundamental theoretical questions surrounding ion and electron swarm experiments have been addressed through rigorous numerical solutions of the Boltzmann kinetic equation[1,6,10,11] in phase space and, in the subject of the present paper, through approximate "moment" or "fluid" equations[12–15] obtained from the Boltzmann equation. Though quite general, and applicable to partially ionized plasmas as well as swarms, the equations were initially limited in their application to the weak gradient, hydrodynamic regime,[10] commensurate with swarm experimental conditions. Furthermore, they were traditionally used to provide physical insight[13] or at most rough semi-quantitative estimates of swarm transport properties, through empirical formulas such Blanc's law, Tonks' theorem, the Wannier energy, and generalized Einstein relations, along with respective refinements.[6] Nowadays, with the increased interest in low temperature plasmas and applications, there has been something of an about face in principle and practice: fluid equations are now often considered accurate and general enough for quantitative purposes, and hydrodynamic swarm transport data are considered as input information. Such a procedure is obviously consistent for correctly formulated fluid equations (i.e., clearly derivable from the governing Boltzmann kinetic equation)[14] which are valid in both the hydrodynamic swarm limit and for the (possibly non-hydrodynamic) conditions prevailing in the low temperature plasma application. This often precludes any physically meaningful or accurate match of swarm data with any of the *ad hoc*, unphysical fluid models which plague plasma physics. On the other hand, a general, physically based fluid formulation based on momentum transfer theory[13] has long been available with the added bonus that it is valid for particles of arbitrary mass. Although it has a distinct and separate history, strategy and motivation, originating in the study of swarms of single charged species ions, electrons, positrons, muons, etc., in a gas, momentum transfer can be applied equally to the electrons and ions of a low temperature, partially ionized plasma making it an eminently suitable candidate as a basis for plasma modeling. This momentum transfer theory formulation, in which the mean energy plays a central and transparent role, provides the starting point for the present discussion on the use of swarm data in fluid equations.

We begin with an overview of key issues in fluid modeling in Sec. II, and emphasize the pivotal role of the mean energy in the collision rates, which are common to both swarms and plasma. Section III outlines the way in which swarm experimental data may be most efficiently incorporated into these rate terms through the direct substitution method. The method overcomes some of the accuracy limitations of standard momentum transfer theory, including the use of smoothing functions and other approximations to treat threshold processes.[18,34] Numerical examples, including a non-hydrodynamic model relating to the Franck-Hertz experiment[16] are given in Sec. IV. In Sec. V, we consider a situation where one requires swarm transport coefficients for a particular type of particle in a specified gas, for which swarm experimental data are either unavailable or difficult to obtain. We show how the fluid equations may be used to infer the required transport data, on the basis of available swarm transport data for another type of particle, in the same gas. Such aliasing of transport data is particularly useful

for obtaining otherwise unknown mobilities of muons μ^+ in H_2, using tabulated data for H^+ ions in the same gas as the surrogate.

II. COLLISION RATES, TRANSPORT COEFFICIENTS, AND MEAN ENERGY

A. Swarm experiments, transport coefficients, and cross sections

Swarm experiments measure transport coefficients as functions of the reduced electric field *E*/*N* (the ratio of the applied dc electric field to gas number density), under carefully controlled conditions, generally corresponding to the weak gradient, hydrodynamic regime.[6,10] The variation of these measured macroscopic transport properties with *E*/*N* reflects the underlying microscopic physics: increasing the field increases the average energy of the particles, and thus a swarm experiment effectively scans the way scattering cross sections,[2] written generically as $\sigma(\varepsilon_{CM})$, depend upon the energy ε_{CM} in the centre-of-mass frame of a charged particle and a neutral molecule. (For light particles, such as electrons, positrons or muons, $\varepsilon_{CM} \approx \varepsilon$, the energy of the particle itself, something which will be implicit in the discussion from now on.) The way in which the field-dependence relates to an energy-dependence is an important question, discussed below, but for now all we need to observe is that the microscopic information (scattering cross sections, interaction potentials) embedded in macroscopic swarm transport coefficient data may be either:

(i) Extracted explicitly, using either Boltzmann's kinetic equation[1,2,6] or the fluid equations;[5,17] or
(ii) Used implicitly, by applying the unprocessed transport data directly to other macroscopic situations.

Either way, the information may be supplemented where necessary by cross sections measured in beam experiments and/or theoretically calculated hydrodynamic swarm transport coefficients, obtained from solution of Boltzmann's kinetic equation.

The present paper explores strategy (ii), i.e., the direct use of swarm transport data in general fluid equations, without reference to cross sections. Exact, general fluid equations, valid for structureless particles of arbitrary mass (atomic ions, electrons, muons, etc.) were formulated in Ref. 13, and subsequently cast into an approximate form suitable for practical application, as shown in Eqs. (1) below. In the present paper, the quantities of most interest are the average collision transfer rates shown on the right hand sides of Eqs. (1b) and (1c).

B. Average collision rates

That the average collision rates are functions of mean energy $\langle\varepsilon_{CM}\rangle$ in the centre-of-mass frame is simply a macroscopic manifestation of the microscopic dependence of scattering cross sections upon CM energy. Since collisions are unaffected by applied fields (unless they are extremely strong), boundaries or the macroscopic state of the plasma or swarm, average collision rates cannot be explicit functions of these external influences. The detailed mathematical expressions for these average collision rates are prescribed uniquely by the collision term in the Boltzmann equation,[6,10,11] which incorporates cross sections but makes no mention of fields (the field term appears only in the left hand side). It is clear that fluid equations derived by taking appropriate velocity moments the Boltzmann equation must have the same mathematical form of collision rates in all circumstances.

Exact general expressions for collision rates in the balance equations are given in Ref. 13, but some approximation (ansatz) is inevitable to mold these in a form suitable for practical application. The ansatz may be in terms of either the moments or the velocity distribution itself, and it is legitimate to ask "which approximation gives the best results, consistent with the constraints described above?" In this paper, we adopt the long established ansatz of momentum transfer theory[6,13,14,19,20] to approximate moments, which in the lowest order of approximation produces Eqs. (1b) and (1c) below. The collision rates have the required general properties, for both ions and electrons, and lend themselves readily to incorporation of swarm data, as explained below.

We acknowledge alternative viewpoints and procedures, especially those with an obvious connection to the Boltzmann equation and clearly stated approximations, which exist for both ions[21] and electrons.[22] Unfortunately, however, *ad hoc* models still dominate the low temperature plasma physics literature, with all their attendant problems,[14] e.g., the mass factor in the momentum transfer term on the right hand side of Eq. (21) of Ref. 23 is incorrect. Other formulations may require extensive numerical calculations to elucidate the pivotal role of mean energy.[24] The local field approximation[23] effectively seeks to replace the explicit and transparent energy dependence in the average collision rates with an artificially imposed field dependence. An extreme case is the so-called drift-diffusion approximation[25] which has nothing whatever to say about mean energy. The papers by Bayle *et al.*[26] claim to have a fluid model based on the Boltzmann's equation, but bear little resemblance to what we consider the correct equations.

C. Mean energy vs *E*/*N*

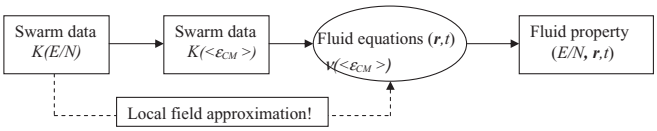
While the role of the mean energy $\langle\varepsilon_{CM}\rangle$ in the centre-of-mass frame of a colliding charged particle and neutral molecule is transparent in the momentum transfer theory formulation of fluid equations[9,10,13–15] in both average collision rates $\nu(\langle\varepsilon_{CM}\rangle)$ (see Eqs. (1b) and (1c) below) and in the transport coefficients which are derived from them (see, e.g., Eq. (5a)), transport coefficients are actually measured as functions of reduced field strength. In order to use these data in the fluid model, one must have a way of relating $\langle\varepsilon_{CM}\rangle$ to *E*/*N*, as discussed in Sec. III. Note that while the momentum transfer formulation is approximate, the central role that it ascribes to mean energy has been established independently. Thus, the equivalence of interpreting transport coefficients as functions of either *E*/*N* or the mean energy $\langle\varepsilon_{CM}\rangle$ in the centre-of-mass of an ion and a neutral particle has been established through rigorous numerical solutions of the Boltzmann equation in

the scaling investigations of Mason and colleagues.[6] (Note that they actually frame their results in terms of an "effective temperature" $T_{eff} = 2\langle\varepsilon_{\rm CM}\rangle/3k_B$, where k_B is Boltzmann's constant.)

III. THE DIRECT SUBSTITUTION METHOD

A. The transition from *E/N* to mean energy

In this section, we show how swarm transport data, measured as a function of a dc field *E/N*, should be recast as a function of mean energy, e.g., mobility $K(E/N) \rightarrow K(\langle\varepsilon_{\rm CM}\rangle)$, for input into the fluid equations. The procedure is shown schematically below:



The fluid equations may then be solved and applied to systems which are quite different to the original swarm experiment. There may be, for example, space and/or time varying fields, strong gradients and non-hydrodynamic conditions in any particular application. This procedure, the direct substitution method (DSM), effectively generalizes an earlier suggestion[18] to include both elastic and inelastic collision rates. As shown in the above schematic, the local field approximation[23] effectively involves substituting transport coefficients and rates as functions of (local and instantaneous) field, rather than mean energy, and hence the approximation, as indicated by its title, cannot accurately model temporal and spatial non-locality.

B. Fluid equations

In general, a charged particle is subject to a electromagnetic force $q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$, in which the fields are generally space and time-dependent, and of either external or internal origin. The exact fluid equations[13] for particles of low number density n, mass m, charge q in a neutral gas of molecules of mass M, number density N, in equilibrium at temperature T_g are perfectly general, but not in a form suitable for practical application, because they are not closed, i.e., there are more unknowns than available equations. Closure generally requires several approximations, starting with the average collision rates, and we begin the present discussion at the point where these have been approximated using first order momentum transfer theory.[6,13,14]

To illustrate the procedure, we shall assume that collisions between particles and gas molecules preserve particle number. (This limitation can easily be removed, using the full set of fluid equations for attachment, ionization, etc., in Ref. 14.) At lowest level of momentum transfer approximation, this results in the following set of balance or fluid equations for particle density n, mean velocity $\langle\mathbf{v}\rangle$ and mean energy $\langle\varepsilon\rangle$, equally valid for both swarms and plasmas:

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

$$nm\frac{d\langle\mathbf{v}\rangle}{dt} + \nabla\cdot\mathrm{P} - nq(\mathbf{E} + \langle\mathbf{v}\rangle \times \mathbf{B}) = -n\frac{mM}{m+M}\nu_m(\langle\varepsilon_{\rm CM}\rangle)\langle\mathbf{v}\rangle, \tag{1b}$$

$$n\frac{d}{dt}\left(\langle\varepsilon\rangle - \frac{1}{2}m\,\langle \mathrm{v}\rangle^2\right) + \nabla\cdot\mathbf{J}_q + \mathrm{P} : \nabla\mathbf{v} = -n\,\nu_e(\langle\varepsilon_{\rm CM}\rangle) \times \left[\langle\varepsilon\rangle - \frac{3}{2}k_BT_g - \frac{1}{2}(m+M)\langle\mathrm{v}\rangle^2 + \Omega(\langle\varepsilon_{\rm CM}\rangle)\right], \tag{1c}$$

where P is the pressure tensor, $\mathbf{J}_q$ is the heat flux vector, and

$$\frac{d}{dt} = \partial_t + \langle\mathbf{v}\rangle\cdot\nabla$$

denotes the convective time derivative. The average collision frequencies for momentum and energy transfer are defined by

$$\nu_m(\langle\varepsilon_{\rm CM}\rangle) = N\sqrt{\frac{2\langle\varepsilon_{\rm CM}\rangle}{\mu_r}}\,\sigma_m(\langle\varepsilon_{\rm CM}\rangle), \tag{2a}$$

where $\mu_r = \frac{mM}{m+M}$ is the reduced mass, and

$$\nu_e(\langle\varepsilon_{\rm CM}\rangle) = \frac{2m}{M}\,\nu_m(\langle\varepsilon_{\rm CM}\rangle), \tag{2b}$$

respectively, where the average momentum transfer cross section $\sigma_m(\langle\varepsilon_{\rm CM}\rangle)$ is, in this, the lowest order of momentum transfer theory, simply the actual cross section evaluated at the mean energy in the centre-of-mass

$$\langle\varepsilon_{\rm CM}\rangle = \frac{M\,\langle\varepsilon\rangle + m\,\frac{3}{2}k_BT_g}{m+M},$$

and k_B is Boltzmann's constant. The quantity

$$\Omega(\langle\varepsilon_{\rm CM}\rangle) = \sum_\alpha \varepsilon_\alpha \frac{\vec{\nu}_\alpha - \overleftarrow{\nu}_\alpha}{\nu_e(\langle\varepsilon_{\rm CM}\rangle)} \tag{3}$$

accounts for inelastic scattering, through channels α which are governed by threshold energies ε_α and average collision frequencies for inelastic and superelastic processes $\vec{\nu}_\alpha$ and $\overleftarrow{\nu}_\alpha$, respectively. These are also functions of $\langle\varepsilon_{\rm CM}\rangle$ but, since the corresponding cross sections are generally steeply rising near threshold, a momentum transfer approximation of the types (2a) and (2b) cannot be used. It is explained below how the functional dependence of the quantities ν_m and Ω upon mean energy may be specified through direct use of swarm data, obviating the need for the input of any cross sections, and avoiding any further approximation.

Solution of Eqs. (1a)–(1c) can, however, proceed only after they are closed, which generally requires an ansatz for both the heat flux $\mathbf{J}_q$ and the pressure tensor P. For light particles, m ≪ M, things simplify considerably, since then $\langle\varepsilon_{\rm CM}\rangle \approx \langle\varepsilon\rangle$, and the pressure tensor is approximately a scalar, $\mathrm{P} \approx 2/3\, n\,\varepsilon\,\mathrm{I}$. A benchmarked ansatz is now available for $\mathbf{J}_q$, and the complete set of closed equations is detailed in Ref. 16.

The question of a general physically based ansatz for each of the heat flux vector $\mathbf{J}_q$ and the pressure tensor P, is quite difficult, and is currently under investigation.[32]

C. Hydrodynamic regime and swarm transport coefficients

Swarm experiments generally operate with static, uniform fields, and in the hydrodynamic regime.[11] Here, the space-time dependence of all quantities is projected onto the number density $n(\boldsymbol{r},t)$, usually in the form of density gradient expansion, e.g., to first order,

$$\Gamma = n\langle \mathbf{v} \rangle = n\mathbf{v} - \boldsymbol{D} \cdot \nabla n \tag{4a}$$

and

$$n\langle \varepsilon \rangle = n\varepsilon - \xi \cdot \nabla n. \tag{4b}$$

The expansions are substituted into the fluid equations, and coefficients of ∇n equated, leading to explicit expressions for the drift velocity $\mathbf{v}$, the diffusion tensor $\boldsymbol{D}$, and the mean particle energy ε in the spatially uniform state. The latter then gives the mean CM energy,

$$\varepsilon_{\mathrm{CM}} = \frac{M\ \varepsilon + m\ \frac{3}{2}k_B T_g}{m+M}.$$

The gradient energy parameter ξ may be similarly calculated, but is not needed here.

The effects of a magnetic field are interesting and varied,[15] but for simplicity we assume $\boldsymbol{B} = 0$ in the remainder of this paper. Thus, we find the mobility coefficient

$$K \equiv \frac{v}{E} = \frac{e}{\mu_r\ \nu_m(\varepsilon_{\mathrm{CM}})} \tag{5a}$$

and the equation for the mean CM energy in the spatially uniform state

$$\varepsilon_{\mathrm{CM}} = \frac{3}{2}k_B\ T_g + \frac{1}{2}M\mathrm{v}^2 - \Omega(\varepsilon_{\mathrm{CM}}). \tag{5b}$$

The famous Wannier energy equation[6,20] is regained in the limit of zero inelastic collisions ($\Omega = 0$). The two components, D_L (longitudinal diffusion coefficient) and D_T (transverse diffusion coefficient), of the diffusion tensor, are related to K through generalized Einstein relations.[6]

For light particles, $\varepsilon_{\mathrm{CM}} \approx \varepsilon$ and Eqs. (5a) and (5b) become

$$K = \frac{e}{m\ \nu_m(\varepsilon)} \tag{6a}$$

and

$$\varepsilon = \frac{3}{2}k_B\ T_g + \frac{1}{2}M\mathrm{v}^2 - \Omega(\varepsilon), \tag{6b}$$

respectively, while the generalized Einstein relation simplifies to

$$\frac{D_T}{K} = \frac{2\varepsilon}{3e}, \tag{7}$$

also known as the Nernst-Townsend relation.[1,6] This may be used to provide approximate values of mean energy from experimental transverse diffusion coefficient data, and can be refined further if required (see the Appendix).

Note that since swarm experiments generally operate in the hydrodynamic regime, they may therefore be analyzed at the fluid level by Eqs. (4)–(7). The hydrodynamic assumption removes any requirement to close the fluid equations and the hydrodynamic transport coefficients then provide the required input into Eqs. (1a)–(1c), which may then be applied to non-hydrodynamic applications. In that case closure is indeed a problem, which can only be dealt with through an ansatz for the heat flux vector.

D. The direct substitution method

We now specialize to light particles, where Eqs. (6a) and (6b) can be employed in two ways, either:

(i) Solved for K and ε as functions of E/N for prescribed cross sections; or
(ii) Interpreted as equations defining

$$\nu_m(\varepsilon) = \frac{e}{mK} \tag{8a}$$

and

$$\Omega(\varepsilon) = \frac{3}{2}k_B\ T_g + \frac{1}{2}M\mathrm{v}^2 - \varepsilon \tag{8b}$$

as functions of ε.

The direct substitution method follows the latter approach.

Suppose that swarm data for both mobility K and D_T/K are available as functions of E/N. This information is entered in the first three columns of the table below, and the mean energy is then calculated as a function of E/N from (7), refined if required as explained in the Appendix, and tabulated in the fourth column.

If swarm experimental data are not available, the entries in columns 1-4 may be supplemented by transport data obtained from solving Boltzmann's equation in the hydrodynamic regime. In either case, the table enables swarm data for K, originally determined as a function of E/N, to be reinterpreted as a function of ε. Equation (8a) then furnishes the elastic collision rate $\nu_m(\varepsilon)$ as a function of ε, where data are then entered in column 5 of the table. The quantity $\Omega\ (\varepsilon)$, which derives from inelastic collision rates, can be evaluated from Eq. (8b) and tabulated accordingly in column 6. Notice that these entries are made without any reference to cross sections and neither is it necessary to assume any *ad hoc* smoothing factor[16] or assumptions[34] to estimate $\Omega\ (\varepsilon)$.

The direct substitution method provides a procedure, based upon hydrodynamic swarm data, for establishing the functional dependence upon ε of both the elastic and inelastic collision terms, ν_m and Ω , respectively, in Eqs. (1b) and (1c), which can then be applied to more general problems, whether a non-hydrodynamic swarm (e.g., the Franck-Hertz experiment[16,27]) or low temperature plasma. Note that the fields in these applications can be space and or time varying.

E. Other fluid parameters

In the linearized version of the general fluid equations[14,16] other parameters emerge, which can also be evaluated directly from swarm experiment data. Thus, if $\Omega(\varepsilon)$ has been found, then $\Omega' = \mathrm{d}\Omega/\mathrm{d}\varepsilon$ can be calculated, and

TABLE I. The "look up" table of experimental swarm data (first three columns) and quantities derived from it required for use in the fluid model equations (1a)–(1c). The quantity γ is defined below in Eq. (9).

E/N	K	D_T/K	ε	$\nu_m(\varepsilon)$	$\Omega\ (\varepsilon)$	γ	
…	…	…	…	…	…	…	…

the key parameter

$$\gamma \equiv \frac{(1+\Omega')\,\varepsilon}{\varepsilon + \Omega - \frac{3}{2}k_B T_g}, \tag{9}$$

which controls the formation of periodic structures in the Franck-Hertz experiment,[12] for example, can be readily found and entered in column 7 of Table I. Further parameters occur in the linearized fluid model and they too can be calculated from experimental data, and entered in Table I for subsequent application.

IV. APPLICATIONS AND BENCHMARKING

A. Benchmarking procedure

The foregoing outlines the recommended procedure for evaluating collision transfer terms, and is essentially encapsulated by Table I. But how accurate is it, and what is the expected improvement over a scheme which merely substitutes cross sections into Eqs. (1b) and (1c) using Eqs. (2) and (3)? To answer this question, we follow standard procedure and benchmark against accurate numerical solutions of Boltzmann's equation, or exact analytical solutions if available. In the following, we take examples for electrons, given that a complete set of physically based ion fluid equations is yet to be formulated.[32] To illustrate the procedure, we take simple model interactions to generate swarm "data" through solutions of the Boltzmann equation. However, we emphasize that the method is tailored explicitly for real cross sections and/or actual experimental swarm data.

B. Elastic collisions: Time-varying field

This simplest application of the method is to electrons undergoing elastic collisions. As in Ref. 18, we take a harmonically time-varying electric field, spatially uniform conditions, and make the substitution (8a) in Eqs. (1b) and (1c), which simplify to

$$\frac{\partial \mathrm{v}}{\partial t} - \frac{e}{m}E(t) = -\frac{e}{mK(\varepsilon)}\mathrm{v} \tag{10a}$$

and

$$\frac{\partial \varepsilon}{\partial t} = -\frac{2e}{MK(\varepsilon)}\left[\varepsilon - \frac{3}{2}k_B T_g - \frac{1}{2}M\mathrm{v}^2\right], \tag{10b}$$

respectively, where $E(t) = E_0 \cos \omega t$ is the magnitude of the applied field directed along the $-$z direction, and v is the z component of the mean electron velocity. The benchmark model in this case is a gas with $T_g = 0$ K, $M = 4.0$ amu, and a constant cross section $\sigma_m = 5\times10^{-20}$ m^2.

The benchmarking proceeds as follows:

a) The swarm "data" for Table I are generated by solving the Boltzmann equation for v and ε as functions of a dc field E/N, and mobilities $K = \mathrm{v}/E$ and ε entered in the second and fourth columns of Table I;
b) The Boltzmann equation is also solved accurately for the electron velocity distribution function, and the required velocity moments v and ε are generated to accuracies of better than 1% as functions of time for the time-varying field $E(t) = E_0 \cos \omega t$, for various reduced frequencies ω/N;
c) The DSM fluid equations (10a) and (10b) are solved under the same conditions;
d) Fluid equations are also solved without the DSM.

The way in which the DSM dramatically improves the accuracy of the fluid model is demonstrated clearly in Table II below for a range of frequencies. The exact values are detailed in the Boltzmann equation column, calculated through a multi-term solution.[18] The DSM results typically agree to within 2% for all transport coefficients at all frequencies considered, whereas discrepancies larger than 10% can arise for no-DSM.

C. Inelastic collisions: Franck-Hertz oscillations

In contrast to the previous example, the Franck-Hertz experiment operates with a dc field, and oscillations in electron properties are generated by inelastic collisions. These enter

TABLE II. Peak velocity and cycle-averaged energy of electrons in a harmonically time-varying field of amplitude $E/N = 1$ Td, for various normalized frequencies $\omega/$N (rad m^3) calculated from solution of (i) the Boltzmann equation, (ii) the DSM form of fluid equations (10a) and (10b), and (iii) fluid equations with cross sections substituted in Eqs. (1b) and (1c). A model gas has been used with temperature $T_g = 0$ K, atomic mass $M = 4.0$ amu and momentum transfer cross section $s_m = 5\times10^{-20}$ m^2.

ω/N (rad m^3/s)	Boltzmann equation v_{max} (m/s) ε_{av} (eV)	Fluid equations (DSM) v_{max} (m/s) ε_{av} (eV)	Fluid equations (no DSM) v_{max} (m/s) ε_{av} (eV)
10^{-18}	5782	5845	6442
	0.4703	0.4512	0.5506
5×10^{-18}	6273	6283	6952
	0.4938	0.4771	0.5775
10^{-16}	6850	6815	7629
	0.5156	0.5006	0.6036

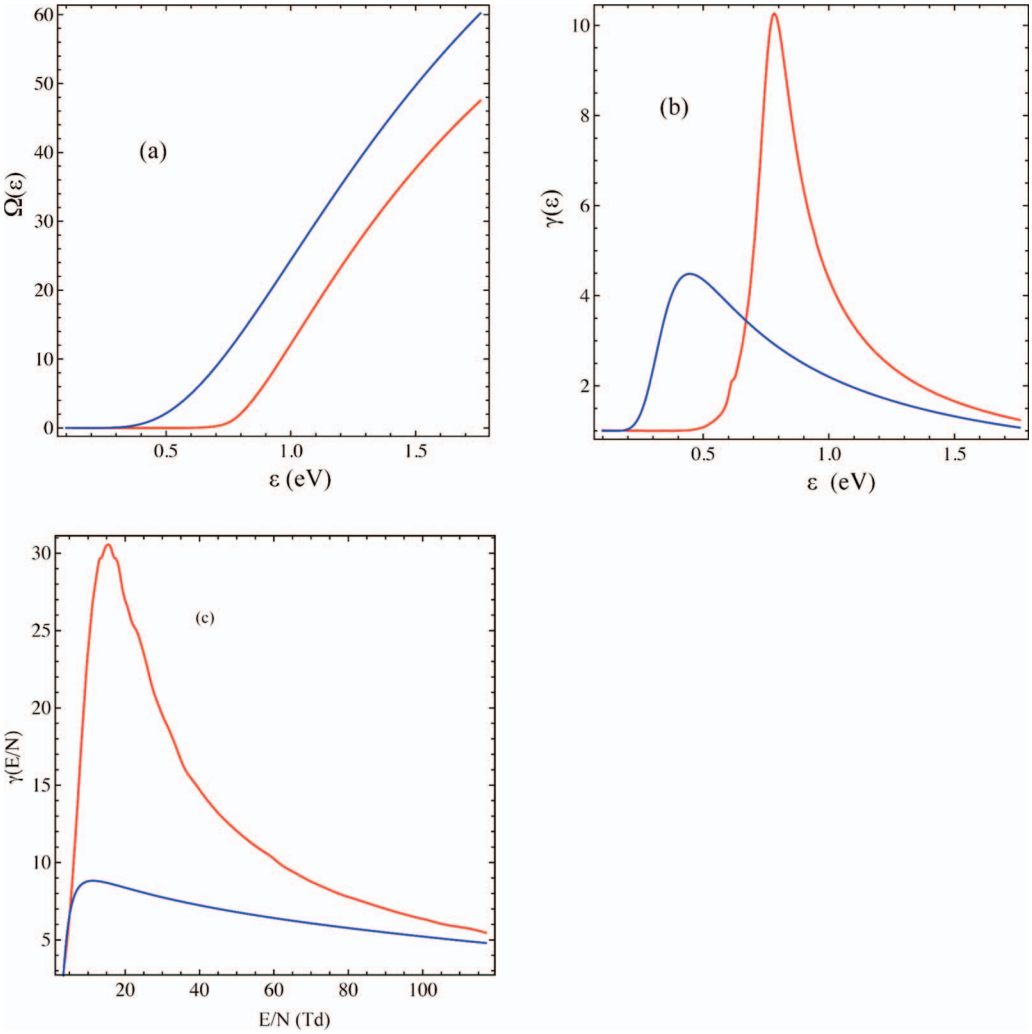


FIG. 1. Fluid parameters Ω and γ for the step-function model, as functions of mean energy (diagrams (a) and (b)) and γ as a function of E/N (diagram (c), where 1 Td $= 10^{-21}$ V/m^2) including the previous empirical prescription[12] (blue curves) and the direct substitution method of the present paper (red curves). Model details: Elastic momentum transfer cross section $\sigma_m = 6\times10^{-20}$ m^2, inelastic total cross section $\sigma_\alpha = 3\times10^{-21}$ m^2, inelastic threshold $\varepsilon_\alpha = 2.0$ eV, gas properties $M = 4$ amu, $T_g = 0$ K.

into the fluid equations through the quantities Ω and γ, as defined by Eqs. (8b) and (9) respectively, which can be evaluated accurately and efficiently using the DSM, without any reference to cross sections. It is important to realize that all quantities in Table I may be considered as functions of either mean energy or E/N, something which is particularly useful for analyzing the Franck-Hertz experiment.

For the benchmark model gas,[16,27] swarm drift velocity and mean energy "data" are again generated by accurate numerical solution of Boltzmann's equation for a range of E/N, and entered into Table I, and the other quantities calculated accordingly. Since the DSM provides a more accurate representation of inelastic collision rates, a correspondingly better representation of Franck-Hertz oscillations may be expected.

Taking the small mass limit of the general equations (1a)–(1c), and assuming a steady state, with spatial variation limited to one dimension (the z-axis), yields the electron fluid equations (1)–(3) of Ref. 12. These equations are then linearized to facilitate an analytic description at large distances z downstream from the cathode, where average electron properties vary as exp (Kz). The wavenumber K, which is found as the solution of a cubic secular equation (Ref. 12, Eq. (7)), is complex within a "window" of E/N. Here, electron properties are oscillatory with a wavelength $2\pi/Im(K)$, determined by the quantized atomic energies, as reflected macroscopically in the quantity γ of Eq. (9), and the Franck-Hertz experiment operates as required. Outside the window, $Im(K)$ is small and $Re(K)$ is large, electron properties are non-oscillatory, and the experiment does not yield useful information about atomic quantization.

In Ref. 16, Ω was calculated by substituting inelastic cross sections as functions of mean energy in (3), incorporating an empirical "smoothing factor" to account for averaging over sharp thresholds. In contrast, the DSM requires no cross sections and avoids completely any empirical assumption. Figure 1 shows Ω and γ calculated in two ways, on the basis of DSM and with the previous empirical formula, respectively, as functions of mean energy. γ is also shown as a function of E/N. It can be seen that the difference is substantial, with DSM yielding a far more pronounced peak in γ (Fig. 1).

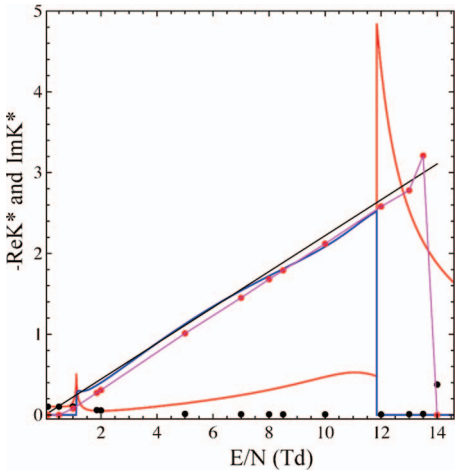


FIG. 2. Real and imaginary parts of the dimensionless wave number $K^* = K\lambda$, as functions of E/N for the step-function model of Fig. 1, calculated by solving the fluid equations with DSM, and Boltzmann's equation,[27] respectively. Length is scaled according to $\lambda = (2^{1/2}N\sigma_0)^{-1}$ with $\sigma_0 = 1$ Å^2 and 1 Td $= 10^{-21}$ V m^2. $-Re(K^*)$: red curve fluid; black points (Boltzmann equation). $Im(K^*)$: blue curve fluid; purple dots (Boltzmann); straight black line "ideal" Franck-Hertz value corresponding to atomic quantization energy of 2 eV.

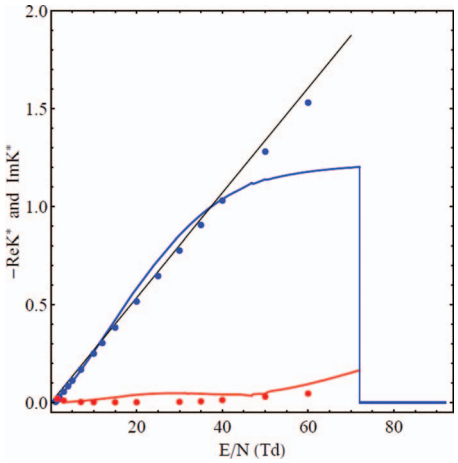


FIG. 3. Real and imaginary parts of the dimensionless wave number K^* as functions of E/N for electrons in neon, calculated by solving the fluid equations with DSM (solid curves), and Boltzmann's equation (dots), respectively, showing also the idealized Franck-Hertz straight line for $Im(K^*)$. A momentum transfer cross section supplied by R. P. McEachran (private communication) has been used, with inelastic processes modeled by a constant cross section of 1.0×10^{-18} m^2 above a threshold energy of 16.6 eV.

Figure 2 shows the dependence of $-Re(K)$ and $Im(K)$ upon E/N for the step function model, calculated by solving the fluid equations with DSM, and Boltzmann's equation,[27] respectively. Comparison with Fig. 1 of Ref. 16 shows that the DSM gives a significantly more accurate estimate of $Im(K)$ overall (mainly due to the increased sharpness in γ) and (due to the increased width of γ) an improved estimate for the upper limit of the window, namely, $E/N = 12$ townsend (Td) (cf. Boltzmann equation 13.8 Td). There is also overall improvement in the accuracy of $Re(K)$, although this is still generally overestimated by the fluid model as compared with the Boltzmann equation.

We have investigated a number of other cases, and find that the pattern shown in Figs. 1(a)–1(c) is typical of the way the DSM results in substantial changes in Ω and γ, with Fig. 2 providing the resulting enhancement of accuracy in fluid equation solutions. For example, Fig. 3 illustrates that the window of Franck-Hertz oscillations is overall quite well prescribed by the fluid equations with DSM for electrons in neon, although $Im(K)$ is somewhat too large at higher E/N.

We now move on to discuss another, quite different scenario, using the same fluid equations, in which transparent role of the mean energy is again central to the discussion.

V. ALIASING OF SWARM TRANSPORT DATA

A. The need for aliasing

We now consider what can be done in circumstances where transport coefficients are required for use in an experiment or technological application, but no swarm data are available for the particles in question. This is the case, for example, in a number of experiments involving muons in gases, such as μ^+ in H_2 in the MuCap experiment,[28] and for producing a high quality beam of μ^+ in He, as discussed by Taqqu.[29] In the discussion below, we formulate a general procedure, based on the approximate formulas of momentum transfer theory plus one key assumption, for obtaining unknown mobilities for one species from known mobility data for another. We refer to this procedure as "aliasing" swarm data.

B. The general prescription for aliasing

Equation (5a) for the mobility of charged particles of arbitrary mass m in a gas of particles of mass M, temperature T_g, along with the expression

$$\nu_m(\varepsilon_{\rm CM}) = N\sqrt{\frac{2\varepsilon_{\rm CM}}{\mu_r}}\sigma_m(\varepsilon_{\rm CM})$$

for the average collision frequency in terms of the average momentum transfer cross section $\sigma_m(\varepsilon_{\rm CM})$, furnishes the reduced mobility coefficient

$$\mathbf{K} \equiv NK = \frac{e}{\sqrt{2\mu_r\varepsilon_{\rm CM}}\,\sigma_m(\varepsilon_{\rm CM})} \tag{11}$$

and the Wannier energy relation (5b) furnishes the average energy $\varepsilon_{\rm CM}$ in the centre-of-mass.

We now wish to apply these general expressions to two different charged species 1 and 2 in the same gas (we have in mind μ^+ and H^+, respectively, in H_2) to find the mobility of species 1, purely on the basis of known mobility data for species 2.

If the nature of the interactions between species 1 and 2 and a gas molecule are known to be similar, then the momentum transfer cross sections for the two different charged species in the same gas may be assumed to be approximately the same, i.e.,

$$\sigma_m^{(1)}(\varepsilon_{\rm CM}) \approx \sigma_m^{(2)}(\varepsilon_{\rm CM}), \tag{12}$$

for all CM energies $\varepsilon_{\rm CM}$. This assumption then implies, with Eq. (11), that the ratio of reduced mobilities of the two species (distinguished by superscripts (1) and (2) in what follows) at

the same mean CM energy $\varepsilon_{\rm CM}$ is

$$\frac{\mathsf{K}^{(1)}}{\mathsf{K}^{(2)}} \equiv \frac{N^{(1)}K^{(1)}}{N^{(2)}K^{(2)}} = \sqrt{\frac{\mu_r^{(2)}}{\mu_r^{(1)}}}. \tag{13}$$

The mass M of the neutral gas molecule is the same in each case and, for simplicity, we will assume that the gas temperatures T_g are also the same. (This assumption can be relaxed if desired.) However, the reduced fields E/N will be different for 1 and 2 even though the energy is the same. Using the Wannier relation (5b) for each species, assuming elastic collisions only ($\Omega = 0$), and equating the mean energies, we find

$$\varepsilon_{\rm CM} = \frac{3}{2}kT_g + \frac{1}{2}M(K^{(1)}E^{(1)})^2 = \frac{3}{2}kT_g + \frac{1}{2}M(K^{(2)}E^{(2)})^2, \tag{14}$$

from which it follows that

$$\frac{(E/N)^{(1)}}{(E/N)^{(2)}} = \frac{\mathsf{K}^{(2)}}{\mathsf{K}^{(1)}} = \sqrt{\frac{\mu_r^{(1)}}{\mu_r^{(2)}}}. \tag{15}$$

Thus, if we know the reduced mobility $\mathsf{K}^{(2)}$ for species 2 at a particular reduced field, $(E/N^{(2)})$, we may use Eqs. (13) and (14) to find the reduced mobility $\mathsf{K}^{(1)}$ of species 1, at a different value $(E/N)^{(1)}$, of reduced field. The procedure is illustrated in the following example.

C. Calculation of the mobility of μ^+ in H_2

No mobility data exist for μ^+ in H_2, but nevertheless it is needed for the MuCap experiment.[28] Of the two possible candidates for aliasing, e^+ and H^+, the mass of μ^+ is closest to the latter, and hence, as far as scaling is concerned, the μ^+-H_2 system is more like H^+-H_2 than e^+-H_2.

Assuming then that a muon and a proton interact with a hydrogen molecule in a similar fashion, the momentum cross sections may be assumed to be approximately the same, as in Eq. (12). If fields are sufficiently low so that elastic collisions dominate, Eqs. (13) and (15) may be applied directly to estimate the unknown mobilities using known swarm mobility data[30] for H^+ in H_2.

With the notation that superscripts (1) and (2) refer to muons and protons, respectively, the reduced masses are

$$\mu_r^{(1)} \approx m_{\mu^+} \quad \text{and} \quad \mu_r^{(2)} = \frac{2}{3}m_H,$$

respectively, and hence $\frac{\mu_r^{(1)}}{\mu_r^{(2)}} \approx 1/6$. If we require the muon mobility at (say) $(E/N)^{(1)} = 0.8$ Td, then Eq. (15) tells us to look up the proton mobility at $(E/N)^{(2)} = 0.8 \times \sqrt{6} \approx 2$ Td. From published tables,[30] the reduced mobility of protons in H_2 at this value field is $\mathsf{K}^{(2)} \approx 2.0\ \mathrm{V\,cm^2\,s^{-1}}$ and hence by Eq. (13),

$$\mathsf{K}^{(1)} = \sqrt{6} \times 2.0 \approx 4.9\ \mathrm{cm^2\ V^{-1}\ s^{-1}}$$

is the reduced mobility of μ^+ in H_2 at 0.8 Td. The procedure can obviously be repeated at other reduced fields for which H^+ mobilities are available.

This method could also be used to investigate the transport properties of μ^+ in He, by aliasing (H^+, He) mobility data,[31] as suggested by Taqqu[29] who, however, has used a different, purely empirical scaling procedure. This is a particularly interesting case because of the runaway phenomenon produced by the sharply falling cross section, but a detailed discussion is beyond the scope of the present paper. Viehland[33] has employed mass scaling equation (13) to calculate mobilities of isotopes of various ions in He, in the special case of zero field, where (15) is satisfied trivially. Although this lacks the generality of the aliasing procedure given above, it nevertheless is interesting to note that Viehland estimates mass scaling to provide zero mobilities accurate to four figures.

VI. CONCLUDING REMARKS

This paper expands on both fundamental and practical questions relating to the general, physically based ion and electron fluid formulation,[13] highlighting the pivotal and transparent role of the mean energy in the collision terms, and illustrating how these may be accurately evaluated through a "direct substitution technique," using swarm transport data alone, without the need for input of cross sections. Mean energy also plays a key role in the "aliasing" procedure reported here, to obtain otherwise unknown transport coefficients for one type of particle from known transport data for another type. Numerical examples have been given in all cases.

While a reasonably accurate, general, closed set of fluid equations exists for light particles, a corresponding formulation for heavier particles (ions) is still needed. Such formulations as presently exist are either (a) general but not closed (i.e., there are more unknowns than equations) or (b) closed but valid only in special cases, e.g., the weak density gradient, hydrodynamic limit, where closure is not a problem. In a paper which follows,[32] we obtain the required ion fluid equations, and thus complete the framework necessary for a general description of a partially ionized plasma.

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APPENDIX: OBTAINING MEAN ENERGY FROM EXPERIMENTAL DATA

The central role of the mean energy ε, both in interpreting swarm data and in the fluid equations themselves, has been emphasized in the text. Approximate estimates may be obtained directly from Einstein relation (7), or more accurately from the modified form,

$$\frac{D_T}{K} = F\frac{\varepsilon}{e}, \tag{A1}$$

where, as specified by Eq. (6-4-22a) and Table 6-4-1 of Mason and McDaniel,[6]

$$F \equiv \frac{2}{3}\left(1 + \Delta_T \frac{K'}{1+K'}\right) \tag{A2}$$

and

$$\Delta_T \equiv \frac{2}{3}\frac{K'}{K'+2}. \tag{A3}$$

The differential logarithmic mobility,

$$K' \equiv \frac{\partial \ln K}{\partial \ln E/N}, \tag{A4}$$

which is ubiquitous in the transport theory literature,[6,13] is obtainable directly from experiment as the slope of measured mobility vs E/N on a log-log plot. The empirical values of ε vs E/N thus obtained may be entered in column 4 of Table I.

Some ideas of the magnitude of the correction factors can be obtained by considering a number of special cases. For a constant elastic collision frequency, or for very weak fields, mobility is constant, i.e., $K' = 0$, the transverse correction factor $\Delta_T = 0$. Then F = 2/3 in Eq. (A1), and Eq. (7) is regained. Otherwise the correction factors may be significant, e.g., for a constant elastic cross section, $K' = -1/2$ at high fields, $\Delta_T = -2/9$ and by Eq. (9), $F = 22/27 = 0.81$ (cf, the exact value[6] of 0.76).

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