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The Effects of Anisotropic Scattering on Electron Transport

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Abstract

The recently developed theory of Lin *et al.* has been used to make a systematic study of calculated electron drift velocities and diffusion coefficients. Differences between the usual two-term solution and the converged results are calculated for a number of cases to demonstrate the effects of anisotropic scattering on the interpretation of swarm experiments.

1. Introduction

Transport coefficients determined in electron swarm experiments have usually been related to microscopic collision processes through solutions of Boltzmann's equation that are based on a two-term spherical harmonics representation of the electron velocity distribution function and matching approximations in the collision operator. Thus, the equation for the electron velocity distribution function, which may be written

$$f(\boldsymbol{v}) = f_0(v) + \sum_{l=1}^{\infty} f_l(v)\,\mathrm{P}_l(\cos\theta), \tag{1}$$

where θ is the angle between $\boldsymbol{v}$ and the electric field $\boldsymbol{E}$, is approximated by

$$f(\boldsymbol{v}) = f_0(v) + f_1(v)\cos\theta. \tag{2}$$

In many circumstances the errors in the transport coefficients calculated using this order of approximation have been shown to be less than experimental error (Braglia 1977; Milloy and Watts 1977), so that the additional complexity associated with the use of more rigorous theory (Lin *et al.* 1979) is usually not necessary. Nevertheless, general arguments have been used (see e.g. Ferrari 1977) to predict that there are combinations of circumstances for which first-order theory may prove inadequate, and later work has produced quantitative illustrations of these predictions (Kleban and Davis 1977, 1978; Lin *et al.* 1979; Reid 1979).

Reid's (1979) work provided a number of examples for isotropic scattering models, and it also demonstrated an enhanced failure of the first-order theory when the scattering is markedly anisotropic. Nevertheless, the Monte Carlo simulation technique he used, while providing valuable bench marks, is too time consuming and costly to be used for systematic surveys, and a number of questions remain to be

answered. Among these is the effect of anisotropy on transport coefficients calculated using first-order theory for low energy electron swarms in H_2 and CO.*

As noted by Reid (1979), the analysis of transport coefficients for these gases has led to unresolved inconsistencies between the results of beam and swarm experiments: in the case of hydrogen there is an unacceptable difference between the threshold behaviour of the $v = 0 \rightarrow 1$ vibrational excitation cross section (for a discussion see Crompton *et al.* 1970), while in the case of CO the two techniques yield different threshold characteristics (see e.g. Schulz 1964) and different overall magnitudes for the vibrational cross sections (Land 1978). For both gases, spot checks made by Reid at a few values of E/N (the ratio of electric field strength to gas number density), using cross sections that modelled the real cross sections, showed that the first-order analytical solution was likely to be adequate provided the scattering was isotropic, but that its use might lead to unacceptable errors in the calculated transport coefficients, at least in the case of CO, when account was taken of anisotropy. However, the problem could not be examined in sufficient detail to provide definitive conclusions.

The object of this paper is a more comprehensive study of the effect of anisotropic scattering on the interpretation of swarm experiments. Such a study has been made possible by the formulation by Lin *et al.* (1979) of a general solution of Boltzmann's equation. Their treatment provides the means of calculating the transport coefficients to any order of accuracy from 'real' cross section data, that is, from differential cross section data whose energy and angular dependences cannot be represented analytically.

The present work consists of three parts. In Section 2 the theory is applied to the calculation of the drift velocity v_{dr} and the perpendicular and parallel diffusion coefficients $D_\perp$ and $D_\parallel$ for one of the models studied by Reid (1979). Here, and in the other cases studied subsequently, comparisons are made between the 'converged' results, that is, results that do not vary as further terms are included in the series representation of the velocity distribution function, and the results obtained when the series is truncated at the second term, corresponding to the results of the usual first-order analysis. Thus, the work in this section parallels but extends Reid's work, with the difference that his 'converged' results were obtained from a Monte Carlo simulation. A comparison of the results where possible provides a test of the consistency of the two approaches.

In Section 3 we examine the effect of increasing anisotropy by using a model in which the total momentum transfer cross section and the total cross sections for inelastic scattering are those for H_2, but artificial anisotropy is introduced through angular dependences which vary as $\cos^n(\frac{1}{2}\theta)$ and $\sin^n(\frac{1}{2}\theta)$ to represent forward and backward scattering respectively. In this way we are able to demonstrate for a real set of integral cross sections the anisotropy required to introduce significant error in the transport coefficients calculated using conventional first-order transport theory.

In Section 4 we present data for H_2 calculated with realistic angular dependences, that is, with data based on the somewhat limited experimental results for angular

* Here we define 'low energy' as referring to swarms in which ionization plays a negligible role. When there is significant electron production (or loss) additional theoretical problems arise, unrelated to the two-term representation of the velocity distribution function, problems whose significance has been the subject of several recent papers (see e.g. Tagashira *et al.* 1977; Reid and Hunter 1979).

distributions in the energy range of our investigation. Finally, in Section 5, we discuss the implications of these results.

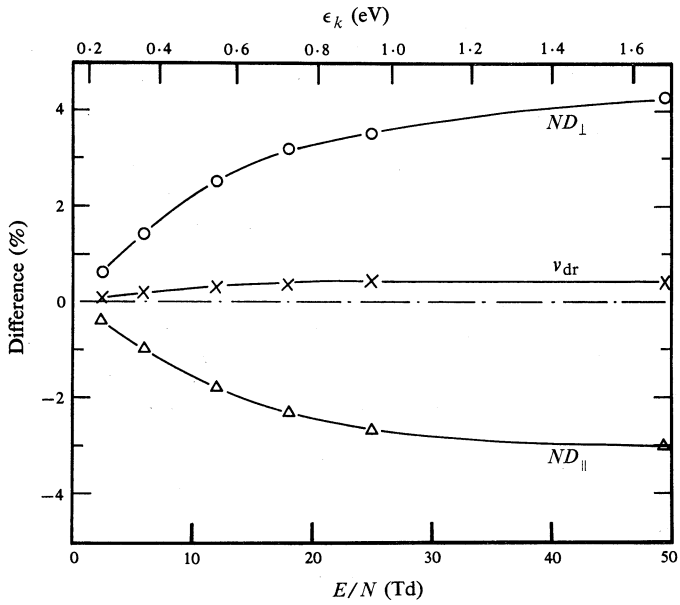

Fig. 1. Differences between the two-term and the converged results for the transport parameters shown, obtained using the cross sections of Reid's (1979) case C. (Differences are positive when the two-term result is the larger.)

2. Transport Coefficients calculated for Reid's Model

The model used in Section 4*b* of Reid's (1979) paper has the following characteristics:

$$\text{Neutral mass } M = 2 \text{ a.m.u.}$$

$$\text{Elastic momentum transfer cross section } \sigma_{m,e} = 10 \text{ Å}^2 \ (\equiv 10\times 10^{-20} \text{ m}^2)$$

$$\text{Total inelastic cross section } \sigma_i = 0{\cdot}4(\varepsilon-\varepsilon_i) \text{ Å}^2 \text{ for } \varepsilon \geqslant \varepsilon_i$$

$$\text{Inelastic threshold } \varepsilon_i = 0{\cdot}516 \text{ eV}$$

$$\text{Gas temperature } T = 0 \text{ K}$$

Four angular distributions for all scattering events were examined:

(A) $I(\theta) =$ constant (isotropic scattering);

(B) $I(\theta) = \cos^4\theta$;

(C) $I(\theta) = \exp\{-1{\cdot}5(1+\cos\theta)\}$;

(D) $I(\theta) = 1$ for $0 \leqslant \theta \leqslant 0{\cdot}134\pi$ and $0{\cdot}75\pi \leqslant \theta \leqslant \pi$,

$= 0$ otherwise.

The total elastic cross section was adjusted in cases C and D (where the scattering is asymmetric about $\frac{1}{2}\pi$) so as to maintain the elastic momentum transfer cross

section $\sigma_{m,e}$ at 10 Å^2. However, since the total inelastic cross section was the same in all cases, the total momentum transfer cross section σ was different (actually somewhat larger) in cases C and D (Reid 1979).

Fig. 1 shows that the differences between the two-term and the converged results become significant when an appreciable number of electrons in the swarm have energies which exceed the threshold energy for the inelastic process.

Table 1. Results for the four models (see text)
Values in parentheses are from Reid (1979)

v	v_{dr} (10^6 cm s^{-1})	kT_i (eV)	$D_\perp/\mu$ (V)	$D_\parallel/\mu$ (V)
		Model A		
2	5·2715 (5·27)	0·8216 (0·821)	0·9496 (0·950)	0·5000
3	5·2597	0·8200	0·9303	0·5096
4	5·2560	0·8200	0·9308	0·5095
5	5·2560 (5·26)	0·8200 (0·823)	0·9308 (0·930)	0·5095
		Model B		
2	5·2715 (5·27)	0·8216 (0·821)	0·9496 (0·950)	0·5000
3	5·2440	0·8178	0·9064	0·5221
4	5·2447	0·8178	0·9080	0·5216
5	5·2447 (5·24)	0·8178 (0·819)	0·9080 (0·905)	0·5217
		Model C		
2	5·1844 (5·27)	0·8145 (0·821)	0·9465 (0·950)	0·4857
3	5·1650	0·8119	0·9162	0·5004
4	5·1655	0·8119	0·9174	0·5001
5	5·1655 (5·13)	0·8119 (0·811)	0·9174 (0·935)	0·5002
		Model D		
2	5·1844 (5·27)	0·8145 (0·821)	0·9465 (0·950)	0·4857
3	5·1341	0·8075	0·8711	0·5234
4	5·1367	0·8076	0·8772	0·5218
5	5·1365 (5·12)	0·8076 (0·807)	0·8771 (0·876)	0·5218

In Table 1 we give our results together with Reid's for all four cases at $E/N = 25$ Td ($\equiv 25 \times 10^{-17}$ V cm^2) to enable a direct comparison to be made. In the first column is the number of Legendre polynomials retained in the calculations, indicated by v. The row for $v = 2$ thus contains the transport coefficients calculated with the usual two-term (i.e. first-order) approximation. The convergences of the results are apparent as v increases from 2 to 5. The values in parentheses are those given by Reid. The accuracies of our calculated transport coefficients for these models are 0·1% for v_{dr} and kT_i (the average electron energy is given by $\frac{3}{2}kT_i$) and 0·2% for $D_\perp$ and $D_\parallel$. In the case $v = 2$, Reid's results were obtained using Gibson's (1970) code based on a solution of Boltzmann's equation due to Holstein (1946; see also Frost and Phelps 1962); these calculated values of v_{dr} and $D_\perp$ are subject to computational errors of less than 0·2%. Reid's Monte Carlo results are shown against the entries for $v = 5$. Errors in the Monte Carlo results for v_{dr} and kT_i were estimated to be less than 1%, and in $D_\perp$ less than 2%.

Apart from the results for v_{dr} and kT_i for $v = 2$ in cases C and D, the agreement with Reid's results are within mutual uncertainties. The enhanced inaccuracy of the two-term results due to anisotropy which Reid noted is confirmed.

The discrepancies between Reid's two-term results and the present ones for cases C and D are due to approximations inherent in the usual application of Holstein's (1946) equation that are not made in the approach of Lin *et al.* (1979). When the scattering is significantly asymmetrical about $\frac{1}{2}\pi$, as in cases C and D, the 'equivalent' momentum transfer cross section that appears in Holstein's equation (see e.g. Reid 1979) may differ significantly from the sum of the momentum transfer cross section for elastic scattering and the *total* inelastic scattering cross sections (contrary to the normal assumption). Thus, the use of an equivalent cross section calculated in this way may lead to significant error in the two-term result, in addition to that which arises from the inadequate representation of the velocity distribution function by the truncated spherical harmonics expansion.

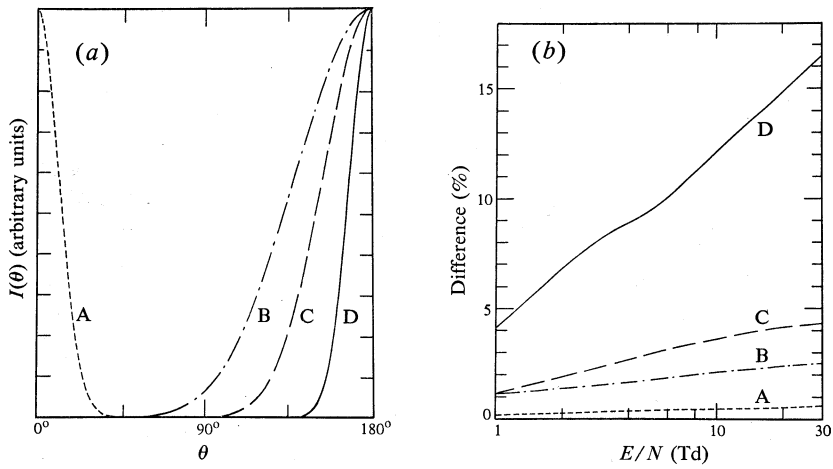

Fig. 2. (*a*) Angular distributions used in the calculation of the transport parameters in (*b*). The curves labelled A, B, C and D correspond to $I(\theta) = \cos^{99}(\frac{1}{2}\theta)$, $I(\theta) = \sin^{8}(\frac{1}{2}\theta)$, $I(\theta) = \sin^{20}(\frac{1}{2}\theta)$ and $I(\theta) = \sin^{99}(\frac{1}{2}\theta)$ respectively. (*b*) Differences between the two-term and the converged results for the transport parameter $ND_\perp$ in 'hydrogen' using a variety of angular distributions, corresponding to those shown in (*a*). (Differences are positive when the two-term result is the larger.)

3. Hydrogen with Artificial Angular Distributions

Fig. 2*a* shows a variety of anisotropies which were introduced into the angular distributions for all scattering channels. Fig. 2*b* presents the results of comparisons of the two-term and converged results for $ND_\perp$ in 'hydrogen' using these anisotropies. The largest changes are seen as the degree of backward scattering is increased, i.e. as n increases with angular distributions of the form $\sin^n(\frac{1}{2}\theta)$. The calculations with isotropic angular distributions show no significant differences.

More specifically, the maximum differences for the calculated values of $ND_\perp$ in the range $1 \leqslant E/N \leqslant 30$ Td increase from approximately 3% for angular distributions of the form $\sin^8(\frac{1}{2}\theta)$ (curve B) to 15% for those of the form $\sin^{99}(\frac{1}{2}\theta)$ (curve D). It should be noted that for the strong forward scattering case $\cos^{99}(\frac{1}{2}\theta)$ (curve A) the differences are only of order 0·5%.

In most cases the values for the drift velocity calculated using the two-term and multiterm solutions are not significantly different. The largest difference is again seen in the backscattering case but is only of order 1%.

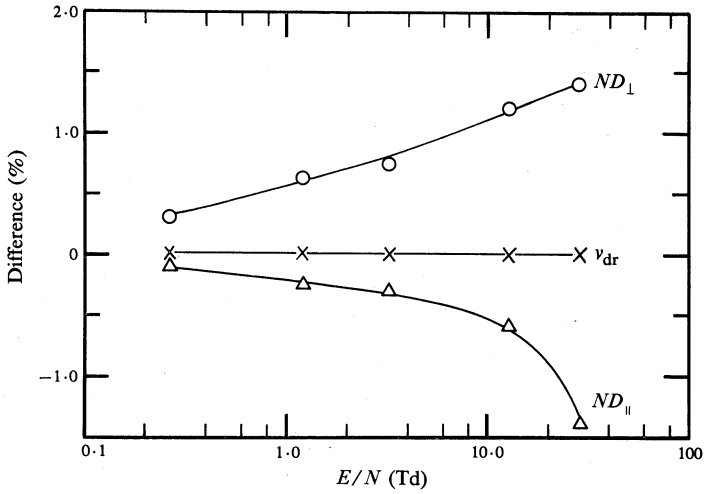

Fig. 3. Differences between the two-term and the converged results for the transport parameters in hydrogen with realistic angular distributions for elastic scattering. (Differences are positive when the two-term result is the larger.)

4. Hydrogen with Realistic Angular Distributions

Fig. 3 shows the differences in the values of ν_{dr}, $ND_\perp$ and $ND_\parallel$ in hydrogen for $0{\cdot}3 \leqslant E/N \leqslant 30$ Td, which have been calculated using the two-term and multiterm solutions of the Boltzmann equation and realistic angular distributions for elastic scattering.

Angular distributions for elastic scattering in hydrogen at several energies have been published by Linder and Schmidt (1971). The angular distributions at the energies required for our calculations were determined from linear interpolations of these data. For all the inelastic processes the angular distribution for the $v = 0 \rightarrow 1$ vibrational excitation process at 4·5 eV (taken from Linder and Schmidt) was used. The choice of a representative angular distribution was permissible as the results were found to be insensitive to this choice.

In Fig. 3 the calculations show no significant difference in the drift velocities calculated using the two methods, but differences of up to 1·5% in $ND_\perp$ and $ND_\parallel$.

Estimates of the errors arising from the use of the two-term solution may be obtained from the formulae given by Lin *et al.* (1979). We have in fact calculated the predicted differences according to these formulae and compared them with the differences between the two-term and converged results. The predictions of errors in the calculation of the drift velocity are remarkably accurate (for example, −0·7% from the prediction formula and −0·5% from the calculations), but are somewhat less reliable in the case of the diffusion coefficients.

5. Conclusions

From the work described in this paper we are able to draw the following conclusions:

(1) The more extensive calculation we have been able to make with one of Reid's (1979) models has confirmed the general conclusions he reached with regard to both

the magnitudes of the errors in the transport coefficients calculated using the two-term approximation and their dependence on the degree of anisotropy in the scattered distribution.

(2) From calculations based on a set of integral cross sections for hydrogen assembled from presently available experimental and theoretical data, but with arbitrarily chosen angular distributions for the scattered electrons, it has been shown that back scattering is responsible for much larger errors than forward scattering when the same degree of anisotropy is assumed. The calculations have also indicated how anisotropic the scattering must be in order to introduce significant error into the two-term results in this case.

(3) The calculations for hydrogen based on realistic angular scattering distributions for the elastic channel have shown that small ($<2\%$) but significant errors result from the use of the two-term approximation in the range $0 < E/N \leqslant 30$ Td. This is the range of E/N used to determine the threshold behaviour of the $v = 0 \rightarrow 1$ vibrational excitation cross section in hydrogen (Crompton *et al.* 1970). The transport data will thus require reanalysis to eliminate the small errors that have been introduced by using the conventional analysis. Since the values of $D_{\perp}/\mu$ calculated using the multiterm analysis are lower than the two-term results, the vibrational cross section will have to be lowered to restore agreement with experiment. Unfortunately this will enhance rather than diminish the disagreement between the beam and swarm results.

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