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Negative differential conductivity of positrons in gases

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ABSTRACT

This paper reports on a new series of calculations of positron transport properties based on current experimental cross section data. It is found that negative differential conductivity (NDC) occurs in the bulk drift velocity W but not the flux drift velocity w. The origin of the phenomenon lies in the "reactive" nature of positron collisions associated with positronium Ps formation, and is quite different in origin to the better known NDC effect in w arising from certain combinations of inelastic–elastic cross sections. Moreover, while the Ps formation process is qualitatively similar (at least from a kinetic theory perspective) to electron attachment, it is characterized by a cross section several orders of magnitude larger and hence the "reactive" NDC effect is correspondingly more pronounced. In this paper we test both established conditions for NDC, and develop new criteria, using simple mathematics and physical arguments where possible.

1. Introduction

Negative differential conductivity (NDC) can be defined as decrease of the drift velocity of charged particles (e.g. electrons, positrons) with increasing driving field. In general conductivity is a product of drift velocity and number density but changes in the number density are controlled by a number of phenomena mostly losses that are geometry dependent while the drift velocity itself is only controlled by the electron distribution function (EDF) and thereby is more fundamental and not a subject of particular properties of the system. Thus in fundamental studies the definition of NDC is confined to the dependence of the drift velocity on E/N only. In what follows we take a system of coordinates in which the z-axis is defined by the direction of the field $\boldsymbol{E}$.

NDC for electrons has been carefully investigated in the last two decades [1–4]. The reason for this is two-fold. On the one hand a number of applications are dependent on it while on the other it can cause undesirable instabilities. For example, the effect is important in gas discharges and for the operation of different kind of lasers. However, it also affects strongly the energy transferred to the plasma by Joule heating.

The conditions for NDC of electron swarms in gases summarized by Petrović et al. [1] and by Robson [3] are the following:

(1) Inelastic processes are necessary.
(2) NDC is favored by increasing momentum transfer cross section.
(3) Decreasing inelastic cross section favors NDC.
(4) Occurrence of NDC depends on relative magnitude of factors (2) and (3), with the precise criterion being given by Eq. (19) of Robson [3].
(5) Superelastic processes will have a tendency to reduce the NDC.

The drift velocity to which these conditions refer is the so-called flux drift velocity w which belongs to that family of transport coefficients defined through flux-gradient equations, in this case, Fick's law. It is also the spatially uniform average velocity, $w = \langle v_z \rangle$. The other type of drift velocity is the so-called bulk drift velocity, W, which belongs to that family of transport coefficients defined through the diffusion equation. It is the time derivative of the center-of-mass of the swarm, i.e. $W = d\langle z \rangle/dt$, where now the average is carried out over space. The two drift velocities differ whenever reactive, non-conservative (with respect to particle number) collisions occur, to a degree determined by the magnitude and energy-dependence of the reactive collision cross section. The difference is more than one of principle, for it is only W which is normally measured in experiments, not w.

Vrhovac and Petrović [4] have pointed out that there are some situations when bulk drift velocity may show NDC when flux drift

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velocity does not. This study was done specifically with electron attachment in mind, and NDC was found to occur only when flux drift velocity almost satisfies the criteria for NDC or at least a plateau in the drift velocity dependence is observed. Given the much larger magnitude of Ps formation cross sections, and the renewed interest in positron behaviour in gases, these calculations now assume a far greater significance.

We have used our new Monte Carlo (MC) code to investigate the transport of positrons in gases, particularly in argon, molecular nitrogen and hydrogen [5–7]. Positrons interactions with atoms and molecules are fundamentally different from those of electrons [8]. The first obvious difference is the absence of the resonance for positrons in nitrogen [6] which leaves very small non-resonant vibrational excitation and also a smaller number of electronic states that may be excited by positron impact. Second, the Ps formation channel, a non-conservative process not present for electrons has a significant cross section for positrons. In fact it can be several orders of magnitude larger than those for the equivalent process of dissociative electron attachment for electrons. The nature of ionization is also different as for positrons it is not a non-conservative process. The most striking feature of our observations was that negative differential conductivity (NDC) is observed in the bulk drift velocity even when the flux drift velocity does not show any signs of NDC. It was shown that the bulk drift velocity NDC is result of the non-conservative nature of Ps formation [5]. Here we check how the manifestation of NDC in positron transport fares against the previously mentioned theoretical conditions for NDC [1,3,4] and use our current results as a guide for modifying those conditions.

2. Monte Carlo results

All drift velocities presented here were calculated by MC simulations, which also produced rates of processes, particularly rates of Ps formation. Data for argon and nitrogen were presented earlier [5,6] while data for hydrogen will be presented later. First, we analyze whether the standard formula defining the difference between the bulk and flux properties [9] works well in this case. The formula is:

$$W = w - \frac{2\varepsilon}{3e}\frac{d\nu_{PF}}{dE}, \tag{1}$$

where ν_{PF} is the positronium formation rate, ε is the mean energy, e is the elementary charge and E is the electric field. We start from the MC flux drift velocity and add to it the second term from this equation where we apply the MC determined rates of Ps formation. The comparisons are presented in Fig. 1.

As can be seen, we obtained a qualitatively good agreement. The best is, of course, for N_2 but that is where the perturbation of the swarm by Ps formation is the weakest.

The next thing to investigate is if our calculated drift velocities satisfies the NDC criteria developed by Vrhovac and Petrović [4] which was the first to consider NDC due to reactive collisions. In the case of positrons the Ps formation takes the role of attachment. The criterion is given as

$$\frac{dW}{dE} = \frac{dw}{dE} - \frac{1}{e}\frac{2}{3}\left[\frac{d\varepsilon}{dE}\frac{d\nu_{PF}}{dE} + \varepsilon\frac{d^2\nu_{PF}}{dE^2}\right] < 0. \tag{2}$$

The region where the drift velocity falls and the predictions of the criterion coincide. The agreement is better for the onset than for the end of the range but overall the qualitatively prediction is good. It is worth checking whether conditions match those from Petrović et al. [1] or from Vrhovac and Petrović [4]:

$$1 + \frac{\frac{2}{3}\varepsilon\nu_1^{(PF)}}{\nu_{el}} + \varepsilon\frac{d}{d\varepsilon}\left[\frac{\frac{2}{3}\varepsilon\nu_1^{(PF)}}{\nu_{el}}\right] < 0. \tag{3}$$

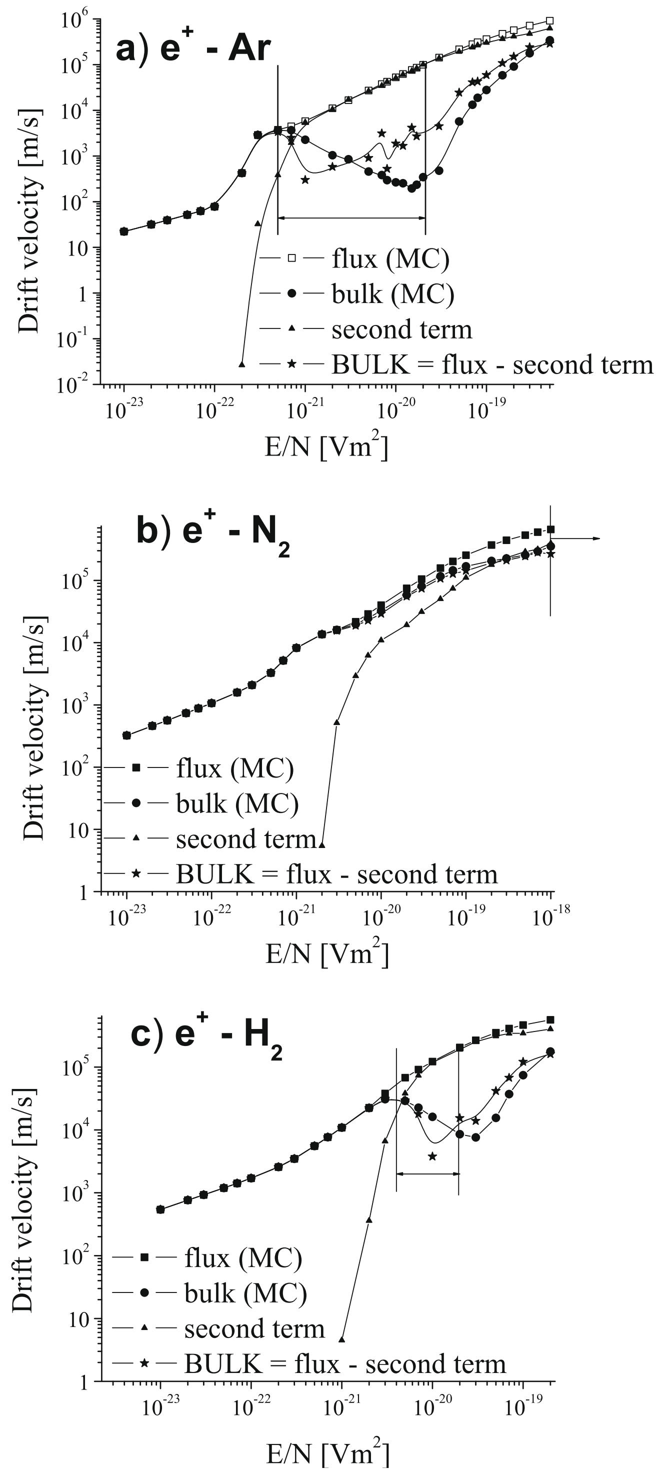

Fig. 1. Comparison between bulk drift velocities calculated using our MC code and predicted by Eq. (1) for positron transport in pure (a) argon [5], (b) nitrogen [6] and (c) hydrogen [7]. The calculations of the bulk drift velocity W were made both directly from MC and by modifying the results of Eq. (1) with calculated Ps formation rates. We also show as vertical lines the ranges of NDC predicted on the basis of the condition given by the Eq. (2).

Both for the flux drift velocity give any prediction of NDC, and in all cases there is no NDC according to these formulae. In Eq. (3) ν_{el} is the rate for elastic collisions while $\nu_1^{(PF)}$ represents the first derivative of the rate for Ps formation with respect to the mean energy. The NDC effect for positron is only for the bulk drift velocity when flux drift velocity is far from satisfying the condition.

In case of electrons it is well known fact that if NDC exist it must be seen in velocity space [4,2]. For positrons it was observed that this criterion is never satisfied.

3. Fluid equation analysis

In this section we apply the fluid equations developed in [9] to study positronium formation and to complement the numerical results obtained from MC analysis. Here the emphasis is on physical understanding, rather than on quantitative analysis, and to this end, we consider the simplest of interaction models, namely a constant elastic momentum transfer collision frequency ν_m and a 'reactive' positronium formation rate which has constant amplitude b above the positronium formation threshold ϵ^* and is zero everywhere else. Inelastic collisions are considered negligible. The analogous case of electron attachment was modelled in a somewhat different reactive collision frequency in [9], but many of the results obtained there can be carried over to the present problem.

In what follows, we concentrate on phenomenology and the more interesting aspects of the NDC phenomena predicted by the MC results, rather than providing any detailed mathematical justification. That will be left to a subsequent publication dealing with kinetic and fluid modelling of reactive effects associated with positrons in gases.

3.1. Drift velocities

For a constant elastic collision frequency model, and assuming

$$\frac{2\varepsilon}{3}\frac{\nu_*'}{\nu_m} \ll 1 \ll \frac{2\varepsilon}{3}\frac{\nu_*'}{\nu_e}, \tag{4}$$

where ν_*' denotes the derivative of the average positronium formation rate with respect to mean positronium energy ε, and $\nu_e = \frac{2m}{m_0}\nu_m$ is the collision frequency for energy transfer, the positron flux drift velocity is given by Robson [9], Eq. (5.53a):

$$w = \frac{eE}{m\nu_m}. \tag{5}$$

Since $w \propto E$ in this model, it is sometimes convenient to use w rather than E as the independent variable. In what follows we use the general reactive energy balance equation ([9], Eqs. (4.28b) and (4.29)) for zero gas temperature and negligible inelastic collisions,

$$\frac{1}{2}m_0 w^2 = \varepsilon + \frac{2\varepsilon^2}{3}\frac{\nu_*'}{\nu_e}, \tag{6}$$

and the general relationship between positron bulk and flux drift velocities ([9], Eq. (5.56)):

$$\frac{W}{w} = 1 - \frac{2\varepsilon}{3ew}\nu_*'\frac{d\varepsilon}{dE}, \tag{7}$$

to obtain

$$\frac{W}{w} \approx \frac{d\varepsilon}{d(\frac{1}{2}m_0 w^2)} \approx \left(1 + \frac{4\varepsilon}{3}\frac{\nu_*'}{\nu_e}\right)^{-1}. \tag{8}$$

To make matters concrete we now discuss results for the step function collision frequency model. In this case, the *average* collision frequency is approximated by

$$\nu_* = bS(\xi), \tag{9}$$

where

$$S(\xi) = (1+\xi)e^{-\xi}, \tag{10}$$

is the "smoothing" function introduced in [3], and $\xi \equiv \frac{3\epsilon_*}{2\varepsilon}$. In this case

$$\varepsilon\nu_*' = b\xi^2 e^{-\xi}, \tag{11}$$

increases from zero at very low mean energies, through to a maximum at $\xi = 2$, corresponding to a mean energy $\varepsilon = \frac{3\epsilon_*}{4}$, and then falls as ε increases above threshold. In other words, well below or well above the threshold energy ϵ^*, ξ is either very large or very small respectively, and $\nu_*' \to 0$ in both cases. In these extremes, reactive effects are small, $\frac{d\varepsilon}{d(\frac{1}{2}m_0 w^2)} \approx 1$ and hence $W \approx w$ as expected. In the intermediate region, however, $\varepsilon\nu_*'$ attains a maximum, and both

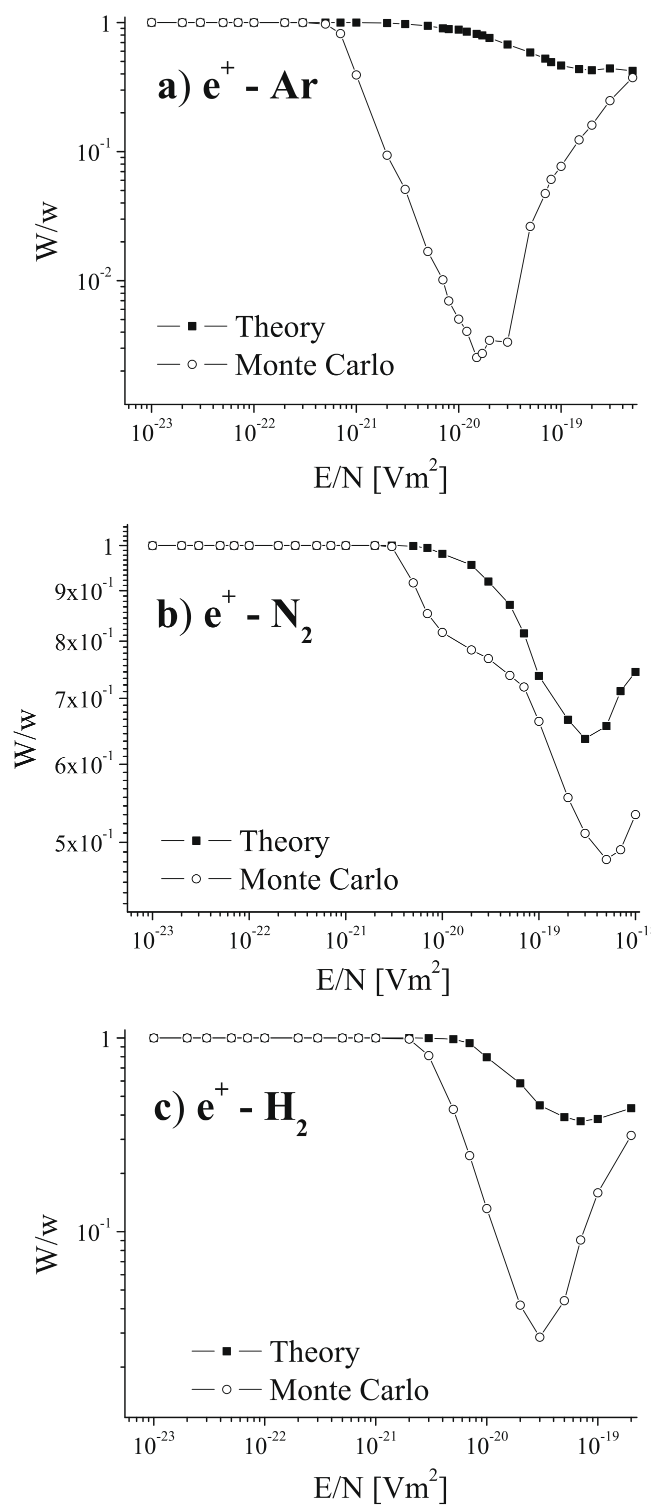

Fig. 2. Ratio between bulk and flux drift velocities: comparison between MC results and theoretical predictions for positron transport in (a) argon, (b) nitrogen and (c) hydrogen.

the variation of mean energy with field and the ratio of bulk to flux drift velocity reach their minimum values here, according to Eq. (8). This is consistent with the MC results which show that the "flat" region of ε versus E/N corresponds to the region of maximum NDC (see Fig. 2).

The comparison of this theory and the MC results is shown through plotting the ratio of the bulk and flux drift velocity. While one could claim that the agreement is far from perfect it is actually very good as the prediction of onsets of the effect of non-conservative processes on drift velocity is given accurately by the theory. Thus the theory contains the basic properties leading to the observed bulk NDC. On the other hand and as it was mentioned in our previous paper [5] the quantitative agreement is affected by the fact that the spatial profile of the swarm is seriously skewed by the Ps formation, which could not be accounted for in the momentum transfer theory. Thus the agreement for N_2 is the best as the spatial profile in that case is not affected considerably. The same is true for the applicability of Eq. (1) as shown in Fig. 1.

3.2. Diffusion coefficients

Generalized Einstein relations for $D_\parallel$ and $D_\perp$ including reactive effects are given by Eqs. (5.33 a,b) of [9], and for the constant elastic collision frequency model these give

$$\frac{D_\parallel}{D_\perp} = \frac{\partial \ln W}{\partial \ln(E/N)} = 1 + \frac{\partial \ln K}{\partial \ln(E/N)}, \tag{12}$$

where $K = W/E$ is the bulk mobility coefficient. This is the same result as obtained for purely conservative collisions, and suffers from the same defect in the case of NDC when $\frac{\partial W}{\partial (E/N)} < 0$, namely, it implies a negative diffusion coefficient and violation of the second law of thermodynamics [3]. The origin of this problem goes back to the assumption in [9] of neglecting heat flux in the energy balance equation. In [3], it was shown that if this term is included, then the generalized Einstein relations yield

$$\frac{D_\parallel}{D_\perp} = 1 + (1+\Delta)\frac{\partial \ln K}{\partial \ln(E/N)}, \tag{13}$$

where

$$\Delta \approx \frac{3Q}{4\varepsilon W}, \tag{14}$$

and Q is the heat flux per particle. This correction term preserves the physical integrity of the generalized Einstein relations and also furnishes a reasonably accurate representation of $\frac{D_\parallel}{D_\perp}$ which, while remaining above zero, nevertheless falls very sharply in the NDC region (see Fig. 4 of [3]). It is thus not surprising that MC simulation shows that $\frac{D_\parallel}{D_\perp}$ falls dramatically when NDC occurs. It might be said that this, like the "flat" region of mean energy variation, is a signature of NDC for positronium formation.

4. Conclusion

In this paper we analyze how the theory of negative differential conductivity works for the case of positrons in gases. The standard form of conditions does not predict NDC as that form is applicable to flux properties only. However if non-conservative collisions are included the conditions work well in predicting the onset of NDC and to some degree its range as well as the ratio of bulk and flux drift velocity. The good qualitative agreement may be followed by a good and more detailed quantitative agreement in all aspects only if major skewing of the spatial profile as shown in [5] is accounted for. However, this would make the theory very complicated and would necessarily lead to numerical rather than analytic calculations for which MC simulations are better suited and accurate.

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