Recent advances in studies of positron swarms in electric and magnetic fields in gases

A. Banković
Institute of Physics, University of Belgrade, Pregrevica 118, POB 68, Zemun, Serbia
ana.bankovic@gmail.com

Abstract. A Monte Carlo simulation technique has been used for the calculation of positron transport properties in neutral gases under the influence of electric and magnetic fields. The high magnitude of the cross section for positronium (Ps) formation process comparing to other collisional processes and its strong energy dependence are two major factors for the development of many interesting kinetic phenomena observed in the positron transport. One of the most striking phenomena is the existence of negative differential conductivity (NDC) in the bulk drift speed component and the absence of any sign of this phenomenon in the profile of the flux component. Along similar lines we have observed that the differences between the flux and bulk components of various transport coefficients, originating from the non-conservative nature of Ps formation, are much higher than those observed for electrons. The influence of magnetic field in a crossed field configuration ($E \times B$) is also investigated. Due to the presence of a magnetic field the number of transport coefficients is increased. Since the longitudinal and transverse components of the drift velocity exhibit different sensitivities with respect to the magnetic field strength, it is found that the NDC effect in a crossed field configuration can be controlled by the magnetic field. The magnetic cooling effect has also been observed – the mean energy of the swarm is a decreasing function of the magnetic field for all electric field strengths considered in this work. In that sense, positrons behave in exactly the same way as electrons. The results of the Monte Carlo simulations are compared with those obtained by the multi-term theory for solving the Boltzmann equation. The excellent agreement between these two entirely independent techniques supports the numerical integrity of our Monte Carlo code.

1. Introduction
Positrons have applications in many research areas ranging from gamma-ray astronomy to biomedicine. In the last few decades there has been growing interest for studying positrons both theoretically and experimentally [1]. One of the major motivational factors for this was the revolutionary improvement of buffer-gas, Penning Malmberg traps for positrons made by Surko and co-workers [2, 3]. The improved positron traps have provided high-flux, low-energy positron beams and thus the new era of positron physics was born. The first response came from the atomic physicists with the provision of accurate cross sections for positron interactions with different gases [4-7], which has opened the possibility to model the transport processes of positrons in neutral gases and soft-condensed matter [8-10, 11], with the principal idea of improving the positron based technologies such as those employed in positron emission tomography. In this paper we investigate the transport properties of positron swarms in neutral molecular gases in a crossed electric and magnetic field configuration. We investigate the positron transport in crossed electric and magnetic fields as possible applications may use combined fields to achieve a better control of properties of the ensemble. It is
well known from the recent comprehensive electron studies that the transport properties of electrons can be significantly affected by the magnetic field, particularly under conditions when the cyclotron frequency dominated the collision frequency \([12]\). Using these arguments as a background, we have been motivated to check the basic features of positron transport in electric and magnetic fields.

In calculations of transport coefficients it is necessary to have a complete set of cross sections \([13]\). In Figure 1 the compilation of the best theoretical \([14 – 16]\) and experimental \([17 – 19]\) cross sections for positrons in hydrogen available from the literature is given. There are three main differences between electron and positron interactions with matter. First, the absence of the resonances for positrons leaves a very small non-resonant vibrational excitation. Second, the absence of the exchange interactions leads to a smaller number of electronic states that can be excited by positron impact. Finally, the Ps formation channel, a non-conservative process unique to positrons, often has a significant cross section.

![Figure 1: Complete cross section set for positrons in hydrogen](image)

The transport properties of positron swarms moving in neutral gases have been studied using a multi-term theory for solving the Boltzmann equation \([20]\) and a Monte Carlo simulation technique \([21]\). Both techniques have been developed for studying the electron swarms in varying configurations of electric and magnetic fields under hydrodynamic and non-hydrodynamic conditions. Numerical codes have passed all well-established benchmarks with high accuracy levels. In the framework of recent positrons studies, however, special attention has been paid to the correct treatment of positronium (Ps) formation. Ps formation is a non-conservative process unique to positrons which often has a cross section larger than the cross sections for elastic and various inelastic collisions and as a consequence it selectively removes the higher energy positrons. The kinetic effects induced by the non-conservative nature of collisions manifest themselves as a difference between the flux and bulk transport properties \([22]\). This duality is an inherent property of all transport coefficients, although it has been systematically ignored for many years in plasma modeling community and related electron studies. The flux transport properties, which are input parameters in fluid plasma models, are defined through the flux-gradient relation and they can be calculated from the spatially uniform average quantities. These quantities are not measurable. On the other hand, bulk transport properties, quantities measurable in swarm-type experiments, are defined through diffusion equation and they can be calculated as the rate of changes of the appropriate averages of the positions of the swarm particles, in the configuration space. The difference between flux and bulk transport coefficients exists only if the number of particles in the swarm changes with time. The differences between the flux and bulk transport properties observed in positron transport are often more pronounced than those for electrons, particularly for those gases with a large Ps formation cross-section. One of the most important kinetic phenomena observed both in electron and positron transport is negative differential conductivity (NDC). This phenomenon can be defined as a decrease in drift velocity of the swarm with increasing...
driving electric field. Both the nature and the manifestation of this phenomenon are different for electrons and positrons. In case of electrons [23-25], NDC is present in both the flux and bulk velocity components while for positrons it has been observed only in the bulk drift velocity. The differences between flux and bulk drift velocities can be more than two orders of magnitude [8-10], while for electrons they are generally 15-20% [12, 20]. Also, NDC is much more pronounced for positrons than for electrons and it originates purely from the non-conservative nature of Ps formation. The interesting situation occurs when the inelastic channels start to open in the vicinity of the threshold of Ps formation. Sometimes, for example in nitrogen [9], the competition between these channels leads to the disappearance of NDC, even though the cross section for Ps formation is as high as it is for the gases with very pronounced NDC. In what follows these issues are illustrated and discussed for positrons in molecular hydrogen and water vapour.

2. Negative differential conductivity (NDC)

The most interesting kinetic effect in positron transport is the existence of the negative differential conductivity (NDC). It represents a decrease in the drift velocity with increasing external electric field. In positron transport this effect appears only in the bulk drift velocity profiles. It has been shown that the origin of the phenomenon lies in the non-conservative nature of positron collisions associated with Ps formation [8] and is quite different in origin to the better known NDC effect in electron transport [23 - 25]. In Fig. 2 we show the bulk and flux drift velocities for both positrons and electrons in molecular hydrogen. In this energy range for electrons in molecular hydrogen the flux and bulk drift velocities are the same, which means that the effects of non-conservative processes are insignificant. On the other hand, the flux and bulk drift velocities for positrons are markedly different, in both quantitative and qualitative way. The maximum difference is of the order of magnitude, similar as for positrons in argon [8], and it is interesting to note that such a huge difference between two types of transport properties has never been observed in electron transport. The NDC effect in bulk drift velocity is well pronounced for positrons, with no sign of it in the profile of the flux velocity.

There is nothing in our experience with electrons that could prepare us for this situation: strong bulk NDC with no sign of flux NDC. We used a standard formula defining the difference between the flux and bulk properties to see if it works well for positrons [25]. The formula is

\[ W = w - \frac{2\epsilon}{3e} \frac{d\nu_{PP}}{dE}, \]  

where \( \nu_{PP} \) is Ps formation rate, \( \epsilon \) is the mean energy, \( e \) 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 comparison is presented in Figure 3. As can be seen we obtained a qualitatively good agreement.

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).
Another criteria against which we tested our results is NDC criteria developed by Vrhovac and Petrović [25], which was the first to consider NDC due to non-conservative collisions. The formula is

\[
\frac{dW}{dE} = \frac{d\nu}{dE} - \frac{1}{e} \left[ \frac{dE}{d\nu} \frac{d\nu_{PF}}{dE} + e \frac{d^2\nu_{PF}}{dE^2} \right] < 0 .
\] (2)

It predicts the region where the drift velocity falls. In Figure 3 this region is marked by vertical lines and we can say that the agreement is better for the onset than for the end of the range but overall the qualitatively prediction is good. In case of electrons it is well known fact that if NDC exist it must be seen in velocity space [25]. For positrons it was observed that this criterion is never satisfied.

![Figure 3: Comparison between bulk drift velocities calculated using our MC code and predicted by Eq. (1) for positron transport in pure hydrogen [27].](image)

3. Transport in a crossed field configuration

The number of transport properties in crossed electric and magnetic field configuration is increased comparing to the case of pure electric field. The drift velocity has two components: the longitudinal \( w_E \) and transverse \( w_{E \times B} \) which behaves in a different manner. If a swarm of positrons is drifting under the influence of electric field only, then the diffusion tensor has three non-zero diagonal elements: one longitudinal component and two transverse components which are by symmetry equal. In a crossed electric and magnetic field configuration there are five non-zero elements of the diffusion tensor. First, there are three diagonal diffusion elements along the \( E \) (\( D_E \)), the \( E \times B \) (\( D_{E \times B} \)), and \( B \) direction (\( D_B \)), respectively. Second, there are also two individual off-diagonal elements which are not the same, but experimentally can not be individually measured. They form the so-called Hall diffusion coefficient and are responsible for the existence of the fluxes known as the Hall current which is experimentally detectable.

3.1. Is there NDC in \( E \times B \) fields?

As emphasized previously, when both the electric and magnetic fields are present, the drift velocity has two components: the longitudinal drift velocity component describes the drift along the electric field direction while the transverse component describes the drift along the \( E \times B \) direction. Therefore, the drift can now be represented in terms of a drift speed and its direction is at some angle to the electric field (magnetic deflection angle). An interesting question arises: how does the magnetic field affect the drift speed under conditions when the cyclotron frequency is much less, of the same order, and much greater than the collision frequency? Figure 4 displays the flux and bulk components of the drift speed as a function of \( E/N \) for different values of \( B/N \) in these different regimes for positrons in
molecular hydrogen. NDC effect has disappeared from the profiles for non-zero magnetic fields. This behavior has been explained in [28]. The longitudinal and transverse components of the drift speed behave in completely different manner so they have to be examined separately. The easiest way to explain the absence of NDC effect in the profiles of the drift speed is by looking at the profiles of the magnetic deflection angle (see Fig 3 of [28]). For B/N of 100 Hx, the flux magnetic deflection angle stays around 45º for the entire range of E/N considered, while the bulk value goes to 90º in the energy region where the Ps formation channel is open. In the energy region where NDC exists for magnetic field free case, for the non-zero magnetic field profiles, the behavior of the drift speed is dominated by the component along the $\mathbf{E} \times \mathbf{B}$ direction. This is the unique situation where due to the nature of collisions the flux and bulk drift velocities differ not only in magnitude, but also in direction.

| $E/N$ [Td] | $0$ Hx | $100$ Hx | $500$ Hx |
|------------|--------|---------|---------|
| $0$        | 100    | 100     | 100     |
| $100$      | 100    | 100     | 100     |

**Figure 4**: Drift speed of a positron swarm in molecular hydrogen as a function of $E/N$ for various B/N. Flux values are represented by full lines and symbols, and bulk by dashed lines and open symbols.

At this point we asked ourselves a question: can these effects be predicted by using the concept of effective field? The basics of this concept have been given in [29]. We used the Tonks’ theorem to calculate effective electric field:

$$E_{\text{eff}}(\varepsilon) = E\sqrt{1 + \left(\Omega / \nu_m \right)^2 \cos^2 \Psi \over 1 + \left(\Omega / \nu_m \right)^2}.$$  \hfill (3)

Using this effective field we have iteratively calculated the mean energy of the swarm, $\varepsilon$, and the drift velocity $W$:

$$\varepsilon(E, B, \Psi) = \varepsilon(E_{\text{eff}}, 0, 0)$$  \hfill (4)

$$W(E, B, \Psi) = W(E_{\text{eff}}, 0, 0)$$

since equations (3) and (4) represents a system of non-linear equations.

In Fig. 5 the differences between flux and bulk components of the drift speed are compared for $\mathbf{E} \times \mathbf{B}$ configuration, and the effective field approximation case (Tonks’ theorem – dashed lines) for positrons in water vapour. We may observe that effective field concept predicts much larger differences between two components of the drift speed. This is more evident for higher values of magnetic field. The lesson from this is that the concept of effective field is not generally appropriate for studying positron transport.
3.2. On diffusion of positrons in gases

In this section we investigate the influence of the non-conservative nature of the Ps formation process on the diagonal elements of the diffusion tensor and also the effects induced by the presence of the magnetic field in a crossed field configuration. Generally speaking, it is hard to fully understand the behavior of diffusion coefficients in electric and magnetic fields since many parallel factors affect them significantly. Among these factors are those associated with the anisotropic nature of the temperature tensor and those associated with the magnetic and electric field anisotropies that are coupled producing different fluxes of positrons along different directions [20]. In addition, the collisions and complex energy dependence of collision frequency further complicate this issue.

Different diagonal elements of the diffusion tensor show different sensitivities with respect to magnetic field, non-conservative collisions and generally to the energy dependence of the cross sections. The diffusion coefficients along the \(E\) and \(E \times B\) directions can vary up to five orders of magnitude in the limit of low values of \(E/N\) where the magnetic field controls the behaviour of the swarm. The longitudinal diffusion coefficient shows the highest sensitivity with respect to the presence of Ps formation, i.e. differences between flux and bulk values are much higher for this diffusion coefficient than those observed for \(D_{E\times B}\) and \(D_B\) components. \(D_B\) component shows the weakest sensitivity to the changes of magnetic field. Essentially, it follows the variation of the mean energy with both \(E/N\) and \(B/N\), and hence the thermal effects play the most important role in the behaviour of this transport property. In Fig. 6 the longitudinal diffusion coefficient is shown for positrons in water vapour. In conclusion, better understanding of the synergetic effects of the magnetic field and non-conservative collisions on the diffusion in \(E\) and \(B\) fields requires knowledge of the spatially resolved data, particularly those associated with the second order variations of the average energy along the swarm [20].

4. Towards application of positrons in medicine

One of the most important applications of positrons is their use in medicine in positron emission tomography (PET). PET is a medical imaging technique, widely and mostly used for tumour diagnostics, but also for studying brain metabolism and brain functions [30]. In spite of the fact that this technique is well developed, the atomic and molecular processes which take place in the human body due to positron interactions are still not well understood and quantified. Currently the PET application is based on models which assume that positrons behave similarly to electrons while interacting with human tissue. This is clearly untrue and in order to have a complete and accurate understanding of PET and other positron based technologies, one must also have a complete knowledge of other secondary processes involved in positron interactions with matter. Investigation of the low energy positron interactions with biologically relevant molecules is of special importance. Certainly the first and the most important among them is the water molecule. Only recently the accurate measurements of the positronium (Ps) formation and total cross section for positron...
interactions with water molecule at low energies have become possible (see Fig. 7 [7]). As a consequence, for the first time a reasonably complete set of cross sections for positrons in water became available.

Modelling of tracks for radiation therapy is one of the interfaces between medical applications and atomic and molecular collision physics. The tracks may be used to envisage the ranges and how therapy proceeds but even for the exactly the same set of cross sections very different tracks may occur depending on the sequence of random numbers. Testing of Monte Carlo codes in such cases proceeds by calculation of standardized benchmark results for averaged properties. The tracks of individual particles are analogous in physics of electron, ion and positron collisions in gaseous background to swarms of particles ensembles of non-interacting particles that do not perturb the background gas. The swarms are best described by transport properties and in the presence of non-conservative collisions the definition of transport properties is ambiguous and one should be aware which property is being calculated. Effects of non-conservative processes on tracks would be profound but difficult to describe in a quantitative manner so one needs averaged properties. The best choices for radiation therapy would be diffusion coefficient/length, range of particles and radial spread. In Figure 6 the longitudinal component of the diffusion tensor for positrons in water vapour is given. In applications to modelling of realistic applications one should be aware that all particles start with very large energies, produce a lot of secondary particles and then reach low energies as well. In other words hydrodynamic definition of transport coefficients may not be valid, although comparisons with such benchmarks are a valid test of the code. In order to test the performance for non-local transport one would need also to use non-hydrodynamic benchmarks such as models of Frank Hertz experiment, Steady state Townsend experiment, Penning-Malmberg-Surko trap and similar experiments.

5. Conclusion
In this work we have calculated various transport properties of positrons in neutral gases in crossed electric and magnetic fields using a multi-term theory for solving the Boltzmann equation and Monte Carlo simulation technique. The results obtained with these two different techniques are in a very good agreement. We hope that present results and the multitude of interesting kinetic phenomena, induced by the synergism of magnetic field and Ps-induced non-conservative collisions, can be a good motivation for a further development of positron swarm experiments.

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