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Theoretical study of the thermalization of the positronium interacting with atoms.

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Abstract. We have investigated the thermalization properties of a gas made by positronium atoms in interaction with a dense gas. Our theoretical model is based on the kinetic Boltzmann formalism that focuses on the microscopical description of the binary positronium-atom collision. We analyze the evolution of the velocity distribution of the positronium atoms during the thermalization process. Our simulations reveal that due to the collision with the heavy mass atoms, the positronium distribution differs significantly from the expected Maxwell-Boltzmann distribution. In particular, a large depletion of ultra-cold atoms is observed.

1. Introduction

One of the challenging of the nowadays antimatter physics concerns the production of cold atoms made by antimatter. An important effort is devoted to the production of anti-hydrogen and dense positronium. The positronium is a hydrogen-like atom composed by one electron and one positron and is the most easily produced atom formed by one antiparticle. It is likely formed in porous materials or aerogel containing fine grains [1]. By diffusing highly energetic positrons in porous materials, thermalized atoms of positronium are formed in less than few nanoseconds after the positron injection [2]. In order to accelerate the production of thermal positronium, the positronium is produced in the presence of noble or heavy mass gases (sometime denoted as remoderators). The thermalization process proceed faster in the presence of the remoderator because the positronium kinetic energy can be transferred to the atoms of the remoderator by elastic collisions [3]. The investigation of the interaction between the positronium and cold atoms is today an active area of research. Experiments have been performed by diffusing low density positronium gas inside a gas of heavy atoms (typically xenon [4, 5]) or helium [6]. In particular, the role played by the quenching, the spin orbit, the pick-off interaction on the modification of the positronium lifetime have been investigated [7, 8, 9, 10, 11, 12].

Measurements of the positronium decay process indicate that the positronium gas in interaction with a remoderator or a solid could thermalize at room or at cryogenic temperature (around 150 K) before the complete annihilation of the positronium. However, few questions remain open and a further investigation of the atomic dynamics is necessary in order to understand the experiments. As an example, in Ref. [13] it is shown that two positronium populations with a large temperature difference can be emitted by silica sample containing cavities that are arranged in the form a regular array of cylindric channels. Moreover, measurements on the spin-orbit interaction between positronium and xenon revealed that the



positronium lifetime is strongly affected by the value of the kinetic energy of the positronium that interacts with the xenon atoms [8].

So far, the theoretical description of the positronium interaction with a solid or a gas is based on the Nagashima's model [3] or on some macroscopic rate equations [10]. One of the basis assumption of these approaches is to consider that the positronium gas is always well described by the equilibrium Maxwell-Boltzmann (MB) distribution. However, since the positronium is typically created in a far-from-equilibrium condition, this hypothesis needs a deeper investigation. With this motivation, on the basis of a theoretical microscopical kinetic model, in the present work we investigate the thermalization of a gas made of positronium atoms interacting with an external gas. With our method, we are able to describe the complete out-of-equilibrium transient evolution of the velocity distribution of the atoms.

2. Results

One of the most efficient way to produce a gas made of positronium is to irradiate a porous material or an aerogel with a highly energetic positron beam. The positrons lose their initial kinetic energies by collisions with the atoms of the solid and the positronium is formed by capturing one electron from one orbital state of the solid. In the case of porous materials, the positronium is mostly formed in the proximity to the internal surfaces of the pores and diffuses inside the solid until it escapes into the void.

Various experiments have established that when the positronium is prepared by using porous materials, the atoms are emitted with a temperature significantly higher than the temperature of the solid. In the case of silica, the positronium atoms are emitted with a characteristic energy that is found to be around 0.5 eV. However, very little is known on the form of the energy distribution of the atoms. It is usually assumed that the positronium thermalize quasi-instantaneously to a MB distribution. Theoretical studies that could confirm such an assumption have not yet been performed. The interest of the present work, is to clarify this point. In a previous study, we showed that the internal positronium thermalization can be rather efficient [14, 15, 16]. By internal thermalization we mean the process through which the total energy of the gas is redistributed among all the atoms leading to the formation of a Maxwell-Boltzmann distribution. Our previous result was derived under the assumption that the positronium is so dense that the probability that two positronium atoms collide is significantly high. In this work, we consider a rarefied positronium gas. Under such condition the bi-positronium collision probability becomes negligible and the only thermalization channel is the collision with the remoderator.

We describe the evolution of the positronium gas interacting with a gas constituted by heavy mass atoms by using the Boltzmann formalism. In this context, the binary heavy-atom positronium collision process is described by the following equation

$$\begin{aligned} \frac{\partial f(\mathbf{p}_1)}{\partial t} = & \frac{2}{(2\pi\hbar)^3} \frac{(M+m)^2}{M^2 m^2} \int \sigma [f(\mathbf{p}_2)g(\mathbf{P}_2) - f(\mathbf{p}_1)g(\mathbf{P}_1)] \delta(\mathbf{p}_1 + \mathbf{P}_1 - \mathbf{p}_2 - \mathbf{P}_2) \\ & \times \delta\left(\frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{P}_1^2}{2M} - \frac{\mathbf{p}_2^2}{2m} - \frac{\mathbf{P}_2^2}{2M}\right) d\mathbf{P}_1 d\mathbf{p}_2 d\mathbf{P}_2 - \frac{f}{\tau}. \end{aligned} \quad (1)$$

Here, f and g denote, respectively, the distribution functions of the positronium and of the external gas. The cross section $\sigma = 4\pi a^2$, a is the scattering length, m is the positronium mass, M is the atomic mass of the external gas and τ is the positronium lifetime. In our simulations, we assume that the scattering cross section is independent from the atomic energy. In the case of highly energetic positrons, some correction to the scattering cross section should be considered [17]. Due to the large mass and density differences, we assume that the remoderator distribution function g is not modified by the presence of the positronium. We assume that g is a constant Maxwell-Boltzmann distribution at room temperature.

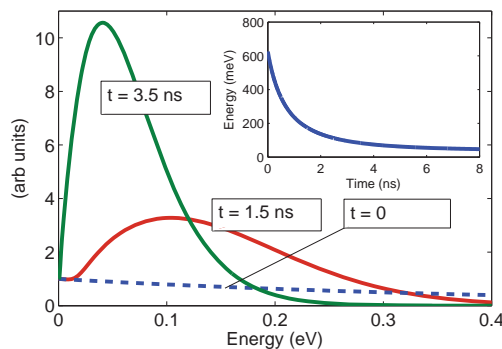


Figure 1. Dynamics of the positronium distribution function induced by collision with a gas made of helium atoms (pressure 1 atm at the room temperature). The dashed-blue line depicts the initial condition (MB distribution at the temperature of 5000 K). The evolution of the mean positronium energy is depicted in the inset.

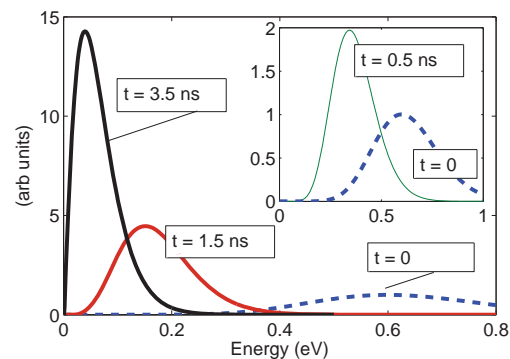


Figure 2. Same case of figure 1 but for an initial gaussian energy distribution of the positronium atoms. Mean energy equal to 0.6 eV and variance equal to 150 meV (dashed-blue line). In the inset we depict the zoom of the initial condition and of the atomic distribution at time $t = 0.5$ ns.

In order to investigate the dynamics of the energetic distribution of the atoms, we consider a low density positronium gas that initially ($t = 0$) is described by a gaussian distribution function with mean energy \bar{E} and energy dispersion ΔE . We investigate the interaction of the positronium with a gas of helium or xenon atoms. Both atoms have already been considered for the experiment of positronium thermalization. In our simulation, we assume that the remoderator density is equal to $6 \times 10^3 \text{ nm}^{-3}$ (250 kPa). The temperature is the room temperature. The scattering cross section of these processes have been measured by various Authors [3, 4]. In our simulations we use the scattering length $a = 2a_0$ where a_0 is the Bohr radius.

The main results of our simulations are displayed in figures. 1-3. In order to illustrate the dynamics of the collision between the positronium and the heavy atom gases, we depict the evolution of the positronium distribution at different times and the evolution of the mean positronium energy (insets of figure 1 and figure 3). We have investigated the influence of the form of the initial positronium energetic distribution on the thermalization dynamics. At this aim, in our simulations we used two different initial conditions for the positronium gas. In the first case (figure 1) we have assumed that the positronium is emitted by the porous material according to the thermal Maxwell-Boltzmann (MB) distribution (dashed-blue line of figure 1) at temperature of 5000 K (that corresponds to the mean emission energy of 600 meV). In the right panel (figure 2) we have depicted the numerical results obtained by taking a Gaussian energy distribution (mean energy $\bar{E} = 0.6$ eV and variance $\Delta E = 150$ meV). We have depicted the positronium distribution function at $t = 1.5$ ns and $t = 3.5$ ns after the positronium formation. The comparison between figure 1 and figure 2 indicates that the memory of the initial condition is lost in less than 3–3.5 ns (note the difference on the energy scale of the two panels). Moreover, our simulations show that the interaction with the gas is able to equilibrate the energy of the positronium with mean room energy (around 27 meV), in a time of round 10 ns that is ten time smaller than the positronium lifetime.

In figure 3 are reproduced the results obtained by assuming that the remoderator is made by xenon atoms. The other quantities are the same as in figure 2. We see that the positronium dynamics is very similar to what obtained in the previous case, except that the time scale is

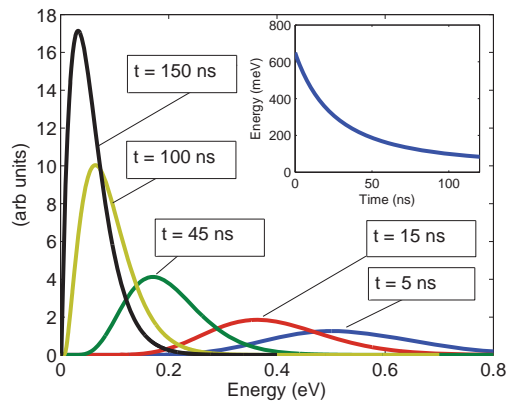


Figure 3. Dynamics of the positronium distribution function induced by collision with a gas made of Xe atoms. The Xe is under the same pressure and temperature conditions as in figure 3. The initial condition for the positronium gas is the same as in figure 2.

considerably increased. It is easy to understand the origin of the difference on the thermalization time when xenon or helium is used. According to the energy and momentum conservation laws, during the bi-atomic collision, we have that the energy transferred by positronium atom to the remoderator atom after one single collision is $\delta E = E_i m/M$ where E_i is the positronium energy before the collision. This consideration shows that the thermalization time scales as the inverse of the mass of the remoderator gas.

Our simulations revealed one important fact concerning the thermalization processes of the positronium induced by collisions with atoms (the same consideration applies also when the positronium collides with a solid or with some other molecules). In agreement with the experimental finding, our simulations show that the positronium energy equals the mean energy of the reservoir after few collision processes. As a conclusion, we can state that the positronium is thermalized before the annihilation. However, a finer analysis of the results reveals that, in contrast to the common assumption, the velocity distribution of the atoms is *not* described by a Bose-Einstein distribution function. A depletion of low velocity atoms can be clearly observed. The final positronium distribution (after 3.5 ns when the remoderator is helium and 150 ns when the remoderator is xenon) is more similar to a gaussian distribution peaked around the room energy (a MB distribution should show a peak when the velocity of the atoms goes to zero). Moreover, this conclusion is independent from the choice of the initial preparation of the positronium gas: even if the positronium is prepared according to the MB distribution with a temperature higher than the remoderator, after the interaction with the thermal bath, the positronium atoms show a non equilibrium configuration, where a depletion of very cold atom is present.

3. Conclusion

We have investigated the thermalization process of the positronium induced by the interaction with a gas (remoderator). We have considered two difference species of gas (Xe and He) characterized by a large mass difference. Our study shows that the positronium main energy becomes comparable with the gas energy in a time shorter than the positronium lifetime. However, the thermalization processe cannot be considered as completed. The numerical simulation show clearly that the positronium during all the thermalization process are not well described by a quasi-equilibrium Maxwell-Boltzmann distribution. In particular, the production of ultracold atoms results inefficient.

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