

Study of the positronium thermalization in porous materials^{*}

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Abstract. We simulate the thermalization process of a high energetic positronium gas trapped in a silica pore. The gas dynamics is reproduced by using a kinetic approach. Our approach includes the two-body scattering interaction and the exchange of energy between the atoms and the internal surface of the pore cavity. We discuss the formation of a quasi-equilibrium state induced by the fast internal thermalization of the gas and the evolution of the gas temperature. We estimate the time necessary to achieve the total thermalization of the gas. The reliability of our model is verified by comparing the numerical results with some experimental data.

1 Introduction

The positron is the most easily produced kind of antiparticle. At low density and temperature, positrons and electrons bound together and form the atom of positronium (Ps). The ground state of positronium consists of triplet states with total spin one and a singlet state with total spin zero. The total angular momentum of the positronium fixes the lifetime and the decay channels of the atom. The triplet state, the ortho-positronium, has a lifetime of 142 ns and annihilates into three photons. The singlet state, the para-positronium, annihilates in 125 ps by emitting two gamma photons. The ortho-positronium can be quickly turned into the para-positronium by using an oscillating magnetic field [1,2].

One of the simplest processes designed for the production of a gas of positronium consists in the implantation of high energetic positrons in a porous medium. During the last decades, many properties of the positronium have been investigated by trapping the gas inside porous materials. In particular, films of porous silica have been employed for the creation of excited atomic states, the di-positronium molecule, and the detection of the quenched lifetime [3–5]. The positrons can be stored in a Surko trap for a around 1000 s and modern devices are able to accumulate up to 10^8 particles [6]. The particles stored in the trap can be compressed and released in a single pulse. It is possible to generate 4–10 ns pulses with kinetic energy of few keV (typical values vary in the range of 1–5 keV [7]),

focused in a spot of 100 μm of radius. The incident beam that enters in the solid target interacts strongly with the lattice. At the distance of roughly 100 nm from the external surface of the material, the particle motion becomes diffusive and the positrons are likely to capture an electron from the solid and form the atom of positronium. The positronium atoms are easily trapped inside solids that contain pores or cavities.

The gas inside the pore thermalizes and transfers energy to the surface of the cavity. Several authors have studied the evolution of the temperature of positronium gases in aggregates of silica aerogel and silica powder [8–10]. Measurements performed by the group of Takada indicate that the time necessary for the full positronium thermalization is around 10 ns for pores with a radius of 5 nm [10]. However, quantum confinement effects could affect the thermalization time in the case of very small pores. In particular, for samples containing pores with a radius of 2.7 nm, no thermalization was observed [11]. In this case, the number of available energy levels for the positronium atoms is reduced, and the gas cannot reach the temperature of the silica sample. The details of the pore structure could affect the capacity to trap the positronium inside the material. If the pores are well separated the positronium can be efficiently trapped. If they are interconnected, the particles diffuse and escape into the vacuum. State-of-the-art techniques of production of porous silica give the possibility to have a good control of the pore characteristics. It is possible to produce well-defined pore structures with, for example, aligned channels in one or two dimensions [12].

The exact nature of the interaction of the positronium gas with the wall surface is not yet known. Experimental data are fitted by simple mathematical models. The validity range of such empirical models is difficult to estimate. In some case they fit only a restricted class of

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experiments. Nagashima et al. developed in reference [13] a theoretical model that describes the time evolution of the positronium temperature in a porous material. The strength of the gas-solid interaction is derived by considering a uniform gas of particles that collide elastically with some heavy molecules of mass M . These molecules are clusters of atoms that cover the surface of the SiO_2 pore. In this approach, the mass M (which is estimated to be around 70 u [9]) is used as a fitting parameter.

In this paper, we investigate the thermalization process of the positronium in porous silica materials. The dynamical evolution of the positronium gas is described by using a kinetic approach. Our model is based on the Boltzmann equation. In particular, we focus on energy the exchange between the gas and the surface of the pore. This aspect plays a crucial role in the evolution of the gas temperature. As an application of our model, we consider a dense positronium gas in a large pore and we estimate the time necessary to reach the critical temperature for the Bose-Einstein condensation process. In the present study, we consider gas of positronium whose density is in the range of $10^{-5} \div 10^{-2} \text{ nm}^{-3}$.

The paper is organized as follows. In Section 1.1 we present the kinetic model that reproduces the gas dynamics. It describes the binary collision of the atoms in terms of the s -wave interaction. We study the internal thermalization of the gas after the injection in the pore. We estimate the initial temperature of the gas and the influence of the initial conditions. In Section 1.2 we propose a mathematical model that reproduces the particle-wall interaction. Our model depends on a free parameter. Sections 1.3–1.4 are devoted to the estimation of this parameter by the comparison of our theoretical predictions with the experimental measurements of Chang et al. [9], Takada et al. [10] and Nagashima et al. [14]. Finally, in Section 1.5 we reproduce the evolution of the temperature of a positronium gas in large silica pore. We investigate the possibility to create a Bose-Einstein condensate made of positronium.

1.1 Thermalization and initial temperature of the Ps gas

We consider the evolution of a hot positronium gas. We assume that the gas is constituted by a single population of ortho-positronium. This can be obtained by using a spin-polarized gas of positron in the process of positronium formation described in the introduction. Some radioactive materials are natural sources of spin-polarized positrons. The preparation of a fully spin-polarized gas of positronium trapped in a porous material has been achieved by the group of Cassidy [7].

We reproduce the dynamics of a gas of positronium by using a kinetic approach. Kinetic models based on the Boltzmann equation have been used by various authors for the description of the evolution and the thermalization process of boson gases in various regimes [15,16]. In the kinetic formalism, the gas is described by the distribution function $f(\mathbf{r}, \mathbf{p}, t)$. It gives the number of atoms

with momentum \mathbf{p} and position \mathbf{r} . The evolution of the distribution function is given by the Boltzmann equation

$$\frac{\partial f}{\partial t} - \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} f = \mathcal{W}[f] - \frac{f}{\tau}. \quad (1)$$

The last term on the right side describes the natural decay process of the ortho-positronium where τ is the lifetime. The two-particle scattering kernel \mathcal{W} is given by [17]:

$$\begin{aligned} \mathcal{W}[f] = & \frac{g^2}{4\pi} \int \delta(E(\mathbf{p}) + E_1 - E_2 - E_3) \\ & \times \delta(\mathbf{p} + \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{p}_3) [(1 + f(\mathbf{p}))(1 + f_1)f_2f_3 \\ & - f(\mathbf{p})f_1(1 + f_2)(1 + f_3)] d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3. \end{aligned} \quad (2)$$

Here, $f_i \equiv f(\mathbf{p}_i)$, $E(\mathbf{p}) = \frac{p^2}{2m}$ is the energy of the atoms, $E_i \equiv \frac{p_i^2}{2m}$ and m is the mass of the positronium. We used physical units where $\hbar = 1$. The presence in the integral of the two Dirac's delta distributions ensures the conservation of the total energy and momentum during each scattering event. The collision term \mathcal{W} describes the two-particle hard sphere interaction. The collision strength is $g = 4\pi a/m$ where $a = 0.16 \text{ nm}$ is the scattering length of ortho-positronium [18,19]. According to the calculations presented in reference [19] where a stochastic variational method is applied, the triplet-triplet scattering section is nearly constant in the range $p \in [0, \hbar a_0/10]$ where a_0 is the Bohr radius. This corresponds to an atomic energy inferior to 5 eV. Since the implantation Ps energy is typically inferior to 1 eV, in our simulations we use a constant scattering section.

The complete thermalization of the system proceeds into two steps. Initially, as a result of the two-particle collisions, the atoms in the gas thermalize and the gas is described by a well defined temperature. Afterwards, due to the contact with the pore surface, the temperature of the gas decreases. These two phases of the dynamics are characterized by two different time scales. In this section we discuss the first part of the thermalization process.

The atoms that are formed in proximity of the pore surface and enter into the cavity are highly energetic. We assume that the initial particle distribution f_i that describes the injection of the atoms in the cavity, is given by a translated Maxwell-Boltzmann distribution

$$f_i(\mathbf{p}) = \frac{n_0}{n_c} e^{-\frac{1}{\Delta E} \frac{(\mathbf{p}-\mathbf{p}_0)^2}{2m}}, \quad (3)$$

where

$$n_c \equiv \left(\frac{\Delta E}{4\pi} \right)^{3/2} \quad (4)$$

and n_0 is the initial particle density. The drift kinetic energy $E_0 \equiv \frac{p_0^2}{2m}$ is typically very high. It is estimated to be around 0.1–0.5 eV [13]. In equation (3), ΔE is the variance of the atomic energy distribution around the mean value E_0 . The particle distribution (3) represents a highly out-of-equilibrium distribution of particles. The two-particle

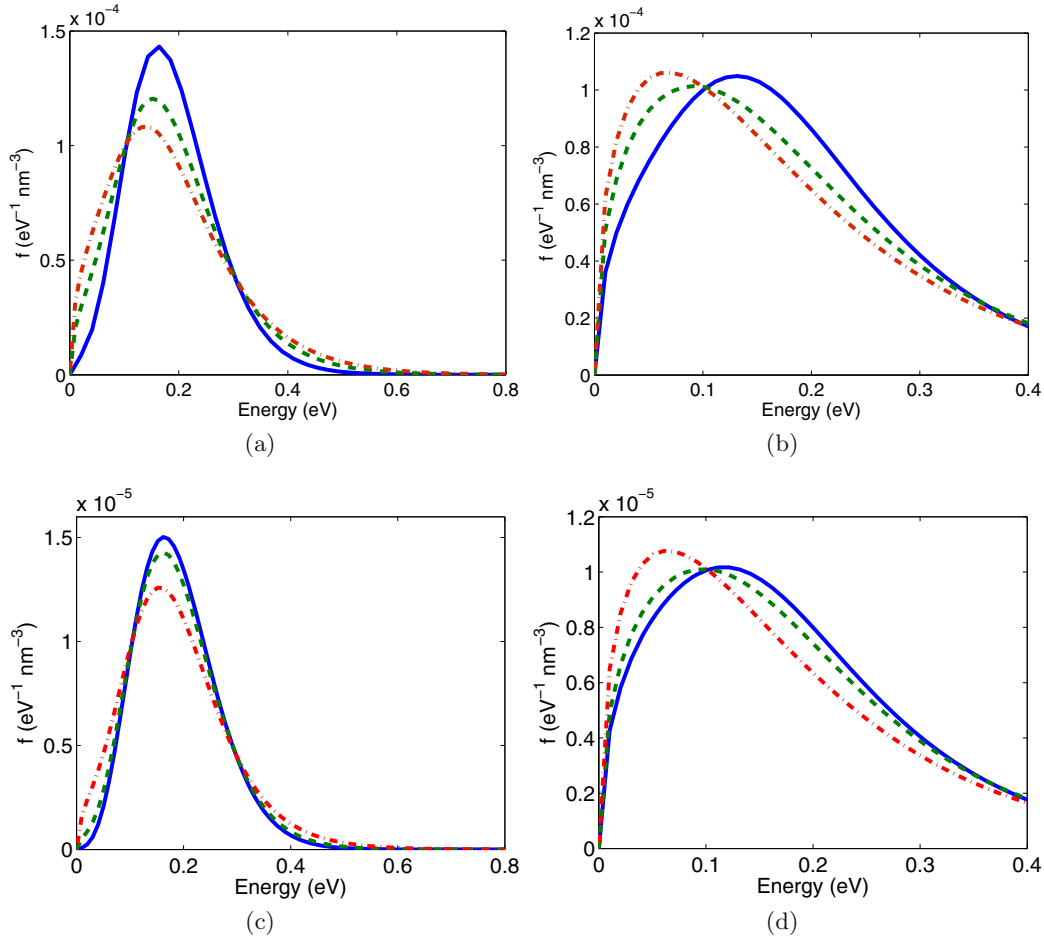


Fig. 1. Time evolution of the particle density during the internal thermalization of the positronium gas. The plots correspond to the following times: panel (a) continuous-blue curve $t = 0$, dashed-green curve $t = 50$ fs, dot-dashed-red curve $t = 90$ fs. Panel (b) continuous-blue curve $t = 100$ fs, dashed-green curve $t = 200$ fs, dot-dashed-red curve $t = 400$ fs. Panel (c) continuous-blue curve $t = 50$ fs, dashed-green curve $t = 150$ fs, dot-dashed-red curve $t = 300$ fs. Panel (d) continuous-blue curve $t = 1500$ fs, dashed-green curve $t = 2000$ fs, dot-dashed-red curve $t = 5000$ fs. The initial particle density is 10^{-2} nm^{-3} (panels a, b) and 10^{-3} nm^{-3} (panels c, d).

hard sphere interaction causes a rapid redistribution of the energy among the particles. As a result, after few scattering events, the gas of positronium is well described by a Bose-Einstein distribution with a certain temperature T_{P_s} that depends only on the initial total energy of the gas. Clearly, we have $T_{P_s} \gg T_l$ where T_l is the temperature of the substrate. The atoms lose energy by impacting with the pore surface. At the end, their temperature equilibrates with the lattice temperature. This process requires a time interval that is much longer than the time necessary for the internal thermalization of the particles in the gas. It will be addressed in the next section.

By using equation (2) we simulate the initial gas thermalization. The main result that emerges from the simulations is that this process is quite fast (it takes around 1–100 ps). After this stage, the resulting particle distribution function is nearly independent from the profile of the initial configuration. It is determined only by the invariants of the motion, the initial total energy and the total number of particles of the gas. This is illus-

trated in Figures 1–2. In Figure 1 we depict the evolution of the particle distribution in the early stage of the dynamics. The continuous-blue curve in the panel a depicts the initial condition of the gas. In the simulations depicted in the panels a and b of Figure 1 we used the following parameters $E_0 = 0.2$ eV, $\Delta_E = 0.1$ eV, and the initial particle density is 10^{-2} nm^{-3} . We plot the evolution of the particle distribution in the time interval 10–400 fs.

After 500 fs the system is completely thermalized (the distribution function becomes identical to the Bose-Einstein distribution). The subsequent modification of the particle distribution proceeds at the nanosecond time scale (see Sect. 1.4) and is characterized by the simple variation of the gas temperature. For the sake of comparison, in the panels c, d of Figure 1, depict the time evolution of a gas with a density which is one order of magnitude smaller than the previous one ($n_0 = 10^{-3} \text{ nm}^{-3}$). In this case the gas is more rarefied and the probability that two particles collide decreases. Consequently, the time necessary for the thermalization increases to nearly 5 ps. However, also in

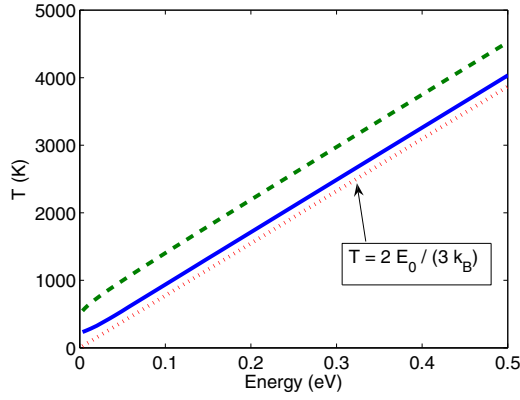


Fig. 2. Temperature of the gas as a function of the mean injection energy E_0 . The dotted-red curve depicts the the temperature $\bar{T} = \frac{2}{3} \frac{E_0}{k_B}$. The continuous-blue (dashed-green) line corresponds to $\Delta_E = 500$ K ($\Delta_E = 1000$ K).

the case of rarefied gases, the internal thermalization time is small compared with the characteristic time of the evolution of the temperature of the gas. In Figure 2 we plot the value of the gas temperature at the end of this stage. The temperature is plotted as a function of the initial particle mean energy E_0 . The two curves correspond to different values of the energy dispersion Δ_E . For the sake of comparison, the dotted-red curve indicates the temperature \bar{T} that corresponds to E_0 , $k_B \bar{T} = \frac{2}{3} E_0$ where k_B is the Boltzmann's constant. As expected, as the variance of the energy increases, the temperature of the gas becomes higher. The simulations show that in this preliminary phase of the dynamics, the total gas energy is nearly constant. In order to quantify more precisely the particle-particle thermalization time t_{pp} , in Figure 3, we depicted the time employed by the gas to reach the Bose-Einstein distribution

$$f_{eq}(\mathbf{p}) = \frac{1}{e^{\frac{1}{k_B T} \left(\frac{\mathbf{p}^2}{2m} - \mu \right)} - 1}, \quad (5)$$

where μ is the chemical potential. We set t_{pp} equals to the minimum time at which the particle distribution can be approximated by f_{eq} with an error smaller than 1%. In the plot, we depict the variation of t_{pp} with respect to the particle density (left panel) and to the initial injection energy E_0 (right panel). Our simulations show that in the typical range of energy and density attained in the experiments where the positronium is trapped in nanometric cavities, the thermalization time is always smaller than 100 ps. In particular, we estimate that when the energy of emission of the Ps gas into the pore is around 0.1–0.3 eV, the gas thermalizes at a temperature in the range of 1000–3000 K.

In order to appreciate the characteristic length scales of the problem, we estimate the mean free path λ between two consecutive Ps-Ps binary collisions. We use the following simple formula [20] $\lambda = \frac{1}{\sqrt{2}\sigma n} = \frac{1}{\sqrt{28}\pi a^2 n}$, where σ is the effective cross section (the factor of 8π instead of the usual 4π arises from the statistical considerations on the indistinguishability of two scattering bosons [19,21]) and n is the gas density. We obtain that the main free

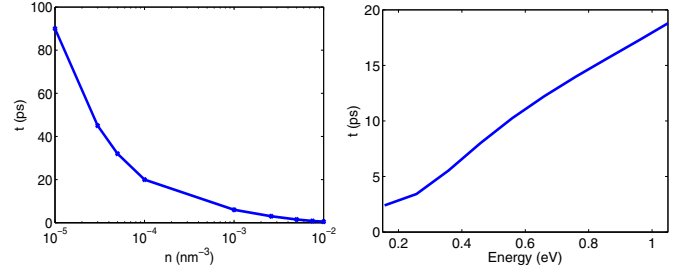


Fig. 3. Thermalization time t_{pp} . Left panel: t_{pp} as a function of the initial atomic density (the density axis is in logarithmic scale). $E_0 = 0.1$ eV. Right panel: t_{pp} as a function of the injection energy E_0 . Particle density 10^{-3} nm^{-3} .

path for a gas density of 10^{-2} nm^{-1} (10^{-3} nm^{-1}) nm, is around 100 nm (1.0 μm). This value is of the same order of the distance between to consecutive interactions of the Ps atom with the pore surface.

1.2 Interaction Ps-surface

In this section we are interested to the evolution of the gas temperature and we model the interaction between the cavity wall and the gas. Since the initial temperature of the gas is nearly two orders of magnitude higher than the substrate, the main mechanism that can be observed is the fast decrease of the positronium temperature. The rate of energy loss of the gas is determined the number of phonons emitted by the atoms when they hit the pore surface. According to the kinetic formalism used in our model, the atom-phonon interaction is described by the following equation (see for example Refs. [22,23])

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_{ph} &= \frac{S}{8\pi^2} \int [(1 + f(\mathbf{p})) f_1 q(\omega) - f(\mathbf{p})(1 + f_1) \\ &\quad \times (1 + q(\omega))] \delta(E_1 - E - \omega) d\mathbf{p}_1 \\ &+ \frac{S}{8\pi^2} \int ((1 + f(\mathbf{p})) f_1 (1 + q(\omega)) - f(\mathbf{p}) \\ &\quad \times (1 + f_1) q(\omega)) \delta(E_1 - E + \omega) d\mathbf{p}_1. \end{aligned} \quad (6)$$

Here, $q(\omega)$ is the phonon distribution, ω is the phonon energy and S is the scattering rate. The phonon distribution is given by the Bose-Einstein distribution $q(\omega) = [e^{\frac{\omega}{k_B T}} - 1]^{-1}$. The scattering rate S describes the strength of the atom-wall interaction. The exact value of S depends on the form of the interaction potential at the interface. The evaluation of this quantity from first principles is a formidable task. In the present work, we estimate S in two different ways. At first (Sect. 1.3), we reduce the complexity of the mathematical description of the gas dynamics, and we obtain a simple model for the evolution of the mean energy of the gas. We refer to the estimation of the atom-surface interaction strength given in references [2,24] and we obtain S . In Section 1.4 we use S as a fitting parameter of the complete model and we compare numerical results

with the experimental data of the positronium thermalization in silica presented in references [10,14].

1.3 Estimation of S: approximated model

As discussed in the previous section, when the gas is injected in the pore, its temperature is high compared to the bulk material. Under this condition, the phonon absorption process can be neglected. As a further simplification of the model, we assume that the particle distribution function is independent on the direction of the momentum (isotropic approximation). In this case, equation (6) can be approximated as follows

$$\left. \frac{\partial f}{\partial t} \right|_{ph} \simeq \frac{S}{\pi} \sqrt{\frac{E+\omega}{2m}} ([1+f(E)]f(E+\omega)q(\omega) - f(E)[1+f(E+\omega)][1+q(\omega)]), \quad (7)$$

where we changed the variables of the distribution and we substituted the momentum with the energy.

By assuming that during each collision the atom has the probability P to emit a phonon with energy ω , the rate of energy loss of the gas is given by:

$$\frac{4\pi R^3}{3} \frac{n\omega P}{\tau_f} = \left. \frac{\partial e}{\partial t} \right|_{ph} = 4\pi R^2 R_i \frac{1}{(2\pi)^3} \int \frac{p^2}{2m} \left. \frac{\partial f(\mathbf{p})}{\partial t} \right|_{ph} d\mathbf{p}, \quad (8)$$

where n is the particle density, e is the energy density, $1/\tau_f$ is the collision frequency with the wall, R is the pore radius and R_i is the range of the potential at the surface. We derived the right side of the equation, by integrating the time derivative of the distribution function over the spatial region where the gas stays in contact with the surface. We assume that the gas interacts with the wall in the small region away from the pore surface delimited by the range of the van der Waals potential. The time of flight τ_f can be estimated as:

$$\tau_f \simeq R \sqrt{\frac{m}{3k_B T}}.$$

In the limit of high temperature, equation (8) gives

$$\begin{aligned} \left. \frac{\partial e}{\partial t} \right|_{ph} &= \frac{n4R^2 R_i S \sqrt{2\pi} (m\beta_{Ps})^{3/2}}{m^2 \pi} \\ &\times \left(\frac{e^{-\beta_{Ps}\omega}}{e^{\beta_l\omega} - 1} - \frac{1}{1 - e^{-\beta_l\omega}} \right) \\ &\times \int E^{3/2} \sqrt{E+\omega} e^{-\beta_{Ps}E} dE \\ &\simeq \frac{n8R^2 R_i S \sqrt{2\pi} (m\beta_{Ps})^{3/2}}{m^2 \pi (\beta_{Ps})^3} \\ &\times \left(\frac{e^{-\beta_{Ps}\omega}}{e^{\beta_l\omega} - 1} - \frac{1}{1 - e^{-\beta_l\omega}} \right), \end{aligned}$$

where we have defined $\beta_l = (k_B T_l)^{-1}$ and $\beta_{Ps} = (k_B T_{Ps})^{-1}$. We can now provide a first estimate of S . According to references [2,24] we assume that the probability

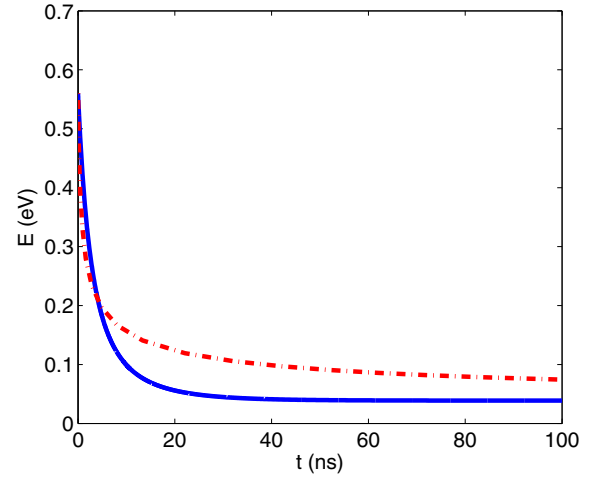


Fig. 4. Temperature evolution of the Ps gas in silica (fit of the experimental data). Continuous-blue curve: equation (9) with $2R = 5.6$ nm (from Ref. [10]). Dotted green curve: equation (9) with $2R = 70$ nm [9].

P to emit a phonon with energy $\omega = 2$ meV is 1%. We expand the exponentials and we use equation (8). We finally obtain

$$S \simeq \frac{\omega P \pi^2}{2R_i \sqrt{6\pi} k_B (T - T_l)} = 1.1 \times 10^{-2} \text{ nm}^{-1},$$

where the gas temperature is chosen equal to 500 K and the range of the potential $R_i = 0.2$ nm [23].

1.4 Estimation of S: full model

In this section we provide a more accurate estimation of S by comparing our numerical results with some experimental data. In Figure 4 we plot the measurements of the gas thermalization presented in references [9,10]. The continuous-blue curve fits the evolution of the energy of a positronium gas in a porous silica with density of 1 g cm^{-3} (that corresponds to an atomic mean free path of around 5.6 nm) [10]. The dotted-green curve fits the Ps energy evolution in a porous silica with density of 1.0 g cm^{-3} (that corresponds to an atomic mean free path of around 70 nm) [9]. The temperature of the substrate is 300 K. The curves are obtained by the following equation and are in good agreement with the measurements

$$E(t) = \left(\frac{1 + Ae^{-bt}}{1 - Ae^{-bt}} \right)^2 \frac{3}{2} k_B T_l. \quad (9)$$

The parameters A and b are given in reference [10], and are quoted here for the sake of clearness

$$\begin{aligned} b &= \frac{1}{RM} \sqrt{3mk_B T_l} \\ A &= \frac{\sqrt{E^*} - \sqrt{1.5k_B T_l}}{\sqrt{E^*} + \sqrt{1.5k_B T_l}}. \end{aligned}$$

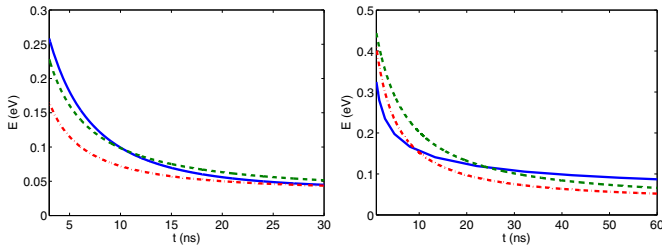


Fig. 5. Evolution of the temperature of Ps obtained with our model. Left panel. Continuous-blue curve: equation (9) for $2R = 5.6$ nm (see Ref. [10]). Dashed-green curve: our model with $S = S_1$. Dotted-dashed red curve: our model with $S = S_0$. Right panel. Continuous-blue curve: equation (9) for $2R = 70$ nm (see Ref. [9]). Dashed-green curve: our model with $S = S_1$. Dotted-dashed red curve: our model with $S = S_0$.

The value of the energy E^* is chosen equal to 0.6 eV. $M = 70$ u is the mass of the SiO_2 clusters that cover the pore surface.

In order to compare the measurements with our numerical results, we display in Figure 5 the evolution of the temperature of the gas obtained with our model for the same cases of Figure 4. Our results are obtained by the numerical discretization of the full kinetic model of equation (2). We use a deterministic method [25–27]. We simulate the evolution of the atomic distribution inside a spherical pore. We assume that the spherical symmetry of the system is preserved. Under this condition, we have that f depends on the three variables (ρ, p, ϑ) , where ρ is the distance from the center of the pore, p is the modulus of the momentum and ϑ is the angle between the momentum and the radius of the sphere. The boundary conditions for $\rho = R$ are provided by equation (6).

In order to find good agreement between our numerical solutions and the experimental data, we use S as a fitting parameter. We find that a S varies in the range $[S_0, S_1]$, with $S_0 \equiv 10^{-2} \text{ nm}^{-1}$ and $S_1 \equiv 0.5 \times 10^{-2} \text{ nm}^{-1}$. In the left panel of Figure 5 we depict the results of our calculations applied to a sample of silica with a density of 1 g cm^{-3} . The continuous blue curve fits the experiments (Eq. (9)). In order to show the sensitivity of our model to the parameter S , we depict the results that correspond to the two extremal values $S = S_0$ (dashed-dotted red curve) and $S = S_1$ (dashed-green curve). In the right panel we consider the case of a silica sample with density of 0.1 g cm^{-3} . In particular, when the parameter S spans in the range $[S_0, S_1]$ the gas thermalization time changes by a factor of around two. When the temperature is elevated, a classical model reproduce the evolution of the particle in the gas in a large cavity as soon its de Broglie wavelength is small in comparison with the dimension of the pore. When Ps energy decreases, the quantum mechanical description of the pore surface becomes necessary. As can be clearly seen by comparison with the experimental data, our model overestimate the cooling process in the final part of the process. We ascribe this discrepancy to the fact that our modeling of the phonon generation-absorption process is not sufficiently accurate at low temperature (the inability to reproduce the correct behavior

of the evolution of the gas energy by a classical model a low temperature was already observed in Ref. [14]). A possible improvement of our results could be obtained by modeling the phonon interaction with the bulk phonon structure. In this case, the deformation potential is proportional to the exchanged momentum and, consequently, the cooling process decreases at low temperature.

1.5 Study of the Ps thermalization time: Bose-Einstein condensation

For the cases presented in the previous section we considered silica samples maintained at room temperature. In this section, we apply our kinetic model to predict the evolution of the temperature of a positronium gas trapped in a nanometric cavity at low temperature. This study has an interesting application: the creation of a Bose-Einstein condensate made of positronium atoms trapped in a silica pore.

The positronium is constituted by two particles with spin one-half. Consequently, its total spin is one and it is a boson. One interesting property of a gas of bosons is that below a critical temperature T_c it undergoes a phase transition called Bose-Einstein condensation process. The main concept at the origin of this phenomenon is that a macroscopic fraction of bosons collapses into the lowest energy state: the zero momentum state in free space or the ground state for a system in a confining potential [28]. The Bose-Einstein condensate is an extended state where Broglie wavelength of the single state particle is comparable to or greater than the average interparticle spacing. The detailed description of the mechanism of the formation of a Bose-Einstein condensate should require a fully quantum formalism. The interaction between two low energy bosons can be modified by the presence of the condensate. However, the simple particle-particle hard sphere interaction is usually considered sufficiently accurate to capture the main physics of the problem (see for example the studies of the condensate formation for the sodium and for the polaritons presented respectively in Refs. [29,30]). The modification of the condensate growth rate induced by the correlation between the condensate and the free positronium wave functions, is investigated in reference [17].

The possibility to create a Bose-Einstein condensate made of positronium has been firstly addressed in reference [2]. The mass of the positronium is considerably smaller than the typical mass of the atoms usually employed in the condensation experiments. Since the condensation temperature is inversely proportional to the atomic mass, a gas of positronium should condensate at a temperature that is several orders of magnitude greater than the critical temperature of, for example, rubidium. However, the positronium lifetime is not sufficiently long to ensure that the condensation process can be completed before the total annihilation of the particles [17]. For that reason, the question whether it is technically possible or not to observe the condensation of a positronium gas trapped inside some porous medium, is still open (see for example

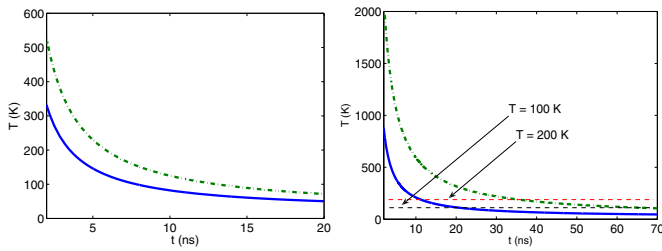


Fig. 6. Time evolution of the temperature of the Ps gas. Pore radius: left panel $R = 100$ nm, right panel $R = 300$ nm. Continuous-blue curve: $S = S_2$ Dotted-green curve: $S = S_1$.

Ref. [31]). In reference [32] Mariazzi et al. presented some experiments where a gas of positronium is cooled down at a cryogenic temperature. They considered a regular array of silica nanochannels (a series of parallel cylinders of diameter of 5–8 nm). Under this condition, they showed that a fraction of around 10% of the injected positrons is converted into a positronium gas at the temperature of 150 K (we note here difference with the cases that we are considering: the pores are connected with the surface and the gas is not trapped inside the silica). The cooling time is estimated to be shorter than 15–20 ns.

We estimate the time necessary to attain a temperature that is sufficiently low to produce a Bose-Einstein condensate. In Figure 6 we display the time evolution of the temperature of a gas injected in a pore of radius 100 nm maintained at the temperature of 30 K. The continuous-blue curve is obtained with the intermediate value of the interaction strength $S = S_2 \equiv 0.8 \times 10^{-2} \text{ nm}^{-1}$. We estimate that the time necessary to reach the temperature of 100 K ($t_{100 \text{ K}}$) is around 7 ns. The dashed-dotted curve is obtained with the more “pessimistic” estimate of $S = S_1$ (“pessimistic” for the formation of a condensate, since lower values of S give longer thermalization times). In this case, $t_{100 \text{ K}}$ is around 13.5 ns. The curves displayed in Figure 6 are evaluated with a density of 0.01 nm^{-3} . The correspondent critical temperature for the Bose-Einstein condensation process is 66 K. We find that the evolution of the gas temperature is quite independent from the particle density. The reason should be ascribed to the fast internal thermalization of the atoms described in Section 1.1. Since the gas is always close to the equilibrium, the frequency of the particle-particle collisions (which is proportional to the gas density), has little influence on the modification of the atomic temperature.

In Figure 6 (right panel), we display the simulations for a pore of size 300 nm. The continuous-blue curve corresponds to $S = S_2$ and the dot-dashed green curve to $S = S_1$. In order to ease the reading of the plot, the horizontal black (red) dashed line indicates the temperature of 100 (200) K. The simulations show that a temperature close to the critical value is attained in the interval between and 10 and 35 ns for $t_{200 \text{ K}}$ and 20–70 ns for $t_{100 \text{ K}}$. In this case, the thermalization time is comparable to the lifetime of the ortho-positronium.

In summary, in this paper we simulated the thermalization process of a high energetic positronium gas trapped in a silica pore. We have discussed the formation of a quasi-equilibrium state of the gas and the time evolution of the gas temperature. We have found that the thermalization process proceeds in two steps. The first is characterized by the formation of a quasi-equilibrium gas state with a well defined temperature. We estimated the characteristic time of the internal thermalization of the gas for different atomic densities and injection energies. We have found that the thermalization time is strongly dependent on the gas density. It is estimated to be equal to few fs for high density gases (with density of 10^{-2} nm^{-3}) and 80 ps for rarefied gases (with density of 10^{-5} nm^{-3}). After having compared the results of our simulations with some experimental results, we used our model to simulate the evolution of the gas in a large trap maintained at a cryogenic temperature. We find that the creation of a Bose-Einstein condensate is compatible with the ortho-positronium lifetime.

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