Positronium-positronium interaction: Resonance, scattering length, and Bose-Einstein condensation

Sadhan K. Adhikari
Instituto de Física Teórica, Universidade Estadual Paulista,
01.405-900 São Paulo, São Paulo, Brazil

October 31, 2018

Abstract

The low-energy scattering of ortho positronium (Ps) by ortho Ps has been studied in a full quantum mechanical coupled-channel approach. In the singlet channel (total spin $s_T = 0$) we find S- and P-wave resonances at 3.35 eV (width 0.02 eV) and 5.05 eV (width 0.04 eV), respectively and a binding of 0.43 eV of Ps₂. The scattering length for $s_T = 0$ is 3.95 Å and for $s_T = 2$ is 0.83 Å. The small $s_T = 2$ scattering length makes the spin-polarized ortho Ps atoms an almost noninteracting ideal gas which may undergo Bose-Einstein condensation.

Pacs Numbers: 34.85.+x, 03.75.Fi, 82.30.Gg
Of the two types of positronium (Ps), the ortho Ps (triplet) of large life time 142 ns, compared to that of the para Ps (singlet) of life time 0.125 ns, has been of great experimental interest. The preparation of ortho Ps from positron interaction with atoms and molecules is well under control. One can study the interaction of Ps, a matter-antimatter bound state, with different atoms and molecules. There has been precise measurement of total cross section of ortho-Ps scattering by H$_2$, N$_2$, He, Ne, Ar, C$_4$H$_{10}$, and C$_5$H$_{12}$. Such processes may take place on the outer surface of a star and are also of astrophysical interest. There have also been studies on bound states of Ps with different atoms as well as of Ps$_2$ molecule.

In addition to the interaction of Ps with matter, the interaction between two Ps atoms is also of general interest. As the anti-atom of Ps is also a Ps, one can study the interaction between matter-antimatter (Ps-Ps) states, where the constituents (Ps) are also matter-antimatter (electron-positron) bound states. In the recent study of hydrogen-antihydrogen interaction, the constituents are, however, not matter-antimatter bound states.

Apart from the theoretical interest in testing fundamental symmetries, (charge conjugation, parity, and time reversal) from a study of Ps-Ps interaction, the Bose-Einstein condensation (BEC) of a collection of spin-polarized ortho Ps (Ps$_\uparrow$) seems to be viable in the laboratory. The critical temperature $T_c$ for BEC of ideal bosons of mass $m$ and density $n$ is given by $T_c = (2\pi^2/m)(n/2.65)^{2/3}$. Hence, a small mass of Ps at a reasonable density should facilitate BEC by leading to a large $T_c$.

Recently, there has been experimental realization of BEC in trapped atoms ($^1$H, $^7$Li, $^{23}$Na, $^{87}$Rb, $^4$He*($^2$S$_1$)) at temperatures of few hundred nK. This initiated intense theoretical and numerical activities on the subject. In actual experiment a trap was needed to increase the density of atoms to a desirable level. However, with the trap emerges a new energy scale $\hbar\omega$($\sim$ few nK) in the problem where $\omega$ is the angular frequency of the trap and a new $T_c = 0.94\hbar\omega N^{1/3}$ where $N$ is the number of atoms. For $N \sim 10^6$ this leads to a $T_c$ of few hundred nK for trapped atoms.

The interaction between the bosonic atoms at low temperature is proportional to the interatomic scattering length $a$. In most cases of trapped atoms above $|a|$ is large which implies a strong interaction and hence a large deviation from an ideal gas. This makes a theoretical investigation via a strongly nonlinear Schrödinger equation extremely complicated.

In the total spin $s_T = 0$ state, the collision between two unpolarized ortho Ps may lead to two para Ps and their quick eventual annihilation. The Ps$_2$ molecule exists in this overall singlet state where both the electron and positron pairs also remain in singlet states. Hence, in a collection of unpolarized ortho Ps the long-lived ortho Ps atoms will disastrously transfer to short-lived para Ps, and for an efficient BEC one should use Ps$_\uparrow$. For two Ps$_\uparrow$, $s_T = 2$ and both the electron and positron pairs remain in triplet states.

The small mass of Ps should enhance BEC, and $10^5$ Ps atoms in a cylindrical
cavity in Si of volume $10^{-13}$ cm$^3$ should allow BEC at tens of Kelvin temperature according to the ideal gas BEC formula for $T_c$ [5, 6], in contrast to hundreds of nK for trapped gas [3, 4]. The advantages of a Si cavity over other metallic cavities for cooling Ps atoms and achieve BEC have been discussed in Ref. [5]. If $n |a|^3 << 1$, the BEC is close to one of an ideal gas [5]. It is interesting to calculate the relevant scattering length for Ps-Ps scattering and see if the BEC of Ps$^+$ can be considered to be ideal or nearly ideal.

In this Letter we present a full quantum mechanical three-Ps-state coupled-channel method with Ps(1s)Ps(1s,2s,2p) states for the study of scattering of ortho Ps by ortho Ps in both $s_T = 0$ (singlet) and $s_T = 2$ states. We do not consider the simultaneous excitation of two Ps atoms in this study. The $s_T = 0$ state is interesting for studying the Ps$_2$ molecule and the $s_T = 2$ state for studying the interaction among the Ps$^+$ atoms to be used in BEC. Similar coupled-channel approach was successfully used in Ps scattering by H [11], He [12], Ar, Ne [13], Li, Na, K, Rb, Cs [14], and H$_2$ [15]. In the Ps-H system we could reproduce the variationally known binding and resonance energies and scattering length in the singlet channel. In Ps-Li, Ps-Na, Ps-K we could reproduce the variationally known binding energies [2] in the singlet channel and predict resonances in S, P, and D waves near the lowest Ps excitation threshold. In Ps-He, Ps-Ar, Ps-Ne, and Ps-H$_2$ we could give a good account of the experimental total cross section at low and medium energies. Hence it seems worthwhile to test this approach in Ps-Ps scattering.

Here we calculate the Ps-Ps scattering lengths, low-energy phase shifts and elastic and inelastic cross sections in both $s_T = 0$ and $s_T = 2$ channels. In the singlet channel ($s_T = 0$) we find resonances in S and P waves below the lowest Ps excitation threshold.

The theory for the coupled-channel method of Ps scattering has appeared in the literature [11, 12]. The relevant coupled Lippmann-Schwinger scattering integral equation in momentum space is given below

$$f_{\nu',\nu}^\pm (k', k) = B_{\nu',\nu}^\pm (k', k)$$
$$- \frac{1}{2\pi^2} \sum_{\mu} \int d\mathbf{q} \frac{B_{\nu',\nu}^\pm (k', \mathbf{q}) f_{\mu\nu} (\mathbf{q}, k)}{k_{\mu}^2/2 - q^2/2 + i0},$$  \(1\)

where $f_{\nu',\nu}^\pm$ is the scattering amplitude, and $B_{\nu',\nu}^\pm$ is the corresponding Born amplitude for $s_T = 0$ and $s_T = 2$ respectively. $\nu$ and $\nu'$ denote initial and final states of one of the Ps while the other being maintained in the 1s state, $k_{\mu}$ is the on-shell relative momentum of Ps-Ps in the channel $\mu$. We present all equations in atomic unit (a.u.) where $\hbar = e = \tilde{a}_0 = m = 1$, where $e$ (m) is the electronic charge (mass) and $\tilde{a}_0$ is the Bohr radius. Because of internal symmetry all direct Born amplitudes with the excitation of only one Ps, as considered in this Letter, are zero and the scattering proceeds solely through exchange interaction by successive exchange of a pair of electrons between two positrons.

3
The exchange Born amplitude for Ps-Ps scattering can be easily derived as in Ref. [12] and the details will be elaborated elsewhere. The time-reversal symmetric exchange Born amplitude is given by

\[ B^\pm_{\nu\nu'}(k', k) = \pm \frac{2}{D} \int \chi^*_\nu(r) e^{-iQr/2} \chi_\nu(r) dr \times \int \chi^*_1(r') e^{iQr'/2} \chi_1(r') dr', \]  

(2)

with \( D = (k^2 + k'^2)/4 + [\beta_1^2 + (\beta_\nu^2 + \beta_{\nu'}^2)]/2 \), where \( Q = k - k' \) is the momentum transfer, \( \chi(r) \) the Ps wave function, and \( \beta_\nu^2 \) and \( \beta_{\nu'}^2 \) are binding energies of initial and final states of Ps in a.u., respectively. The exchange amplitude with the + sign in Eq. (2) refers to an attractive interaction and corresponds to overall \( s_T = 0 \) state mentioned above where the electron and positron pairs are in singlet states. The exchange amplitude with the – sign refers to a repulsive interaction and corresponds to the overall \( s_T = 2 \) state with both the positronium pairs in the triplet state. This exchange Born amplitude for Ps-Ps scattering is considered to be a symmetrized generalization of the Ochkur-Rudge exchange amplitude for electron scattering [16].

After a partial-wave projection of Eq. (1), the resultant one-dimensional scattering equations are solved by the method of matrix inversion. Forty Gauss-Legendre points are used in the discretization of each momentum-space integral.

First we study the binding of Ps\(_2\) using the present coupled-channel approach with Ps(1s)Ps(1s,2s,2p) states. In the singlet channel, this approach leads to a Ps\(_2\) molecule of binding 0.43 eV in excellent agreement with the accurate binding of 0.435445 eV [3] obtained by Frolov and Smith, Jr. using variational method.

In Fig. 1 (a) we present the Ps-Ps singlet \((s_T = 0)\) phase shifts at different Ps-Ps center of mass energies \((E_{\text{c.m.}} = 13.6k^2 \text{ eV})\) in S, P, and D waves. It should be noted that \( E_{\text{c.m.}} = 5.1 \text{ eV} \) corresponds to the first excitation threshold of one of the Ps. In Fig. 1 (b) we present the same for the \( s_T = 2 \) channel. From Fig. 1 (a) we find that there are S- and P-wave resonances in the singlet channel below the lowest excitation threshold of the Ps where the phase shifts jump by \( \pi \). The position and the width of the resonances are obtained by fitting the corresponding cross sections to a Breit-Wigner form. The present S- and P-wave resonance energies are 3.35 eV (width 0.02 eV) and 5.05 eV (width 0.04 eV), respectively. The appearance of these resonances in the electronic singlet state of Ps scattering by atoms with a single active electron seems to be a general phenomena and similar resonances have been found in Ps scattering by H [1] and alkali-metal atoms [4]. The ability of the present approach to reproduce the precise binding of Ps\(_2\) as well as to predict resonances in S and P waves assures us of its realistic nature and the legitimacy to use it in the \( s_T = 2 \) channel, where one has essentially the same set of coupled equations [1] with a change of sign of the exchange Born amplitudes imposed by the condition of antisymmetrization for identical fermions.
Next we report the results for scattering lengths. In the singlet channel $a_0 = 7.46$ a.u. = 3.95 Å, and in the $s_T = 2$ channel $a_2 = 1.56$ a.u. = 0.83 Å. The first is in agreement with the prediction of Platzman and Mills [5] based on qualitative argument: $a_0 \simeq 3$ Å, and should be considered to be refinement over this estimate. In the interaction of two Ps$, only a_2$ is pertinent as the two electrons as well as two positrons have their spins aligned parallel (triplet states) in two Ps$. It is this scattering length which governs the BEC of Ps$.

We exhibit in Fig. 2 the present elastic Ps$(1s)$Ps$(1s)$, and inelastic Ps$(1s)$Ps$(2s)$ and Ps$(1s)$Ps$(2p)$ cross sections at different c.m. energies for Ps-Ps scattering in the two spin states: $s_T = 0$ (full line) and 2 (dashed line). The corresponding exchange Born contribution (dashed-dotted line) to the cross sections is also shown. At high energies the cross sections for both $s_T = 0$ and $s_T = 2$ states tend to the corresponding first Born results and hence to each other as the two Born estimates are the same. We find from Fig. 2 that the energy-dependence of the elastic cross section is similar to that for Ps scattering by H [11] and alkali-metal atoms [14]. The cross section has a monotonic slow decrease with increasing energy. In the $s_T = 0$ channel it also has a local minimum and maximum below the lowest Ps excitation threshold manifesting the S- and P-wave resonances.

Let us see the consequence of the present calculation on the proposed BEC of Ps$^\uparrow$ [5, 6] of $10^5$ Ps$^\uparrow$ atoms in a Si cavity of macroscopic volume $10^{-13}$ cm$^3$ leading to a density $n$ of $10^{18}$ atoms/cm$^3$. The interaction between these atoms will be governed by the scattering length $a_2 \sim 0.8$ Å and $n|a_2|^3$ gives a good measure of the nonideal nature of the condensate. In this case $n|a_2|^3 \sim 10^{-6} << 1$, and the ideal gas BEC critical temperature formula without trap should hold good. The smallness of the scattering length $a_2$ for Ps$^\uparrow$ makes it an excellent candidate for very weakly interacting BEC. We recall that for the experimentally observed BEC in trapped atoms, the relevant scattering length for $^{23}$Na is 27.5 Å, for $^{87}$Rb is 57.7 Å, for $^7$Li is $-14.5$ Å, for $^4$He*(2$^3S_1$) is 16 Å [8, 9]. The larger scattering lengths make these atoms strongly interacting and their condensates should have larger deviation from ideal-gas BEC. In the case of $^7$Li the large negative scattering length implies strong attraction between the atoms which leads to condensate which even experience collapse as the condensate grows in size [9].

Next we study the profile of the BEC of $N$ atoms of Ps$^\uparrow$ in a spherical Si cavity of radius $R$ in the ground S state described by the following mean-field Gross-Pitaevskii (GP) equation in atomic units [10]

$$\left[ -\frac{1}{4}\frac{d^2}{dr^2} + \frac{N a_2}{2} \frac{\phi(r)}{r} \right] \phi(r) = \mu \phi(r),$$

(3)

where $\mu$ is the chemical potential and the radial wave function $\psi(r) = \phi(r)/r$ is normalized according to $\int_0^R |\phi(r)|^2 dr = 1$. As proposed [5] we consider $N = 10^5$ in a spherical cavity of volume $10^{-13}$ cm$^3$ which corresponds to $R = 5440$ a.u.
We solve Eq. (3) variationally subject to the boundary condition $\phi(0) = \phi(R) = 0$ as in a spherical box. In the ideal gas case $a_2 = 0$ and the normalized solution of Eq. (3) is $\phi(r) = \sqrt{2/R} \sin(\pi r/R)$ with $\mu = \pi^2/(4R^2) = 8.34 \times 10^{-8}$ a.u. In Fig. 3 we plot the variational solution of Eq. (3) for $N = 10^5$ and $R = 5440$ a.u. and compare with this ideal-gas result. The variational result for $\mu$ is $4.18 \times 10^{-6}$ a.u. The increase in the value of $\mu$ compared to the ideal-gas case is due to the repulsion among the atoms, which contributes positively. In the ideal gas case the center of the spherical cavity is the region of maximum density. In case of $\text{Ps}^\uparrow$ the region of maximum density has moved away from the central region due to the repulsive interaction between the $\text{Ps}^\uparrow$ atoms. However, as the repulsion among the atoms is weak the wave function of the BEC of $\text{Ps}^\uparrow$ atoms is qualitatively similar to the ideal gas solution. For BEC of trapped bosons because of the attraction of the trapping potential the center of the trap is the region of maximum density for both attractive and repulsive atomic interactions \cite{10}.

In conclusion, we have studied the $\text{Ps}-\text{Ps}$ scattering in a coupled-channel framework allowing the excitation of one of the $\text{Ps}$ atoms to $\text{Ps}(2s,2p)$ states. We report the results for scattering lengths for total spin $s_T = 0$ (3.95 Å) and $s_T = 2$ (0.83 Å), and $\text{Ps}_2$ binding energy (0.43 eV). We also present results for phase shifts in lower partial waves and elastic $\text{Ps}(1s)\text{Ps}(1s)$ and inelastic $\text{Ps}(1s)\text{Ps}(2s,2p)$ cross sections for $s_T = 0$ and $s_T = 2$. We find resonances in S and P waves in the singlet state. The consideration of scattering length shows that $\text{Ps}^\uparrow$ atoms are extremely weakly interacting and constitute excellent candidates for nearly ideal-gas BEC in macroscopic Si cavity without magnetic trap at a relatively high temperature of tens of Kelvin. By explicitly solving the GP equation we show that the wave function of the $\text{Ps}^\uparrow$ in a spherical cavity of volume $10^{-13}$ cm$^3$ is similar to that of ideal gas atoms in the same cavity.

The work is supported in part by the CNPq and FAPESP of Brazil.

References

[1] N. Zafar, G. Laricchia, M. Charlton, and A. Garner, Phys. Rev. Lett. 76, 1595 (1996); M. Skalsey, J. J. Engbrecht, R. K. Bithell, R. S. Vallery, and D. W. Gidley, ibid. 80, 3727 (1998); A. J. Garner, G. Laricchia, and A. Özen, J. Phys. B 29, 5961 (1996); Y. Nagashima, T. Hyodo, K. Fujiwara, and A. Ichimura, ibid. 31, 329 (1998).

[2] N. Jiang and D. M. Schrader, J. Chem. Phys. 109, 9430 (1998), D. M. Schrader, F. M. Jacobsen, N. P. Frandsen, and U. Mikkelsen, Phys. Rev. Lett. 69, 57 (1992); Y. K. Ho, Phys. Rev. A 17, 1675 (1978).

[3] N. Jiang and D. M. Schrader, Phys. Rev. Lett. 81, 5113 (1998); K. Varga, J. Usukura, and Y. Suzuki, ibid. 80, 1876 (1998); A. M. Frolov and V.
H. Smith, Jr., Phys. Rev. A 55, 2662 (1997); D. B. Kinghorn and R. D. Poshusta, ibid. 47, 3671 (1993); Y.-K. Ho, ibid. 33, 3584 (1986).

[4] P. Froehlich, S. Jonsell, A. Saenz, B. Zygelman, and A. Dalgarno, Phys. Rev. Lett. 84, 4577 (2000).

[5] P. M. Platzman and A. P. Mills, Jr., Phys. Rev. B 49, 454 (1994); Physica B 165, 491 (1990).

[6] J. Golovchenko, “11th workshop on low-energy physics with positron and positronium”, Santa Fe, 25–27 July, 2001, to appear in Nucl. Instrum. Method Phys. Res. B.

[7] K. Huang, Statistical Mechanics (Wiley, New York, 1963).

[8] J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 77, 4984 (1996); K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, ibid. 75, 3969 (1995); D. G. Fried, T. C. Killian, L. Willmann, D. Landhuis, S. C. Moss, D. Kleppner, and T. J. Greytak, ibid. 81, 3811 (1998); F. Pereira dos Santos, J. Léonrd, J. Wang, C. J. Barrelet, F. Perales, E. Rasel, C. S. Unnikrishnan, M. Leduc, and C. Cohen-Tannoudji, ibid. 86, 3459 (2001).

[9] C. Sackett, H. T. C. Stoof, and R. G. Hulet, Phys. Rev. Lett. 80, 2031 (1998).

[10] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999); S. K. Adhikari, Phys. Rev. A 63, 043611 (2001); Phys. Lett. A 281, 265 (2001); Phys. Rev. E 62, 2937 (2000); 63, 054502 (2001).

[11] S. K. Adhikari and P. K. Biswas, Phys. Rev. A 59, 2058 (1999).

[12] P. K. Biswas and S. K. Adhikari, Phys. Rev. A 59, 363 (1999).

[13] P. K. Biswas and S. K. Adhikari, Chem. Phys. Lett. 317, 129 (2000).

[14] S. K. Adhikari and P. Mandal, J. Phys. B 34, 1361 (2001); S. K. Adhikari, Phys. Lett. A 283, 224 (2001); P. K. Biswas, Phys. Rev. A 61, 012502 (2000).

[15] P. K. Biswas and S. K. Adhikari, J. Phys. B 33, 1575 (2000).

[16] M. H. R. Rudge, Proc. Phys. Soc. London 86, 763 (1965); V. I. Ochkur, Zh. Eksp. Teor. Fiz. 45, 734 (1963) [Sov. Phys. JETP 18, 503 (1964)].
Figure Caption

1. S- (full line), P- (dashed line), and D-wave (dashed-dotted line) phase shifts of Ps-Ps scattering at different c.m. energies in the (a) $s_T = 0$ and (b) $s_T = 2$ states.

2. Cross section of Ps-Ps scattering at different c.m. energies in the $s_T = 0$ (full line) and $s_T = 2$ (dashed line) states. The corresponding Born contributions (dashed-dotted line) are also shown.

3. The wave function $\psi(r) = \phi(r)/r$ of the BEC of Ps↑ atoms (full line) contrasted with the ideal gas solution (dashed line) in atomic units.
Figure 1 (a)

Phase Shift (radian)

$E_{c.m.} (eV)$

$s T = 0$

S-wave

P-wave

D-wave
Figure 1 (b)
Figure 2

Partial Cross Section (units of πa₀²)

Ps(1s)  
Ps(2p)  
Ps(2s)  

E_c.m. (eV)
