DOUBLY EXCITED RESONANCES IN THE POSITRONIUM NEGATIVE ION

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ABSTRACT

The recent theoretical studies on the doubly excited states of the Ps^- ion are described. The results obtained by using the method of complex coordinate rotation show that the three-lepton system behaves very much like an XYX tri-atomic molecule. Furthermore, the recent investigation on the positronium negative ion embedded in Debye plasma environments is discussed. The problem is modeled by the use of a screened Coulomb potential to represent the interaction between the charge particles.

INTRODUCTION

This paper describes some of the recent research activities on the doubly excited states of the positronium negative ion. The positronium negative ion, Ps^-, is a three-lepton system consists of two electrons and a positron, and interacting with Coulomb potential. Theoretical calculations of the ground state energy of Ps^- have a long history ever since the early work of Wheeler [1]. Activities have been intensified due to, in part, the discovery of such a system by Mills [2], and his measurement of its annihilation rate [3]. The earlier activities on this system have been summarized and discussed in several reviews and papers [4-8]. The present paper reviews the activities starting, for the most part, from the early 1990s. Since that time, precision calculations on the ground state energy of Ps^- have started. Most of the calculations on the non-relativistic ground state energy have achieved accuracy with uncertainty to within 10^{-10} a.u. These include calculations using the Hylleraas basis by Bhatia and Drachman [9] and by Ho [10] with the latter that employed a double sum for the Hylleraas expansions. Other groups have also calculated the ground state energy of Ps^-. These include Ackemann and Shertzer [11] who used a finite-element method, Krivec *et al* [12] used a stochastic variational method, Korobov [13] used a variational method, Frolov and Smith [14] used a variation method with exponential variational expansions, and Drake and co-workers used a variational method with multi-sum Hylleraas basis [15]. Two very recent works --- Drake *et al* used a triple-sum Hylleraas basis [16] and Frolov used an extensive exponential variational expansion [17] --- have obtained accuracy for the non-relativistic ground state energy with uncertainty to within 10^{-20} a. u..

From the experimental side, the Ps^- ion was first observed by Mills [2] in 1981. Very recently, progress has been reported in some new experiments to investigate this system. A group from FRM II in Munich, Germany, has tried to improve the measurement on the annihilation rate of the Ps^- ion [18]. Another group in Aarhus Positron Facility, Denmark, has planned a series of measurements to study such a system [19]. A proposal in their agenda is to determine the binding energy of this ion. Also, a recent experimental development [20] in positron trapping and accumulation technology has opened up the door to study various properties of atomic systems involving positrons and positronium atoms. For a related system that consists of only leptons, the positronium molecule Ps_2 might have been produced in laboratory by Mills and co-workers [21]. All these experimental activities enhance the motivation for theoretical investigations of this pure-lepton system. Another interesting aspect of this system is the calculations of photo-detachment cross sections that have been carried out by several groups

(Bhatia and Drachman [22], Ward, Humberston and McDowell [23], Frolov [24], and Maniadaki, Nikolopoulos, and Lambropoulos [25]). Accurate photo-detachment cross sections would help experimental determination for the binding energy of the Ps$^-$ ion.

The positronium negative ion in many aspects is very similar to its counter-part of hydrogen negative ion. They both have only one bound state, the $1s^2\ ^1S^e$ state, denoted by the usual spectroscopic notation. Many years ago, Drake [26] and Bhatia [27] have calculated the $2p^2\ ^3P^e$ state as a meta-stable state lying below the H (N=2) threshold. A natural question for Ps$^-$ was raised that should there be a similar $2p^2\ ^3P^e$ meta-stable state lying below the Ps (N=2) threshold. Mills [28], and Bhatia and Drachman [29] have addressed such a question and concluded that due to the mass effect, the $2p^2\ ^3P^e$ state could not form binding lying below the Ps (N=2) threshold. Using the hyperspherical coordinates, Botero [30] calculated this state as a shape resonance immediately lying above the Ps (N=2) threshold. Bhatia and Ho [31] using the method of complex-coordinate rotation and employing highly correlated Hylleraas basis have determined the energy and width for the $2p^2\ ^3P^e$ shape resonance of Ps$^-$. In the following the complex-coordinate rotation method will be briefly described, and the applications of this method in calculations of high-lying doubly excited states of the Ps$^-$ ion with differ angular momentum are discussed.

RESONANCE CALCULATIONS

The first theoretical investigation [32] of the resonances in Ps$^-$ was reported in 1979 in which the $2s^2\ ^1S^e$ and $3s^2\ ^1S^e$ resonances were calculated using the method of complex-coordinate rotation [33]. For illustrative purpose, the work is briefly described here. The Hamiltonian of Ps$^-$ is

$$\hat{H} = \hat{T} + \hat{V}, \tag{1}$$

with

$$\hat{T} = -\frac{1}{m_1}\nabla_1^2 - \frac{1}{m_2}\nabla_2^2 - \frac{1}{m_p}\nabla_p^2 \tag{2}$$

and

$$\hat{V} = -\frac{2}{r_{1p}} - \frac{2}{r_{2p}} - \frac{2}{r_{12}} \tag{3}$$

where 1, 2, and p denote the electrons 1,2, and the positron, respectively. The mass for particle i is m_i; and r_{ij} represents the distance between particles i and j. For $^{1,3}S^e$ states, wave functions of Hylleraas-type were used with the form

$$\Phi = \sum_{k\,l\,n} C_{k\,l\,n} \exp[-\alpha(r_{1p} + r_{2p})] r_{12}^n (r_{1p}^k r_{2p}^l \pm r_{1p}^l r_{2p}^k), \tag{4}$$

with $k+l+n \leqq \omega$, where ω, k, l, and n are positive integers or zero. In Eq. (4), the upper sign is for the singlet-spin states, and the lower sign for the triplet-spin states. Also, for the $^1S^e$ states, the summation indexes in Eq. (4) are $k \geqq l \geqq 0$ and $n \geqq 0$. For $^3S^e$ states, the indexes are $k > l \geqq 0$ and $n \geqq 0$. In the complex-rotation method [33], the radial coordinates are transformed by

$$r \rightarrow r\,e^{i\Theta} \tag{5}$$

and the transformed Hamiltonian becomes,

$$\hat{H}_\theta = \hat{T}\exp(-2i\theta) + \hat{V}\exp(-i\theta), \tag{6}$$

where $\widehat{T}$ and $\widehat{V}$ are the kinetic and the Coulomb part of the potential energies, respective, and

$$N_{ij} = \langle \psi_i | \psi_j \rangle \tag{7}$$

are the overlapping matrix elements
and

$$H_{ij} = \langle \psi_i | H(\Theta) | \psi_j \rangle. \tag{8}$$

The complex eigenvalues problem can be solved with

$$\sum_i \sum_j C_{ij} \left(H_{ij} - E N_{ij} \right) = 0 \ . \tag{9}$$

The complex resonance energy is given by

$$E_{res} = E_r - \frac{i\Gamma}{2}, \tag{10}$$

where E_r is related to the resonance energy and Γ the width.

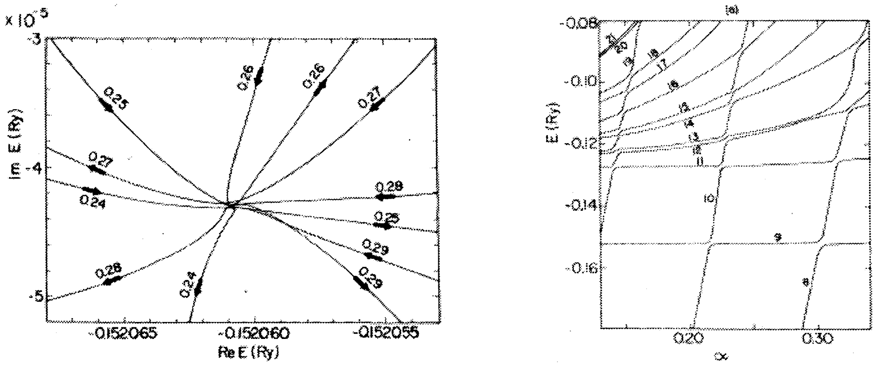


Fig.1. Lowest resonance $2s^2\ {}^1S^e$ of Ps$^-$ below the Ps (N=2) threshold (see Ref. [32]).

Fig. 1(a) shows the lowest resonance $2s^2\ {}^1S^e$ state of Ps$^-$ below the Ps (N=2) threshold obtained by using the method of complex-coordinate rotation (with 161 terms, ω=10). The arrow indicates the direction of the path coming from different directions for increasing rotational angle θ, as various non-linear parameters from the stabilization plateau (Fig. 1(b)) were used. The paths are nearly stationary for θ=0.2 to 0.35 rad when they come across the resonance position [32]. The recent theoretical calculations of some S-wave resonances in Ps$^-$ included the calculations using the method of complex-coordinate rotation by Ho [34] with Hylleraas-type basis, by Usukura and Suzuki [35] with correlated Gaussians and stochastic variational method, and by Li and Shakeshaft [36] using the Pekeris-type basis wave functions. Several groups have also investigated the resonances in Ps$^-$ from scattering approaches. These include the works by Basu and Ghosh [37] using the close coupling method, by Gilmore *et al* [38] using the pseudo-state close coupling approach, and by Igarashi and Shimamura [39] using the close coupling approximation in hyper-spherical coordinates. A different approach was carried out by Papp *et al* [40] to study the resonances in Ps$^-$ using the Faddeev integral equations with Coulomb-Sturmian basis wave functions.

For angular momentum states with L=1 and L=2, Bhatia and Ho [31, 41] have obtained resonance energies and widths using the complex rotation method and employing correlated Hylleraas basis. For high-angular-momentum doubly excited states ($L \geqq 3$) as the two electrons are further apart, the products of Slater orbitals were used to construct the wave functions [42],

$$\begin{aligned}\Psi(\vec{r}_1,\vec{r}_2) = {} & \phi_{n_1 l_1}(r_1)\phi_{n_2 l_2}(r_2) Y^{L,M}_{l_1,l_2}(1,2) S(\sigma_1,\sigma_2) \\ & - \phi_{n_1 l_1}(r_2)\phi_{n_2 l_2}(r_1) Y^{L,M}_{l_1,l_2}(2,1) S(\sigma_2,\sigma_1)\end{aligned}, \tag{11}$$

with
$$\phi_{nl}(r) = r^n \exp(-\xi_l r) \tag{12}$$

and
$$Y^{L,M}_{l_1,l_2}(1,2) = \sum_{m_{l_1} m_{l_2}} C(l_1, l_2, L, m_{l_1}, m_{l_2}, M) Y_{l_1 m_1}(1) Y_{l_2 m_2}(2) , \tag{13}$$

where the $Y_{l_2 m_2}$ etc., are the spherical harmonics. Ivanov and Ho [42] have calculated high-angular-momentum resonances with up to L=8 (L-states) and associated with the Ps (N=3, 4, and 5) thresholds. The results were used to construct supermultiplet structures of the doubly excited states of Ps$^-$.

From the available theoretical results [31, 41, 42], it is apparent that this ($e^- e^+ e^-$) three-body system behaves very much like a tri-atomic XYX molecule, as illustrated in Figs 2-6. Due to the vibrational character of such a molecule, the $^3P^e$ and $^1P^0$ states (see Fig. 2) that have the same "quantum numbers" would be nearly degenerate [43]. This indicates that both the $^3P^e$ and $^1P^o$ states in Ps$^-$ are shape resonances. The rotational character of Ps$^-$ implies that the $^1S^e$, $^3P^0$, and $^1D^e$ states having the same quantum numbers would belong to the same rotor series. In Figs 2-6, each state is classified by a set of quantum numbers (K, T, N, n, L, S, π) where $L, S, N, n,$ and π have the usual spectroscopic meanings. The quantum numbers K and T are "approximately good" quantum numbers, and can be described briefly as follows: K is related to $<-\cos\,\theta_{12}>$, where θ_{12} represents the angle between the two electron vectors. The more positive the value of K, the closer the value of $<-\cos\theta_{12}>$ is to unity. The two electrons in this situation are located near the opposite sides of the position. The quantum number T describes the orientations between the orbitals of the two electrons. For example, a state with T=0 implies that the two electrons are moving on the same plane. The quantum numbers K and T hence describe the angular correlations between the two doubly excited electrons. States having the same KT quantum numbers, hence belonging to the same rotor series, are grouped together. For a given set of K, T, and N, the allowed L values for the doubly excited states are

$$L = T, T+1, \cdots\cdots, K+N-1. \tag{14}$$

The highest L value for a given [K, T] rotor series is therefore governed by the relationship $L_{(max)} = K + N - 1$. For example, when K=4 and N=5 (the [4, 0] series in Fig. 6) the highest L states is an L =8 state (the $^1L^e$ state). Also in Figs. 2-5, we use the results for the doubly excited intrashell states associated with the positronium N=2, N=3, N=4 and N=5 thresholds, respectively, to construct the I-supermultiplet structures [43]. The quantum number "I" is defined as

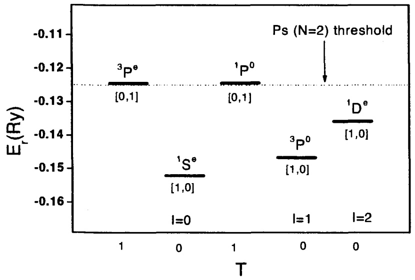


Fig.2. Supermultiplet structures of doubly excited intra-shell states associated with the N=2 Ps threshold. (see Ref. [41, 42]).

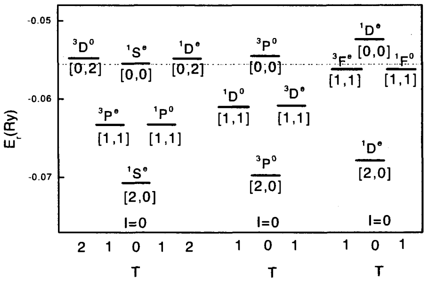
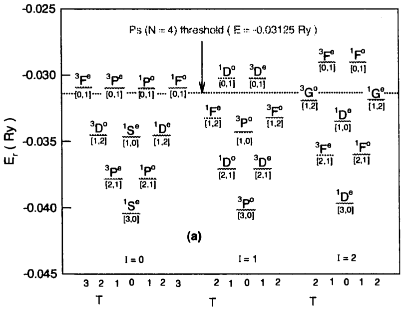


Fig. 3. Supermultiplet structures of doubly excited intra-shell states associated with the N=3 Ps threshold. (see Ref. [41, 42]).



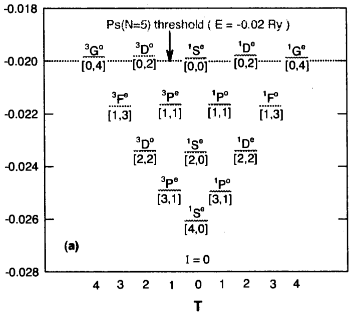


Fig. 4. Vibrational character of the spectra of the doubly excited intrashell states of Ps$^-$ associated with the Ps (N=4) threshold, I values ranging from $I=0$ to $I=2$ [41, 42]

Fig. 5. Vibrational character of the spectra of the doubly excited intrashell states ($I=0$) of Ps$^-$ associated with the Ps (N=5) threshold (see Ref. [42]).

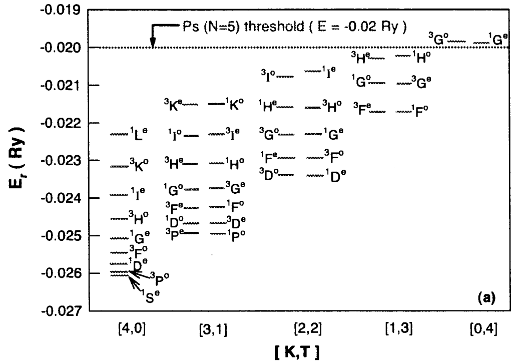


Fig. 6. Rotational character of the spectra of the doubly excited intrashell states of Ps$^-$ associated with the Ps (N=5) threshold. (see Ref. [42]).

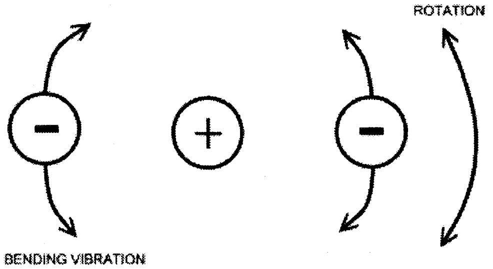


Fig. 7. Doubly excited Ps$^-$ behaves like an XYX tri-atomic molecule.

$$I = L - T, \tag{15}$$

and has the same meaning as the ro-vibrational quantum number R used in molecular physics [43]. For example, states with I=0 are the ground states of various rotor series. From these figures, the vibrational characters of the "molecule" are evident, as shown here in Fig. 7 (Ref.[43, 44]). Other workers have also examined the "molecular" aspects of the positronium negative ion in the literature [45, 46].

In addition to the calculations of the resonance energies and widths for the doubly excited states, the electric-field effects on such states have also been investigated [47]. Fig. 8 shows the Stark effect on the positions of the ${}^1S^e(2)$ and ${}^1P^0(1)$ resonances as a function of the external electric field strength. As these two resonance states are nearly degenerate for the field-free case, they will repel each other when the external field is turned on.

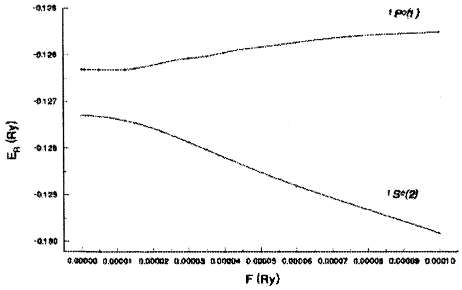


Fig. 8. Positions of the ${}^1S^e(2)$ and ${}^1P^0(1)$ resonances as a function of external electric field intensity (see Ref. [47]).

PLASMAS-EMBEDDED POSITRONIUM NEGATIVE IONS

Very recently, the Ps^- embedded in an external environment such as that of plasma has attracted some attention [48]. With the recent developments in laser plasmas produced by laser fusion in laboratories [49], and the continued interest of helium abundances in astrophysics plasmas [50], as well as the recent activities on cold plasmas, it is important to have accurate atomic data available in the literature for helium atoms in various plasma environments [51, 52]. In the Debye-Hückel model for plasmas, the interaction potential between two charge particles is represented by a Yukawa-type potential,

$$\phi(r_a, r_b) = Z_a Z_b \exp(-\mu|r_a - r_b|)/|\bar{r}_a - \bar{r}_b|, \tag{16}$$

where r_a and r_b represent respectively the spatial coordinates of particles A and B, and Z_a and Z_b denote their charges. The screening parameter μ is given as a function of the temperature T and the charge density n by $\mu = \sqrt{e^2 n / \varepsilon_0 k_B T}$ where n is given as the sum of the electron-density N_e and the ion density N_k of k^{th} ion species having the nuclear charge q_k as $n = N_e + \sum_k q_k^2 N_k$. For laser plasma conditions we have $T \sim 1$ keV, $n \sim 10^{22}$ cm^{-3}, and $\mu \sim 0.1$ to 0.2. Such conditions can now be achieved in the laboratories. The model is appropriate for "hot and dense" and "low-density and warm" plasmas [53, 54].

The non-relativistic Hamiltonian describing the three-lepton system (e^+, e^-, e^-) embedded in Debye plasmas characterized by the parameter D is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{2}\nabla_3^2 - \frac{\exp(-r_{31}/D)}{r_{31}} - \frac{\exp(-r_{32}/D)}{r_{32}} + \frac{\exp(-r_{12}/D)}{r_{12}} \tag{17}$$

For the ${}^1S^e$ states of Ps^- ion, we have employed the wave function [55]

$$\Psi = (1 + P_{12}) \sum_{i=1}^{N} C_i \exp[(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21})\omega] \tag{18}$$

where ω is a scaling constant for calculations of resonances, and P_{12} is the permutation operator defined by $P_{12}f(r_{32},r_{31},r_{12}) = f(r_{31},r_{32},r_{12})$. We have used a quasi-random process to choose the non-linear variational parameters α_i, β_i and γ_i (see Ref. [56]). For the ${}^{1,3}P^o$ states of Ps$^-$, we have employed the wave functions [57]

$$\Psi = (1+S_{pn}P_{12})\sum_{i=1}^{N} C_i r_{31}\cos\theta_1 \exp[(-\alpha_i r_{31} - \beta_i r_{32} - \gamma_i r_{21})\omega]\cdot \tag{19}$$

To extract the resonance energy E_r and the resonance width Γ, we have calculated the density of the resonance states using the stabilization method [58]. For a single energy level the following formula has been used,

$$\rho_n(E) = \left| \frac{E_n(\omega_{i+1}) - E_n(\omega_{i-1})}{\omega_{i+1} - \omega_{i-1}} \right|^{-1}_{E_n(\omega_i)=E} \tag{20}$$

where the index i is the i^{th} value for ω and the index n is for the n^{th} resonance. After calculating the density of resonance states $\rho_n(E)$ with the above formula (18), it can be fitted to the following Lorentzian form that yields resonance energy E_r and total width Γ, with

$$\rho_n(E) = y_0 + \frac{A}{\pi}\frac{\Gamma/2}{(E-E_r)^2 + (\Gamma/2)^2}, \tag{21}$$

where y_0 is the baseline offset, A is the total area under the curve from the base line, E_r is the center of the peak and Γ denotes the full width of the peak of the curve at half height. The method has been used and well tested for resonance calculations in other systems [59]. Fig. 9(a) shows a stabilization plot for the $2s^2\ {}^1S^e$ state of the Ps$^-$, and Fig. 9(b) shows the calculated density of resonance states and a fit to the Lorenztian function with which the resonance energy and width were determined [55, 57]. Fig. 10 shows the ${}^{1,3}P^o$ (1) resonances energies as functions of the Debye length D and of the screening parameter $\mu=1/D$. Depending on the nature of the autoionization mechanism, the width would decrease for the "+" states and increase for "-" states when the screening effect is increased, as shown here in Fig. 11(a) and (b), respectively. Fig. 12(a) illustrates such autoionization mechanism for the "+" and Fig. 11(b) for the "-" states. A more detail discussion for the screening effect on the autoionization widths can be found in Ref. [57].

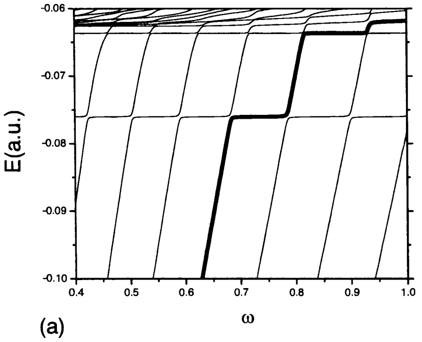


Fig.9a. Stabilization plots of the $2s^2\ {}^1S^e$ state of the Ps$^-$.

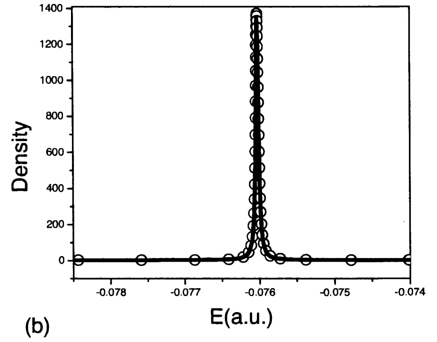


Fig.9b. Calculated density (circles) and in the fitted Lorenztian (solid line) (Ref. [55]).

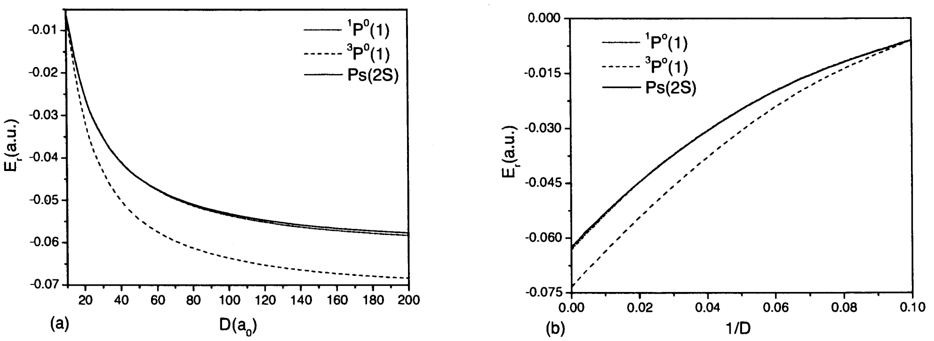


FIG 10. The $^{1,3}P^o$ (1) resonances energies in terms of Debye length D in (a) and in terms of Debye parameter, $1/D$ in (b) along with the $Ps(2s)$ threshold energies (solid line) (Ref. [57]).

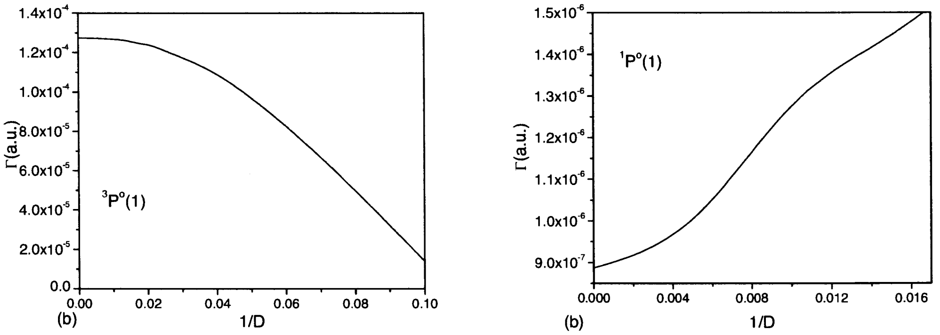
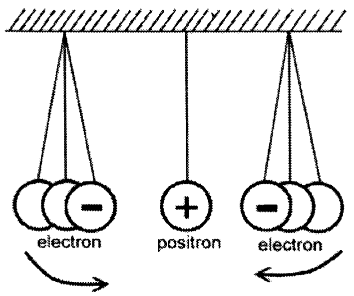


FIG 11. The $^3P^o$ (1) and $^1P^o$ (1) resonances widths as a function of $1/D$ (see Ref. [57]).



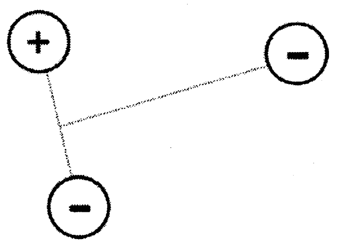


Fig.12 (a) The autoionization mechanism for the "+" states, in which the two electrons are moving toward the positron "in phase."

Fig. 12(b) The autoionization mechanism for the "-" states. An electron is bound temporary to the dipole field of the excited positronium atom.

SUMMARY AND DEDICATION

This paper describes the recent theoretical studies on the doubly excited states of the Ps$^-$ ion using the method of complex-coordinate rotation and the stabilization method. Results show that the doubly excited positronium negative ion behaves very much like a XYX tri-atomic molecule. In addition, the recent investigations on the positronium negative ion embedded in the Debye plasmas have been discussed. Our works has been supported by the Nation Science Council of Taiwan, ROC, and I thank Dr. A. K. Bhatia, Dr. I. A. Ivanov, and Dr. S. Kar for their collaborative works on this interesting system. Last, but not the least, I would like to express my sincere gratitude for being invited to the Temkin-Drachman Retirement Symposium. As a postdoctoral research associate spending two years with this wonderful group during the 1975-1977 periods, I am indebted to Dr. Temkin, Dr. Drachman, and Dr. Bhatia for numerous discussions with them. I got interested in the problem of resonances in Ps$^-$ ion [32] after I have worked with Dr. Temkin and Dr. Bhatia on the benchmark calculation in a related problem, the lowest S-wave resonance in electron-hydrogen scattering using the Feshbach projection operator formalism [60]. I was also benefited from being exposed to the method of complex-coordinate rotation, then a state-of-the-art computational tool for resonance calculations, by discussions on many occasions with Dr. Drachman, who was working on the problem of positronium–hydrogen resonance scattering using this method [61]. It is, therefore, most appropriate to dedicate the present paper to Aaron and Dick on this occasion for Temkin-Drachman Retirement celebration. Here, I wish Aaron and Dick happy retirement, and thank them for their great contributions to the areas of atomic physics and positron physics.

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