Ground state and resonance state of Ps^- in plasmas with various Debye lengths

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We have made an investigation on the resonances for positronium negative ion Ps^- in various model plasma environments. The $2s^2\,{}^1S^e$ autoionization resonance state in Ps^- ion is determined by calculating the density of resonance states using the stabilization method. We have also performed accurate variational calculations to obtain ground-state energy eigenvalues of Ps^- for various Debye lengths. A screened Coulomb potential obtained from the Debye model is used to represent the interaction between the charged particles. A correlated wave function has been used to represent the correlation effect between the three charge particles. The calculated resonance energies and widths for various Debye parameters ranging from infinity to a small value along with the ground-state energies are reported.

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I. INTRODUCTION

The effect of external environments such as that of plasmas on atomic systems are currently interesting topics of research [1–10]. Few theoretical studies have been performed to estimate the ground states [1–8] and resonant states [9,10] of two-electron atoms in Debye plasma environments. In the present investigation, we have made calculations for resonance energies and widths of positronium negative ion Ps^- in model plasma environments. The Ps^- ion consisting of three leptons (e^+,e^-,e^-) is the simplest three-body system. Few experimental investigations [11–14] and several theoretical studies [15–20] are available for the case of a free Ps^-. Mills made an experimental measurement for the annihilation rate of Ps^- [11,12]. An attempt to improve the measurement on the annihilation rate is currently being prepared [13]. Recently, Balling *et al.* [14] discussed the status of the facility and proposed experiments, e.g., multiphoton ionization of Ps and photodetachment of Ps^-. Several calculations are available on the bound state of Ps^- [15–17]. Ho investigated the autoionization states of Ps^- using the complex coordinate rotation method [18,19]. Very recently, Igarashi and Shimamura [20] made a theoretical investigation on the resonances in Ps^- by calculating the time-delayed matrices. Saha *et al.* [21] studied the effect of Debye plasma on the structural properties of a compressed positronium atom. It should be mentioned in this regard that Roussel *et al.* [22] performed a variational calculation of Schrödinger's equation for atomic hydrogen in static screened Coulomb potentials and Rogers *et al.* [23] investigated the bound eigenstates for a two-particle system interacting through a static screened Coulomb potential. The importance of the screened Coulomb potential in the modeling of atomic potential has been discussed in the work of Stein *et al.* [24]. Recently Saha *et al.* [7] calculated the electron affinity of positronium embedded in Debye plasma. In our earlier works, we investigated the $2s^2\,{}^1S^e$ autoionization resonance states of H^- [9] and He [10] in the Debye plasma environments. However, in our earlier study of the $2s^2\,{}^1S^e$ autoionization resonance state in H^- [9], the electron-electron screening was not included. It is also worthy of mention in this context that Wang and Winkler carried out an investigation on resonances for a model screened Coulomb potential [25]. They presented an analytic method for the calculation of shape resonances for a model problem.

In the present work, we have made a theoretical investigation on the ground state and the lowest resonance state of Ps^- when it is embedded in model plasma environments. To our knowledge, no investigation on the *S*-wave autoionization states of Ps^- in Debye plasmas has been reported in the literature. A screened Coulomb potential of Debye type has been chosen to represent the interaction in the Hamiltonian. Correlated wave functions expanded in terms of product basis sets involving inter-particle coordinates are used to represent the correlation effects between the three charge particles. The density of resonance states has been calculated using the stabilization method proposed by Mandelshtam *et al.* [26]. In the course of studying resonances, we have performed accurate variational calculations to obtain the ground state energy eigenvalues of Ps^- for various Debye lengths. Our calculated ground state energies are comparable with the reported results of Saha *et al.* [7]. The convergence of the calculations has been examined with the increasing number of terms in the basis expansion. All the calculations have been preformed on DEC-ALPHA machines using the quadruple precision arithmetic (32 significant figures) in the UNIX environments.

II. THE METHOD

The nonrelativistic Hamiltonian describing the positronium negative ion embedded in Debye plasmas characterized by the parameter D is given by

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

where 1, 2, and 3 denote the two electron 1, 2 and the positron respective and r_{ij} is the relative distance between the

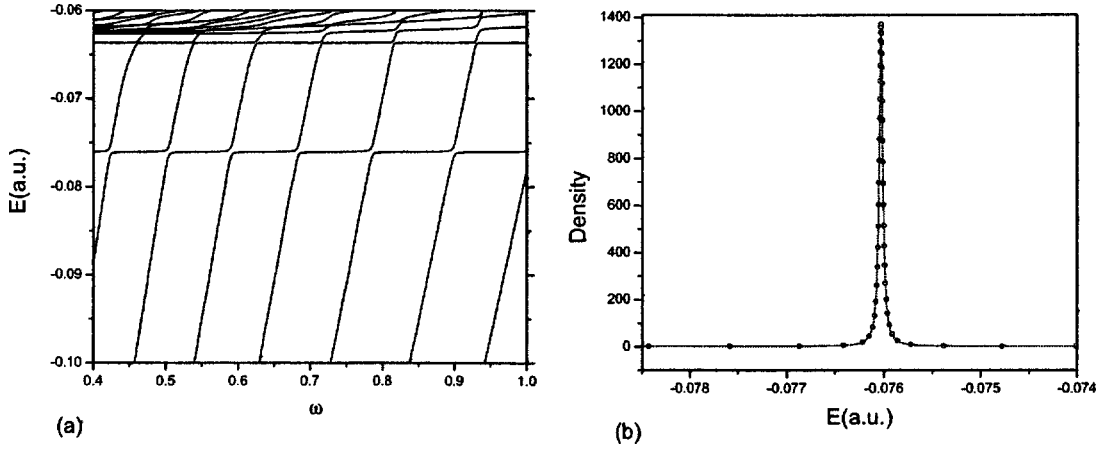

FIG. 1. (a) Stabilization plots for the $2s^2\,{}^1S^e$ state of Ps^-. (b) Calculated density (circles) and the fitted Lorenztian (solid line) corresponding to the $2s^2\,{}^1S^e$ state of Ps^-.

particle i and j. A particular value of the screening parameter D corresponds to the range of plasma conditions, as the Debye parameter is a function of electron density and electron temperature. The smaller values of D are associated with stronger screening. A parametrized screening potential approximated the effects of the plasma charges on the interaction between a bound electron and the atomic nuclei, as well as that between the two electrons.

For the ${}^1S^e$ states of the Ps^- atom, we have employed the wave function

$$\Psi = (1 + P_{12})\sum_{i=1}^{N} C_i \exp[(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21})\omega], \quad (2)$$

where $\alpha_i, \beta_i, \gamma_i$ are the nonlinear variational parameters, $C_i (i=1,\ldots,N)$ are the linear expansion coefficients, ω is a scaling constant to be discussed later in the text, and P_{12} is the permutation operator defined by $P_{12} f(r_{32}, r_{31}, r_{12}) = f(r_{31}, r_{32}, r_{12})$. To obtain the ground-state energy of Ps^- we first set $\omega=1$. The wave functions of Eq. (2) have been widely used in the several bound states calculations of two electron systems in model plasma environments [6,7,10]. Following the work of Frolov [27], we have used a quasirandom process to choose the nonlinear variational parameters α_i, β_i, and γ_i. According to the multibox strategy for constructing highly accurate bound state wave function for three-body systems [27], the parameters α_i, β_i, and γ_i will be chosen from the three positive interval $[A_1^{(k)}, A_2^{(k)}]$, $[B_1^{(k)}, B_2^{(k)}]$, and $[C_1^{(k)}, C_2^{(k)}]$; where $k=\mathrm{mod}(i,3)+1$, $1 \leqslant i \leqslant N$:

$$\alpha_i = \eta_1^{(k)}\left[\left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{2}\right\rangle\right\rangle (A_2^{(k)} - A_1^{(k)}) + A_1^{(k)}\right],$$

$$\beta_i = \eta_2^{(k)}\left[\left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{3}\right\rangle\right\rangle (B_2^{(k)} - B_1^{(k)}) + B_1^{(k)}\right],$$

$$\gamma_i = \eta_3^{(k)}\left[\left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{5}\right\rangle\right\rangle (C_2^{(k)} - C_1^{(k)}) + C_1^{(k)}\right], \quad (3)$$

where the symbol $\langle\langle\cdots\rangle\rangle$ designates the fractional part of a real number. The positive scaling factors $\eta_1^{(k)}$, $\eta_2^{(k)}$, and $\eta_3^{(k)}$ will be equal to 1 in the first stage and in the second stage it will be varied. But for the present problem we have set

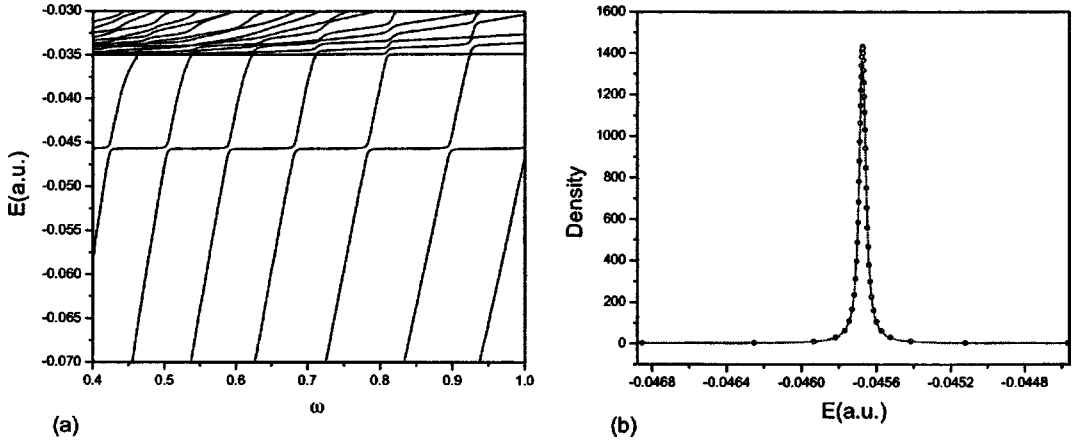

FIG. 2. (a) Stabilization plots for the $2s^2\,{}^1S^e$ state of Ps^- in Debye plasma environments for $D=30$. (b) Calculated density (circles) and the fitted Lorenztian (solid line) corresponding to the $2s^2\,{}^1S^e$ state of Ps^- for $D=30$.

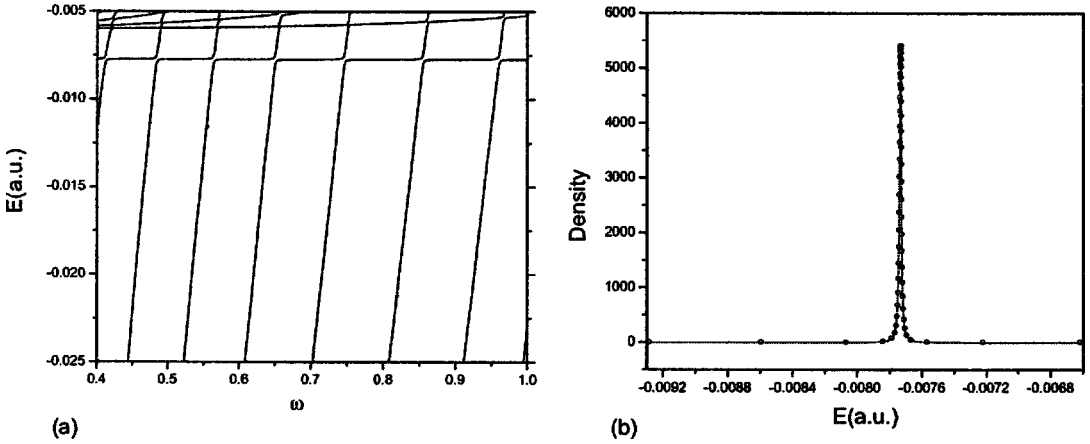

FIG. 3. (a) Stabilization plots for the $2s^2\ ^1S^e$ state of Ps^- in the Debye plasma environments for $D=10$. (b) Calculated density (circles) and the fitted Lorenztian (solid line) corresponding to the $2s^2\ ^1S^e$ state of Ps^- for $D=10$.

$A_1^{(k)}=0, A_2^{(k)}=a$; $B_1^{(k)}=0, B_2^{(k)}=b$; $C_1^{(k)}=0, C_2^{(k)}=c$; and $\eta_1^{(k)}=1, \eta_2^{(k)}=1, \eta_3^{(k)}=\lambda$. Ultimately, four variation parameters a, b, c, and λ are used in the entire calculations.

III. RESULTS AND DISCUSSION

We have used the stabilization method to extract resonance energies and widths by calculating the density of resonance states. After diagonalization of the Hamiltonian (1) using the basis functions (2) with different ω values, we obtained the energy levels $E(\omega)$ which leads to a stabilization plot from which resonance position can be identified. The scaling parameter ω in the wave function [Eq. (2)] can be considered as the reciprocal range of a "soft" wall [28]. Detail discussions are available in the recent work of Kar and

TABLE I. The convergence of resonance energies (E_r) and widths (Γ) using the basis expansion 300, 400, and 500 for Debye parameters $D=1.8$, 2, 4, 9, 10, 20, 50, and infinity, along with the ground-state energies (E_{Ps^-}). The notation A[−B] stands for $A\times10^{-B}$.

		N		
D (a.u.)	Ground-state and resonance energies and width (a.u.)	300	400	500
∞	$-E_{Ps^-}$	0.2620050686	0.2620050701	0.2620050702
	$-E_r$	0.076030	0.076030	0.076030
	Γ	4.30[−5]	4.32[−5]	4.31[−5]
50	$-E_{Ps^-}$	0.2424865646	0.2424865663	0.2424865663
	$-E_r$	0.057024	0.057025	0.057025
	Γ	4.22[−5]	4.27[−5]	4.26[−5]
20	$-E_{Ps^-}$	0.2149738338	0.2149738357	0.2149738358
	$-E_r$	0.033172	0.033172	0.033172
	Γ	3.62[−5]	3.66[−5]	3.64[−5]
10	$-E_{Ps^-}$	0.1736181575	0.1736181598	0.1736181600
	$-E_r$	0.007736	0.007736	0.007736
	Γ	1.17[−5]	1.16[−5]	1.16[−5]
9	$-E_{Ps^-}$	0.1651598570	0.1651598595	0.1651598596
	$-E_r$	0.004629	0.004629	0.004629
	Γ	7.5[−6]	6.31[−6]	6.32[−6]
4	$-E_{Ps^-}$	0.0798460693	0.0798460754	0.0798460757
3	$-E_{Ps^-}$	0.0449254087	0.0449254114	0.0449254117
2	$-E_{Ps^-}$	0.0059655900	0.0059656590	0.0059656643
1.8	$-E_{Ps^-}$	0.0011178572	0.0011183487	0.0011184443

TABLE II. Comparison of the ground-state energies of $Ps^-(E_{Ps^-})$ with the reported results of Saha *et al.* [7] along with the electron affinity $(E_{Ps}-E_{Ps^-})$ of positronium.

D	$-E_{Ps^-}$	$-E_{Ps}$	$E_{Ps}-E_{Ps^-}$
∞	0.2620050702	0.250000000	0.012005070
	0.2620050702[a]	(exact)	0.012005068[b]
	0.262005068[b]		
100	0.2521260115	0.240148053[b]	0.0119779585
	0.252126009[b]		0.011977956[b]
70	0.2479656736		
50	0.2424865663	0.230584818[b]	0.0119017483
	0.242486564[b]		0.011901746[b]
40	0.2377556768		
30	0.2300010975		
20	0.2149738358	0.203529015[b]	0.0114448208
	0.214973833[b]		0.011444818[b]
15	0.2005771456		
10	0.1736181600	0.163340426[b]	0.0102777340
	0.173618156[b]		0.010277730[b]
9	0.1651598596		
8	0.1549479742		
7	0.1423956851		
6	0.1266427187		
5	0.1064096775	0.099188041[b]	0.0072216365
	0.106409646[b]		0.007221605[b]
4	0.0798460757	0.074058510[b]	0.0057875657
	0.079845972[b]		0.005787462[b]
3	0.0449254117		
2	0.0059656643	0.005142875[b]	0.0008227893
	0.005908326[b]		0.000765451[b]
1.8	0.0011184443		

[a]Refs. [15–17].
[b]Ref. [7].

Ho [28]. Varying the Debye length D from infinity to small values, different resonance parameters (energy and width) have been obtained.

To extract the resonance energy E_r and the resonance width Γ, we have calculated the density of resonance states for a single energy level with the help of the following formula;

TABLE III. The resonance energy (E_r) and width (Γ) of the Ps^- ion for various Debye parameters. The notation A[$-B$] stands for $A\times10^{-B}$. Results are in atomic units.

D	$-E_r$	Γ
∞	0.076030	4.31[−5]
	0.07603044[a]	4.3034[−5][a]
	0.076029[b]	4.3[−5][b]
100	0.066260	4.31[−5]
70	0.062231	4.29[−5]
50	0.057025	4.26[−5]
40	0.052633	4.21[−5]
30	0.045674	4.09[−5]
20	0.033172	3.64[−5]
15	0.022642	2.95[−5]
10	0.007736	1.16[−5]
9	0.004629	6.32[−6]

[a]Ref. [19].
[b]Ref. [20].

$$\rho_n(E) = \left| \frac{E_n(\omega_{i+1}) - E_n(\omega_{i-1})}{\omega_{i+1} - \omega_{i-1}} \right|^{-1}_{E_n(\omega_i)=E}, \tag{4}$$

where the index i is the ith value for ω and the index n is for the nth resonance. After calculating the density of resonance states $\rho_n(E)$ with the above formula (4), we fit it to the following Lorentzian form that yields resonance energy E_r and total width Γ, with

$$\rho_n(E) = y_0 + \frac{A}{\pi} \frac{\frac{\Gamma}{2}}{(E-E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}, \tag{5}$$

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.

To construct the stabilization plot, we have used an expansion length of $N=500$ in the basis function (2). The stabilization diagram [in Fig. 1(a)] corresponding to the Debye length D tends to ∞ (a.u.) in the range of $\omega=0.4-1.0$ shows the stabilization character near $E=-0.076$ (a.u.). We use 301 points to cover the range of ω from 0.4 to 1.0 in the mesh size of 0.002. We have calculated the density of resonance states for the individual energy levels in the range $\omega=0.4$ to 1.0, with one energy level at a time. The calculated density of resonance states from the single energy eigenvalue is then fitted to Eq. (5), and the one that gives the best fit (with the least chi square) to the Lorentzian form is considered as the desired results for that particular resonance. Figure 1(b) shows the fitting of the density of resonance states for the

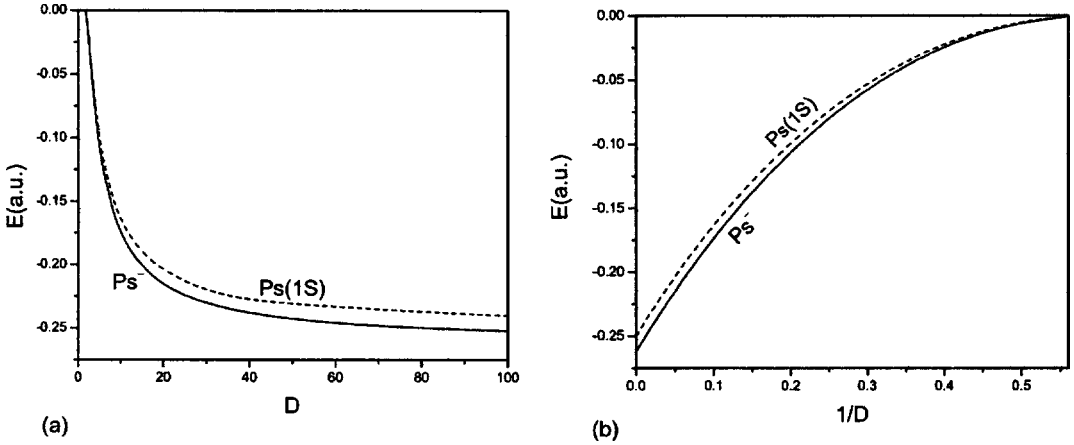

FIG. 4. (a) The ground state energy of Ps^- for various Debye length D. (b) The ground-state energy of Ps^- for different values of $1/D$. Dashed line denotes the Ps(1S) threshold energy.

20th eigenvalue of the stabilization plot. From the fit, we obtain the resonance energy $E_r=-0.076030$ a.u. and the corresponding width as $\Gamma=4.31\times10^{-5}$ a.u. The resonance energy and width are nicely comparable with the reported results of Ho [19] and Igarashi *et al.* [20]. The circles are the results of the actual calculations of the density of resonance states using formula (4) and the solid line is the fitted Lorentzian form of the corresponding $\rho_n(E)$. The stabilization plots in Figs. 2(a) and 3(a) for $D=30$ and $D=10$, respectively, show the stabilization character near the energy $E=-0.046$ (a.u.) and $E=-0.0077$ (a.u.). Figures 2(b) and 3(b) show the fittings of the density of resonance states for the 21st and 17th eigenvalues, respectively, corresponding to the stabilization plots in Figs. 2(a) and 3(a).

Table I shows the convergence of the ground state energies, resonance energies and the widths for $N=300$, 400, and 500 basis terms with $D=1.8$, 2, 3, 4, 9, 10, 20, 50, and infinity. For $N=300$ and 400 terms we have used the same parameters as those for the 500-term basis functions. It is seen from Table I that the convergence of the resonance energies and widths are quite good. In the present work, before we calculate the resonances for Ps^- in Debye plasmas, we first optimize the nonlinear parameters in Eq. (2) to obtain an accurate ground state energy of Ps^- for different Debye parameters. The ground-state energies of Ps^- ion (E_{Ps^-}) obtained from our calculations for various Debye lengths are presented in Table II, along with the ground-state energies of Ps (E_{Ps}) and the calculated electron affinity ($E_{Ps}-E_{Ps^-}$) of the positronium atom. The ground state energies of positronium atom (E_{Ps}) are taken from the reported results of Saha *et al.* [7]. For the Debye length tends to infinity, our calculated ground-state energy value of −0.2620050702 a.u. reported in Table II compares well with the best results of −0.2620050702 a.u. available in the literature [15–17]. We have compared our calculated ground-state energies of Ps^- ion with the available results of Saha *et al.* [7] for various Debye lengths in Table II, along with the electron affinity of the Ps atom. Our calculated ground-state eigenenergy values for $D=2,\ldots,100$ are lower than those published in the literature. All the results presented in Table II are for the $N=500$ basis function of Eq. (2).

It is also interesting to mention here that the same set of nonlinear parameters are needed in our calculations for the optimization of the ground-state energies up to $D=4$. The best values of this parameters are $a=2.84$, $b=2.34$, $c=0.30$, and $\lambda=0.44$. For $D\leqslant3$, we have observed that the only

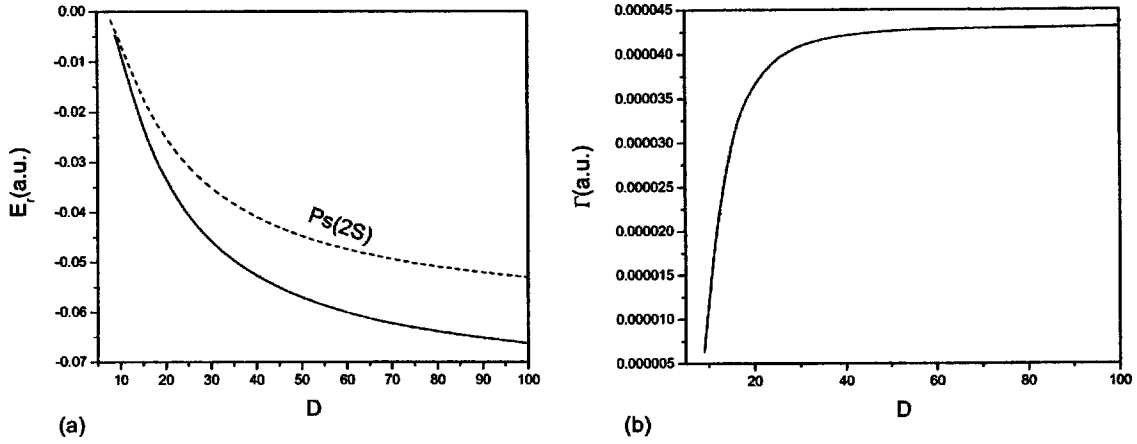

FIG. 5. (a) The $2s^2\,{}^1S^e$ resonance energy E_r for different values of Debye parameter D (solid line). The dashed line denotes the Ps(2S) threshold energy. (b) Resonance width Γ corresponding to the resonance energy in (a) for different values of Debye parameter D.

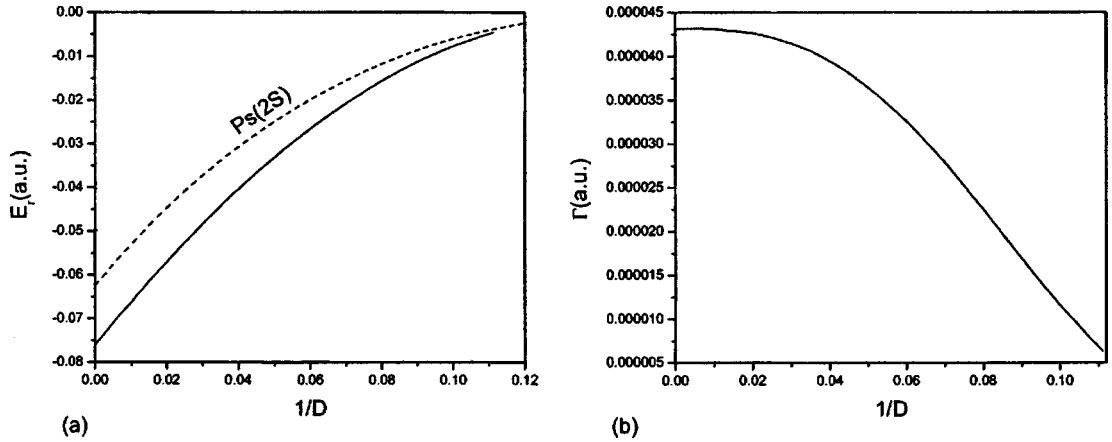

FIG. 6. (a) The $2s^2\,{}^1S^e$ resonance energy E_r as a function of $1/D$ (solid line). The dashed line denotes the Ps($2S$) threshold energy. (b) Resonance width Γ corresponding to the resonance energy in (a) as a function of $1/D$.

variations in the scaling factor λ are sufficient for optimization of the ground-state energies using 500 basis terms. The value of λ is equal to 0.3, 0.24, and 0.16 for $D=3$, 2, and 1.8 respectively. We have not optimized the ground-state energies using 300 or 400 terms.

Table III presents the resonance energies and widths for various Debye lengths ranging from infinity (corresponding to no screening) to a small value 9 (corresponding to strong screening) along with the nonlinear parameters used in the wave functions. The results for the $2s^2\,{}^1S^e$ resonant state of Ps^- ion are comparable with the reported results of Ho [19] and Igarashi and Shimamura [20].

All the results shown in Figs. 1–6 and Tables II and III are obtained using the 500-term wave functions. The ground-state energies of Ps^- obtained from our calculations are presented in Figs. 4(a) and 4(b) as functions of D and $1/D$, respectively, along with the Ps($1S$) threshold energy. The Ps($1S$) threshold energy values are taken from the reported results of Saha *et al.* [7]. Our calculated resonance energies associated with the Ps($N=2$) threshold are shown in Figs. 5(a) and 6(a), along with the Ps($2S$) threshold energies for different values of D and $1/D$, respectively, with the corresponding widths are plotted in Figs. 5(b) and 6(b). The values of Ps($2S$) energy are taken from the reported results of Rogers *et al.* [23] by considering the Ps($2S$) threshold energy as the half of $H(2S)$ threshold with the proper scaling of D. It is apparent from Table II and Fig. 4 that the system will be gradually destabilized with stronger Debye screening and ultimately the system will be ionized. The threshold value of Debye length for which the system will be ionized is about $D=1.8$.

From Fig. 5(b) and Table III, it is seen that the resonance width Γ decreases with decreasing value of D. The situation can be explained in the following way: The $2s^2\,{}^1S^e$ state in Ps^- is a "+" state, and the two electrons are located on opposite sides of the positron. The movements of the two electrons are moving toward the positron "in phase." The autoionization of such a state is through the momentum transfer, as one of the electrons is "knocked out" by the other via the positron. Apparently, when the electron-positron screening is increased (decreasing D, increasing $1/D$), the movement of the electrons will be slowed down. As a result, the lifetime of the autoionization process will be prolonged, leading to the narrowing of the resonance width, a consequence of the uncertainty principle.

It should be mentioned here that we have not found any resonances for $D\leqslant 8$. If a resonance were to exist for $D\leqslant 8$, it would be located at a region very near the Ps($2S$) threshold. However, calculations for such resonances would require more extensive basis sets in the wave functions, and no attempt is made to carry out large-scale calculations here. It is of interest to search for such resonances in future investigations.

IV. CONCLUSIONS

This work presents a calculation of the $2s^2\,{}^1S^e$ autoionization resonance for positronium negative ion embedded in Debye plasma environments. The $2s^2\,{}^1S^e$ state resonance energies and widths for various Debye parameters ranging from infinity to small value (up to 9) have been reported. The accurate ground state energies have also been reported for the Debye length ranging from infinity to small values (up to 1.8). The stabilization method is used to extract resonance energies and widths. This method is a practical method to calculate resonance parameters (E_r,Γ). Our present work will provide useful information to the plasma physics research community, as well as to the positron physics community that is interested in such a three-lepton system.

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