Resonances in positronic lithium in hot and dense plasmas

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Low-lying S-wave resonances in positronic lithium (e^+Li) under hot and dense plasmas are investigated by the stabilization method. The screened interaction in plasma is represented by the Debye-Hückel model. Two resonances are located lying below the Ps($n = 2$) excitation threshold. It is found that resonance positions are lifted with increasing plasma screening strength. For the free atomic system, our reported results are in agreement with the results of other reliable calculations.

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I. INTRODUCTION

Theoretical calculations show that a positron can bind itself to the ground state of a lithium atom to form a positronic lithium atom (e^+Li) [1–8]. In fact, positronic lithium is the first atom that showed that a positron is able to bind itself to the ground state of a neutral atom [1]. The ground state of positronic lithium has a binding energy of 0.002 484 a.u. and is electronically stable against decay into both the Li-e^+ and Li^+-Ps channels [6]; however, it is not stable against electron-positron annihilation. Besides the ground state of lithium, the positron can also attach itself to a number of excited states of the lithium atom [1]. Such states can be viewed as excited states of e^+Li and would open the possibility of spectroscopic detection of this system [1]. There is also calculational evidence that positrons can form bound states with a variety of atoms such as positronic sodium and positronic calcium [9–14]. The existence of positron bound states with neutral atoms and molecules has important implications for positron and positronium (Ps) chemistry [15]. One possible signature for positron-atom binding is the existence of resonant structures associated with atomic excited states in the positron scattering spectrum. The bound or quasibound (resonance) of positron and Ps to atoms and molecules has been a subject of extensive study (see [2–26] and references therein). Large Feshbach resonances have been observed in annihilation cross sections corresponding to the formation of positron-molecule bound states, providing strong evidence that such states also exist for molecules [27]. However, experimental evidence of positron-atom bound states has proven to be evasive [9]. In the case of the positron-lithium system, experimental results relating to cross sections have been found [28,29], but their energy resolution is not adequate to map out the resonance structure.

In this paper we look for S-wave resonances lying below the Ps($n = 2$) excitation threshold in positronic lithium under hot and dense plasmas. The existence of such low-lying S resonances, as a rule, leads to a resonant radiative recombination (RRR) process, which is bound to take place in dense plasma. The RRR process is likely to dominate recombination rates in the low-energy regimes where the wavelength of the electron is much larger than the range of the potential. Moreover, the observational evidence of the existence of positrons in several astrophysical plasma environments [30–33] suggests that we examine positron scattering phenomena in plasma environments. In astrophysical environments, such as of compact objects and inertial confinements, plasma remains hot and dense. The ranges of density N_e and temperature T_e are around 10^{20}–10^{23} cm^{-3} and 10^7–10^8 K, respectively [34,35], whereas the Debye length λ_D for such plasmas is known to be $\lambda_D \geqslant 10a_0$, where a_0 is the first Bohr radius of the hydrogen atom. These plasmas can be classified as Debye plasmas or weakly coupled plasmas. For these plasmas, the coupling parameter Γ (ratio of the potential energy to the average kinetic energy) is much less than unity. These conditions are also fulfilled in a wide class of laboratory plasmas. In a Debye-type plasma, it is known that the short-range potential around a unit test charge scales as the Debye-Hückel potential or static screened Coulomb potential (SSCP) [36] (in a.u.)

$$V(r) = e^{-r/\lambda_D}/r. \tag{1}$$

Here $\mu = 1/\lambda_D$ is called the plasma screening parameter. The Debye length is related to the thermal velocity v_T and plasma frequency ω_P by the formula $\lambda_D = v_T/\omega_P$. In a Debye plasma the interaction screening is the collective effect of the correlated many-particle interactions and in the lowest particle correlation order it reduces to a SSCP of the form (1). This paper aims at looking for S-wave resonances lying below the Ps($n = 2$) excitation threshold in the e^+-Li system under Debye-type plasmas by applying a stabilization method. Atomic units will be used in the rest of the paper unless explicitly stated otherwise.

II. THEORY AND CALCULATIONS

Carrying out calculations on resonances by applying the stabilization method in a multibody system such as the positron-lithium system requires enormous computational effort. In order to reduce computational effort, here we resort to the model potential method to treat the positron-lithium system as a three-body system. In the model potential method, the lithium atom is treated as a two-body system consisting of a positive ionic core (Li^+) together with an electron (active). The interaction between the electron and the ionic core is then represented by a model potential, whereas the core includes the average effect of all other electrons (passive). Considering

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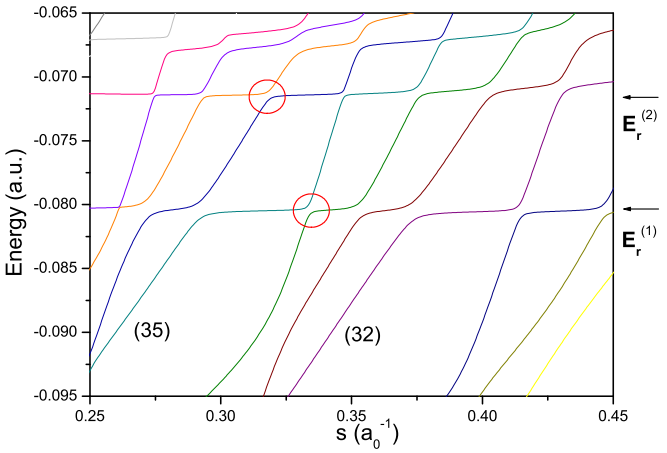

FIG. 1. Stabilization plot for $\mu = 0.0$ and $\omega \leqslant 14$ ($N = 680$). The number in parentheses next to the solid line shows the order of appearance of the eigenvalues (energy levels). The arrows indicate the positions of resonances. The circles show the point of avoided crossing.

the interactions among the electrons in the atom, the potential between the ionic core and the active electron is so constructed that it corresponds to the energy of the original atom. We assume that the ionic core Li^+ is infinitely heavy. Let $\vec{r}_1$ and $\vec{r}_2$ denote, respectively, the coordinates of positron and the active electron relative to the core and $\vec{r}_{12}$ $(= \vec{r}_1 - \vec{r}_2)$ is the coordinate of the positron relative to the active electron. The average effect of the passive electrons is taken care of by simulating the multielectron core interaction with the single valence electron in an analytical modification of the Coulomb potential such that

$$\lim_{r_2\to\infty}\left[V_m^{(e^-)}(\vec{r}_2)\right] = \lim_{r_2\to\infty}\left(-\frac{\tilde{Z}}{r_2}\right),$$
$$\lim_{r_2\to 0}\left[V_m^{(e^-)}(\vec{r}_2)\right] = \lim_{r_2\to 0}\left(-\frac{Z}{r_2}\right), \tag{2}$$

where Z is the nuclear charge and $\tilde{Z}$ is the ionization stage defined by $\tilde{Z} = Z - N_c$, with N_c being the number of electrons in the core shell. Details of various aspects of the model potential method have been considered in several studies [37–40]. In the present work, to represent the interaction between the ionic core Li^+ and the electron in vacuum we use the following model potential:

$$V_m^{(e^-)}(\vec{r}_2) = -\frac{1}{r_2}[\tilde{Z} + N_c(e^{-2\alpha r_2} + \beta r_2 e^{-2\gamma r_2})], \tag{3}$$

where α, β, and γ are parameters to be determined. This model potential function satisfies the asymptotic conditions (2). In order to determine the parameters α, β, and γ we solve the corresponding one-electron Schrödinger equation within the framework of the Rayleigh-Ritz variational principle by employing Slater-type orbitals

$$\phi_{nlm}(\vec{r}_2) = R_{nl}(r_2)Y_{lm}(\theta_2,\phi_2) = \left[\sum_i C_i e^{-A_i r_2} r_2^{l_i}\right] Y_{lm}(\theta_2,\phi_2), \quad l_i = 0,1,2,\ldots, \tag{4}$$

where C_i are the normalization constants and A_i are variational parameters. The values of the parameters are then obtained by optimizing the Hamiltonian matrix elements with respect to the parameters so that the resulting energies are in agreement with the experimental results. In view of Eqs. (1) and (3), we represent the interaction between the ionic core and the electron in Debye plasma by the potential (in a.u.)

$$V_m^{(e^-)}(\vec{r}_2) = -\frac{e^{-r_2/\lambda_D}}{r_2}[\tilde{Z} + N_c(e^{-2\alpha r_2} + \beta r_2 e^{-2\gamma r_2})]. \tag{5}$$

The above potential with opposite sign is used to represent the interaction potential between the core and the positron $V_m^{(e^+)}(\vec{r}_1)$, that is,

$$V_m^{(e^+)}(\vec{r}_1) = \frac{e^{-r_1/\lambda_D}}{r_1}[\tilde{Z} + N_c(e^{-2\alpha r_1} + \beta r_1 e^{-2\gamma r_1})]. \tag{6}$$

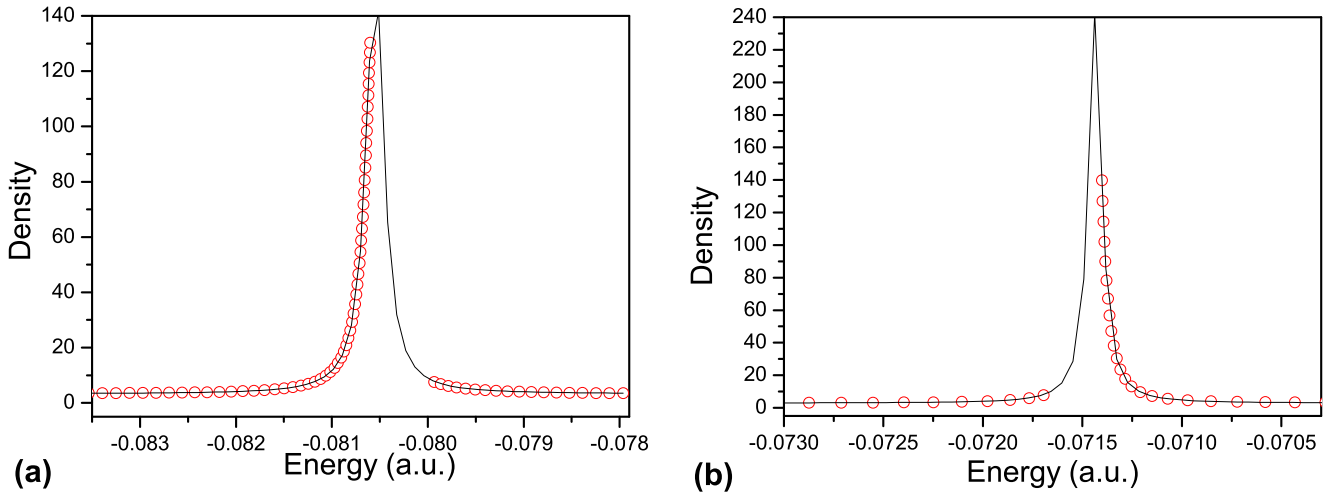

FIG. 2. Fittings of the density of resonance states to the Lorentzian form for the lowest two resonances below the Ps($n = 2$) threshold in positronic lithium for $\mu = 0$. The circles are the calculated values and the solid line is the fit function. (a) The resonance parameters are determined to be $E_r = -0.080\,550$ a.u. and $\Gamma = 0.000\,22$ a.u. using 34th and 35th eigenvalues. (b) The resonance parameters are determined to be $E_r = -0.071\,436$ a.u. and $\Gamma = 0.000\,08$ a.u. using 38th and 39th eigenvalues.

TABLE I. Energy levels (in a.u.) of lithium relative to ionization limit for various Debye lengths $\lambda_D = 1/\mu$.

	States				
μ	$2s$	$3s$	$4s$	$5s$	$6s$
0.00	−0.198141	−0.074310	−0.038677	−0.023640	−0.015642
[a]	−0.19816	−0.07419	−0.03862	−0.02364	−0.01595
[b]	−0.19814	−0.07418	−0.03862	−0.02364	−0.01594
[c]	−0.19815	−0.07415	−0.03862	−0.02364	−0.01595
[d]	−0.198141				
0.01	−0.188122	−0.064751	−0.029567	−0.015063	−0.007446
[d]	−0.188122				
0.02	−0.178471	−0.056104	−0.022068	−0.008887	−0.001872
[d]	−0.178471				
0.03	−0.169174	−0.048288	−0.015946	−0.004601	
0.04	−0.160220	−0.041237	−0.011022	−0.001742	
[d]	−0.160220				
0.05	−0.151597	−0.034894	−0.007156		
[d]	−0.151597				
0.06	−0.143293	−0.029211	−0.004234		
0.07	−0.135299	−0.024144	−0.002146		
0.08	−0.127606	−0.019655	−0.000755		
0.09	−0.120206	−0.015710			
0.10	−0.113089	−0.012276			
[d]	−0.113089				

[a]Experimental results of Johansson [47].
[b]Experimental results of Bashkin and Stoner [48].
[c]Theoretical results of Laughlin and Victor [38].
[d]Theoretical results of Sahoo and Ho [49].

As this interaction includes the effect of exchange between the positron and the electron, it is a bit more repulsive than the real physical situation, so our reported energies may lie a bit higher than the true resonance energies. With this choice of model potential, the nonrelativistic Hamiltonian (in a.u.) of positronic lithium under a Debye plasma, characterized by the Debye-Hückel potential (1), is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + V_m^{(e^+)}(\vec{r}_1) + V_m^{(e^-)}(\vec{r}_2) - \frac{e^{-r_{12}/\lambda_D}}{r_{12}}. \quad (7)$$

We now apply stabilization method to determine resonances in positronic lithium. Various aspects of the stabilization method that we use in the present work have been described in detail in a number works by Ho and co-workers [41–45], so here we just state the salient features of the method, which are required for implementation of the method. Implementation of the method consists of four major steps. In the first step, eigenenergies of the Hamiltonian are calculated, for a certain range of the scaling parameter $0 < s < 1$, by employing an extensive wave function Ψ that includes the scaling parameter. In the present investigation we choose the following wave function:

$$\Psi(\vec{r}_1,\vec{r}_2) = \sum_{i=1}^{N} \psi_i(r_1,r_2,r_{12}) = \sum_{l_i+m_i+n_i=0}^{\omega} C_{l_i m_i n_i} e^{-s(r_1+r_2)} r_1^{l_i} r_2^{m_i} r_{12}^{n_i}, \quad (8)$$

where $C_{l_i m_i n_i}$ is linear expansion coefficient and l_i, m_i, n_i, $\omega \in \mathbb{Z}^*$ is the set of non-negative integers. Thus $\omega = 0$ corresponds to $N = 1$, $\omega = 1$ corresponds to $N = 4$, and so on. In the second step, energy eigenvalues of the Hamiltonian are plotted as a function of the scaling parameter. This plot is referred to as a stabilization plot or stabilization diagram (shown in Fig. 1). The appearance of a stabilized energy level (slowly varying energy level) at the energy E_r indicates the existence of a resonance state with energy E_r. It should be mentioned that the wave function should be an extensive one in order to be able to predict a resonance. In the third step, the density of the resonance state is calculated for each energy level near the avoided crossing at E_r by the formula

$$\rho_n(E) = \left[\frac{s_{i+1} - s_{i-1}}{E_n(s_{i+1}) - E_n(s_{i-1})}\right]_{E_n(s_i)=E}, \quad (9)$$

where the index i is the ith value for s and the index n is for the nth resonance. In the fourth step, the resonance energy E_r and width Γ are determined by fitting the density of the resonance state $\rho_n(E)$ for each pair of consecutive energy levels near the avoided crossing (indicated in Fig. 1) to the following Lorentzian form:

$$\rho_n(E) = y_0 + \frac{A}{\pi}\frac{\frac{\Gamma}{2}}{(E - E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}, \quad (10)$$

where y_0 is the baseline offset, A is the total area under the curve from the baseline, E_r is the center of the peak, and Γ denotes the full width of the peak of the curve at half height (as shown in Fig. 2). From the above Lorentzian fitting we obtain the resonance energy E_r and resonance width Γ corresponding to each stabilized energy level. Out of all those fittings, the one that corresponds to the best fitting is considered the desired result for that particular resonance. The best fitting means that fitting for which the value of the coefficient of determination (the square of the correlation coefficient between the sample and predicted data) is closest to unity. It should be mentioned that Hazi and Taylor [46] used the stabilization method for calculating resonance energies of model problems.

TABLE II. Lowest S-wave resonance energy and width below the Ps($n = 2$) threshold in positronic lithium.

	$-E_r^{(1)}$ (a.u.)			$\Gamma^{(1)}$ (a.u.)		
μ	$N = 455$ ($\omega = 12$)	$N = 560$ ($\omega = 13$)	$N = 680$ ($\omega = 14$)	$N = 455$ ($\omega = 12$)	$N = 560$ ($\omega = 13$)	$N = 680$ ($\omega = 14$)
0.00	0.080400	0.080454	0.080550	0.00024662	0.00019317	0.00021503
0.01	0.070629	0.070683	0.070781	0.0002414	0.00019122	0.00021308

TABLE III. Comparison of the S-wave resonance energy E_r and width Γ for positronic lithium in vacuum. The quoted values of resonance energy E_r are relative to the Li($2s$) state with an energy of -0.198141 a.u.

Parameter	Present work	Ref. [19]	Ref. [17]	Ref. [16]	CC5 of [21]	MP1 of [24]	Potential V of [25]
$E_r^{(1)}$ (a.u.)	0.117591	0.117483	0.117451	0.110615	0.110836	0.117517	0.117498
$\Gamma^{(1)}$ (a.u.)	0.00022	0.00020[a]	0.00021	0.00147	0.00276	0.00023	0.00013
$E_r^{(2)}$ (a.u.)	0.126705	0.124209	0.125609	0.123661	0.124029		
$\Gamma^{(2)}$ (a.u.)	0.00008	0.00004	0.00008	0.00004	0.00096		

[a]This number is taken from the text of Han *et al.* [19]. The number reported by them in Table I is 2.93 eV.

III. RESULTS AND DISCUSSION

We have examined the fitness of the model potential (5) by calculating the binding energies of the lithium atom. The optimized values of the parameters in the potential (5) have been obtained as $\alpha = \beta = \gamma = 1.6559$. It should be mentioned that the equality of the parameters α, β, and γ is a mere coincidence. The same model potential (5) can be used to represent Na($1s^2 2s^2 2p^6 nl$). In this case α, β, and γ have been found to be $\alpha = 1.8321$, $\beta = 1.0591$, and $\gamma = 1.3162$, respectively. The ground-state energies of the lithium atom for various Debye lengths are shown in Table I. From Table I we notice that our present results for the binding energies of the lithium atom are in close agreement with the experimental observations [47,48] and the theoretical predictions [38,49]. Below the Ps($n = 2$) excitation threshold we have found two S-wave resonances. The positions of those resonances are indicated by arrows in the stabilization plot in Fig. 1. The convergence of the resonance parameters with an increase in the number of terms of the wave function (8) for the lowest S-wave resonance below the Ps($n = 2$) excitation threshold is shown in Table II. It should be mentioned that for each best fitting the value of the coefficient of determination R^2 is at least of the order of 0.999 996, which is an indication of good fitting. In all cases, the scaling parameter s is given an increment of 0.0005. From Table II it is apparent that it is possible to obtain convergent results for the resonance energies correct up to three significant digits by using $N = 680$ ($\omega = 14$) terms in the wave function (8). The uncertainty in our reported results lies in the fourth significant digit. All other reported results of resonance parameters have been obtained by using 680 terms in the wave function (8). For a given Debye length all 680 eigenvalues of the Hamiltonian (7) have been calculated for various values of the scaling parameter s within the range $0.25 \leqslant s \leqslant 0.45$ with a mesh size of 0.0005 to prepare stabilization diagram. It should be mentioned that energy of the core (which is -3 a.u.) has to be added with the reported value of the resonance energy in order to get the exact resonance position.

For a free atomic system ($\mu = 0$), we make a list of the resonance parameters for the lowest two S-wave resonances below the Ps($n = 2$) excitation threshold, obtained by various methods, in Table III. From this table we note that our reported resonance positions agree nicely with the others. Also, the reported resonance widths agree with [17,19,24]. As far as the width is concerned, we note that there is significant disagreement between the results of stabilization calculations [17,19,24] and the results of close-coupling calculations [16,21]. In particular, the CC5 results of Liu *et al.* [21] seem to be overestimated. This is, according to the authors [21], due the effect of the channel coupling scheme.

In Table IV we report the results of the resonance energies and widths for various Debye lengths. A graphical representation of our present results is given in Fig. 3. From Table IV and Fig. 3(a) it can be seen that the resonance energy increases steadily with decreasing Debye length and ultimately tends to merge with the Ps($n = 2$) excitation threshold. It is expected that resonance energy would increase with increasing screening effect, as the interaction potential becomes weak with increasing screening effect. Moreover, from Fig. 3(b) we note that with decreasing Debye length the width of both resonances decreases; however, the width of the lowest resonance decreases rapidly, whereas the width of the other resonance decreases slowly. It should be noted that resonances are of Feshbach type. The effect of increasing screening on a Feshbach resonance is in general to decrease its width because in a screening environment the movements of particles slow down, which results in the lifetime of the resonance process being elongated. Thus the resonance width becomes narrow as a consequence of the uncertainty principle [50,51].

TABLE IV. Lowest two S-wave resonances (in a.u.) below the Ps($n = 2$) threshold in positronic lithium under Debye plasma for various values of the screening parameter μ (in a_0^{-1}) corresponding to $kT = 4.0$ eV. The notation $x[y]$ means $x \times 10^y$.

N_e (cm^{-3})	μ	$-E_r^{(1)}$	$\Gamma^{(1)}$	$-E_r^{(2)}$	$\Gamma^{(2)}$
0.00	0.00	0.080550	0.00022	0.071436	0.00008
7.82[18]	0.01	0.070781	0.00021	0.061824	0.00007
3.13[19]	0.02	0.061576	0.00021	0.053069	0.00007
7.04[19]	0.03	0.052992	0.00019	0.045154	0.00007
1.25[20]	0.04	0.045068	0.00017	0.038031	0.00007
1.96[20]	0.05	0.037827	0.00014	0.031643	0.00007
2.82[20]	0.06	0.031284	0.00011	0.025934	0.00007
3.83[20]	0.07	0.025440	0.00008		
5.01[20]	0.08	0.020287	0.00005		
6.34[20]	0.09	0.015806	0.00003		

IV. CONCLUSION

We have identified two Feshbach resonances in positronium lithium embedded in a Debye plasma lying below the Ps($n = 2$) excitation threshold. With an increase in plasma screening strength, the positions of these resonances are lifted and their widths narrow. The existence of these resonances predicts the positron-lithium bound system. Nowadays energetic

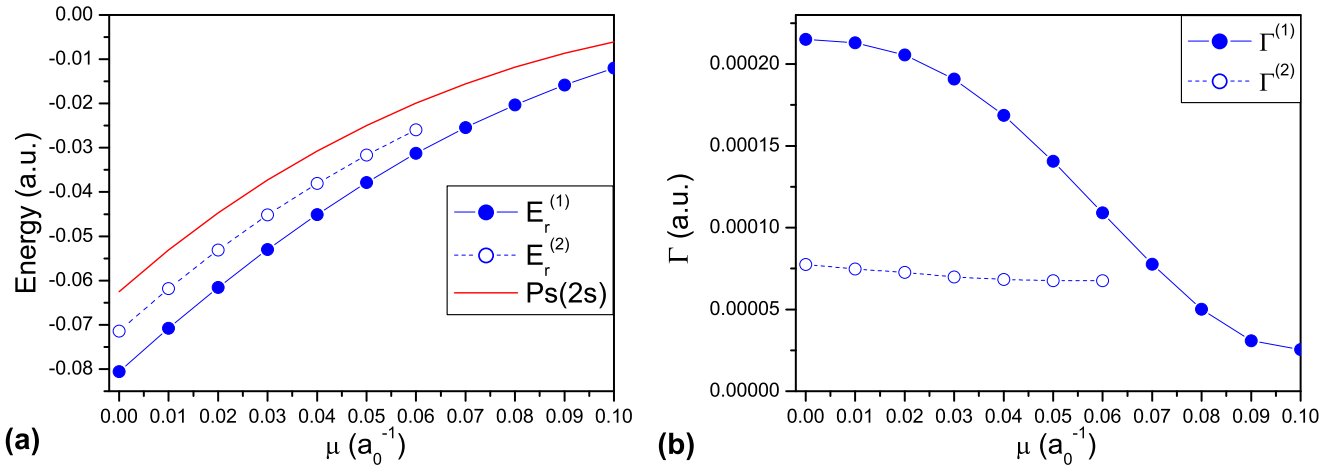

FIG. 3. (a) Lowest two resonance energies $E_r^{(1)}$ and $E_r^{(2)}$ below the Ps($n = 2$) threshold in positronic lithium for different values of the screening parameter μ. The red line denotes the Ps($2s$) threshold energy. (b) Resonance widths $\Gamma^{(1)}$ and $\Gamma^{(2)}$ corresponding to the resonance energies in (a) for different values of the screening parameter μ.

positron beams are available in different positron research laboratories around the world [52–54]; we expect that our results may stimulate an experimental search for resonances in the positron-lithium system. We hope that our present investigation of resonances will provide useful information to astrophysics, plasma physics, and positron physics.

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