Determination of resonance parameters for the e^+-H system in Debye plasma environments using the complex-coordinate-rotation method

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In the present work, we have carried out an investigation on the *S*-wave resonances of e^+-H in plasma environments based on the Debye model for weakly coupled plasmas. We employ the complex-coordinate-rotation method with highly correlated Hylleraas-type wave functions. For resonant states below the respective H($n=2s$) and Ps($n=2s$) thresholds, good agreement has been found with an earlier calculation using the stabilization method. Results for the other five *S*-wave autoionization states up to and below the H($n=4s$) threshold of the e^+-H system immersed in a Debye plasma are reported here.

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I. INTRODUCTION

One recent interesting research topic for atomic physicists is atomic processes in the presence of a plasma. Several studies have been carried out on bound states of one-electron [1,2] and two-electron [3] atomic systems surrounded by plasmas. Autoionizing resonant states play a considerable role in plasma physics. Ho and co-workers [4–12] have performed several calculations with different degrees of plasma screening. Because of the presence of the plasma environment, the electrostatic potentials between the charged particles of atomic systems deviate from their original Coulomb potentials. The effective potential is represented by a screened Coulomb potential of Debye type, $\exp(-r/D)/r$ [13]. The Debye screening model gives an important characteristic length D (in units of a_0^{-1}, with a_0 the Bohr radius) that depends on the temperature and density of the plasma. Smaller values of the Debye parameter D correspond to stronger screening according to the Debye-Hückel model. It is widely accepted that the static Debye-Hückel model is valid for weakly coupled high-temperature and low-density plasmas. Here, we present a calculation for resonance parameters in the plasma-embedded positron-hydrogen system using the Debye screening model. In the presence of a plasma, a resonance lying below the H($n=2s$) threshold and another associated with the Ps($n=2s$) threshold were calculated by Kar and Ho [11] using the stabilization method. There are other resonance states in the unscreened positron-hydrogen scattering system lying below, and associated with, the higher thresholds of the hydrogen atom, as documented in the literature [14–16]. This system consists of a positron, an electron, and a proton, and such a three-body system does not form a bound state. However, there exist many quasibound states that lie in the positron-hydrogen scattering continua. The resonance due to the attractive dipole potential, which behaves like r^{-2} asymptotically in e^+-H scattering below the H($n=2s$) threshold, is the same as that in the e^--H system. Moreover, in the e^+-H case, there exists also a lower-lying positronium formation channel. In the present work, we are interested in investigating the higher-lying *S*-wave resonances for this system with a screened Coulomb potential using the Debye plasma model. We employ the method of complex-coordinate rotation (also called the complex-rotation (CR) method [17]). It is a powerful method to search for resonant positions and widths for higher excited states. Our study includes a search for the existence of resonance states up to and below the H($n=4s$) threshold. With the CR method, we have calculated the energy positions and widths for seven resonances with various plasma-screening effects. These resonances are one [H($2s$-1)] below the H($n=2s$) threshold, two [Ps($2s$-1) and Ps($2s$-2)] associated with the Ps($n=2s$) threshold, two [H($3s$-1) and H($3s$-2)] below the H($n=3s$) threshold, and two [H($4s$-1) and H($4s$-2)] below the H($n=4s$) threshold. Throughout the text, notation like $A(ns-m)$ implies the following: A is either the hydrogen atom or the positronium atom, ns means the nth threshold of the two-body subsystem, and m is the mth resonance associated with the ns threshold, with $m=1$ the lowest member for that series. Highly correlated Hylleraas-tpe wave functions are used in the present work.

II. THEORY

The nonrelativistic Hamiltonian for the positron-hydrogen system surrounded by a plasma, and with the proton infinitely heavy, is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{\exp(-r_1/D)}{r_1} + \frac{\exp(-r_2/D)}{r_2} - \frac{\exp(-r_{12}/D)}{r_{12}}, \tag{1}$$

where r_1 and r_2 are the position coordinates of the electron and the positron, respectively, and r_{12} denotes the relative distance between these two. In the method of complex-coordinate rotation [17], r is transformed as

$$r \rightarrow |r|e^{i\theta} \tag{2}$$

and

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TABLE I. Comparison of present H(2*s*-1) and Ps(2*s*-1) resonance energies ($-E_r$) and widths (Γ) of the e^+-H system for various Debye parameters (D) with earlier predictions [11]. All the results are in atomic units. The notation $a(-b)$ stands for $a\times 10^{-b}$.

Resonant state	D	Present (method of complex-coordinates rotation)		Kar and Ho [11] (stabilization method)	
		$-E_r$	Γ	$-E_r$	Γ
H(2*s*-1)	∞	0.128687	6.67(−5)	0.128685	6.65(−5)
	100	0.118841	6.65(−5)	0.118840	6.60(−5)
	50	0.109343	6.52(−5)	0.109345	6.50(−5)
	30	0.097295	6.15(−5)	0.097295	6.10(−5)
	20	0.083325	5.26(−5)	0.083325	5.25(−5)
	16	0.073705	4.30(−5)	0.073705	4.28(−5)
	10	0.049720	2.25(−5)	0.049720	2.24(−5)
Ps(2*s*-1)	∞	0.075159	3.34(−4)	0.07515	3.34(−4)
	100	0.065381	3.33(−4)	0.06535	3.32(−4)
	50	0.056127	3.27(−4)	0.05610	3.28(−4)
	30	0.044744	3.17(−4)	0.04475	3.21(−4)
	20	0.032206	2.84(−4)	0.03225	2.91(−4)
	16	0.024021	1.98(−4)	0.02415	2.05(−4)
	10	0.006820	1.01(−4)	0.00685	1.02(−4)

$$H(r,\theta) = Te^{-2i\theta} + V_1 \tag{3}$$

where T is the kinetic energy operator and the rotated potential V_1 is

$$V_1 = \left(-\frac{\exp(-r_1 e^{i\theta}/D)}{r_1} + \frac{\exp(-r_2 e^{i\theta}/D)}{r_2} - \frac{\exp(-r_{12} e^{i\theta}/D)}{r_{12}}\right) e^{-i\theta}.$$

The basis set is constructed using the Hylleraas wave functions

$$\Psi_{klm} = \sum_{klm} C_{klm} \exp[-\alpha(r_1 + r_2)] r_{12}^k (r_1^l r_2^m + r_1^m r_2^l), \tag{4}$$

where $k+l+m \leqslant \omega$, and ω, k, l, and m are positive integers or zero. We have performed complex eigenvalue calculations with $\omega=16$ ($N=969$) and 17 ($N=1140$) separately to examine convergence behavior, and obtained the resonance energies E_r and widths Γ. The challenging aspect of the present problem, which differs from the earlier complex-scaling approach for pure Coulomb potentials, is that the dynamic variables r_{ij} now appear in the screened Coulomb potentials. Under the complex transformation, one must also scale such dynamic variables as a function of θ, and, as such, the matrix elements for $H(r,\theta)$ are calculated separately for different values of θ.

III. RESULTS AND DISCUSSIONS

In the present investigation, we first reproduced the existing values that were obtained by using the stabilization method [11] for the resonant positions and widths associated with the H($n=2s$) and the Ps($n=2s$) thresholds. Table I shows good agreement between these two sets of calculations. Next, we employ the complex-rotation method to extract higher-lying resonances. Calculations of high-lying resonances using the present CR method are as straightforward as those used for low-lying resonances. Our calculations are performed with $N=969$ and 1140 individually in order to test the convergence. Details of the computational procedure were discussed in our earlier work [12]. All the present results associated with the H($n=2s,3s,4s$) and the Ps($n=2s$) states are well converged with basis length $N=1140$ except for the resonant states of H(3*s*-2) and of H(4*s*-2). Since these two resonant states can be identified properly only when the basis length has reached $N=1140$, and for practical and economical reasons, we have not extended our calculations beyond those using $N=1140$. We have obtained two members of resonant states below the Ps($n=2s$) threshold, whereas in the earlier calculation for a screened potential [11], only one resonance was reported. The second resonant state Ps(2*s*-2) associated with the Ps($n=2s$) excitation threshold for different D values along with its corresponding threshold energies are tabulated in Table II. As a function of decreasing value of D (increasing $1/D$) the resonant energies increase gradually from their free-atom values, while their corresponding widths decrease for increasing screening effects. The Ps(2*s*-2) resonances can be predicted up to $D=30$, and all the results are very close to but lower than its threshold throughout the energy region mentioned. Other resonances associated with the H($n=3s$) and H($n=4s$) states along with their corresponding threshold energies as a function of D are also presented in Table II. It is apparent from Table II, that the resonance positions E_r of H(3*s*-1) are located lower than their corresponding threshold

TABLE II. The Ps($2s$-2), H($3s$-1), H($3s$-2), H($4s$-1) and H($4s$-2) resonance energies ($-E_r$) and widths (Γ) of the e^+-H system and their corresponding threshold energies ($-E_{H(nS)}$) for various Debye parameters (D). All results are expressed in atomic units. The notation $a(-b)$ stands for $a\times 10^{-b}$.

Resonant states	D	$-E_r$	Γ	$-E_{H(ns)}$
Ps($2s$-2)	∞	0.065838[a]	1.62(−4)[a]	0.0625000
		0.065838[b]	1.63(−4)[b]	
	100	0.056109	1.60(−4)	0.0530750
	50	0.047060	1.50(−4)	0.0447050
	30	0.036258	1.24(−4)	0.0350100
H($3s$-1)	∞	0.058050[a]	6.28(−4)[a]	0.0555500
		0.058065[b]	6.3(−4)[b]	
		0.05803[c]	6.2(−4)[c]	
	100	0.048346	6.12(−4)	0.0462000
	50	0.039441	5.58(−4)	0.0380200
	30	0.029160	3.86(−4)	0.0287200
	20	0.019212	2.60(−4)	0.0193500
H($3s$-2)	∞	0.056064[a]	1.60(−4)[a]	0.0555500
		0.056063[b]	1.34(−4)[b]	
		0.05603[c]	1.4(−4)[c]	
	100	0.046438	1.50(−4)	0.0462000
	50	0.037920	1.16(−4)	0.0380200
H($4s$-1)	∞	0.038544[a]	4.72(−5)[a]	0.0312500
		0.038544[b]	4.74(−5)[b]	
	100	0.028938	4.66(−5)	0.0223550
	50	0.020454	4.20(−5)	0.0153800
	30	0.011319	2.99(−5)	0.0085050
	20	0.003713	1.24(−5)	0.0030900
H($4s$-2)	∞	0.033947[a]	4.74(−5)[a]	0.0312500
		0.033947[b]	4.75(−5)[b]	
		0.033934[d]	4.8(−5)[d]	
	100	0.024427	4.60(−5)	0.0223550
	50	0.016349	3.60(−5)	0.0153800

[a]Present work.
[b]Reference [16].
[c]Refernece [14].
[d]Reference [15].

energies $E_{H(3s)}$ in the range of Debye parameter from $D=\infty$ to about 30, whereas the resonance energy E_r for $D=20$ is located higher than its threshold value. In other words, the resonances from $D=\infty$ (the unscreened case) to $D=30$ are Feshbach-type resonances (lying below threshold), and beyond $D=30$, there exist shape resonances lying above the corresponding threshold. We are able to determine the resonance parameters for one shape resonance with $D=20$ using the present CR method. Similarly, for the case of the H($3s$-2) autoionization state, the resonance positions are lower than the threshold energies for $D=\infty$ and 100, i.e., these are Feshbach resonances, and when the Debye length is decreased to about $D=50$, shape resonances start to appear. For the case of the H($n=4s$) state, all the resonance energy positions for various plasma-screening parameters are located lower than the corresponding threshold energies. The smallest values of Debye lengths used here are $D=20$ and 50 for H($4s$-1) and H($4s$-2), respectively. We present all the corresponding resonance widths in Table II. The widths of H($3s$-1) for all **D** values are greater than those of H($3s$-2). Furthermore, the width for each state decreases with increasing value of $1/D$ as is shown in the Ps($2s$-2) state. To explain such behavior for the widths, we conclude that the lifetimes of the resonances in the collision processes will be increased with increasing screening effect (decrease of the Debye length D), due to the slowing down of the movements of the charged particles. As a result, the autoionization processes will be prolonged by ejection of a particle (or composite of particles). When the lifetime of a resonance is prolonged, its width will become narrower, a consequence of the uncertainty principle. Table II also compares our present resonant parameters for the unscreened potential with the corresponding values of other calculations, and there is very good agreement between the two sets of results. For other possible decay routes, once such resonances are formed, readers are referred to Ref. [11] for a more detailed discussion.

We now discuss the relevance of our present investigation, and the possible experimental observations of our present results. The predicted behavior for the resonances in positron collisions with plasma-embedded hydrogen atoms might be observed in positron collisions with hydrogen atoms that are embedded in partially ionized hydrogen plasmas. While there have been very limited studies of positron-atom collisions in plasmas environments, there has been considerable interest and activity in the investigations of electron collisions with atoms or ions in weakly coupled plasmas. Such studies include work on electron-hydrogen collisions in partially ionized plasmas [18–20]. Other investigations include electron-impact excitation of hydrogenic ions in dense plasmas [21,22], inelastic electron-ion scattering in dense plasmas [23–25], and studies of plasma effects on electron-impact ionization [26]. We hope that the present work will stimulate further investigations of positron-atom scattering in plasma environments. Last, we should also mention that, from the theoretical aspect, our present work is a different approach to investigating atomic resonances with Yukawa potentials. It has been a challenging theoretical problem to use the complex-scaling method to investigate resonances with Yukawa potentials, as the interparticle coordinate r_{ij} appears as a dynamical variable. An exploratory complex-coordinate L^2 calculation of three-body photoproduction cross sections was carried out for model three-body systems, which mimic He and H^- with Yukawa potentials [27]. The authors in Ref. [27] approximated the three-dimensional problem by a collinear version of the Hamiltonian. Very recently, a calculation for the resonance levels of the Yukawa potential in a one-electron (two-body) atomic system has been reported [28]. Our present approach using a complex-scaling treatment for a realistic three-body system interacting with Yukawa potentials represents a major advance in the field.

IV. CONCLUSION

In conclusion, this work presents a calculation of resonance energies and widths for some S-wave autoionization

states below and up to the H(n=4s) threshold of the positron-hydrogen system as a function of the Debye length. For the screened cases, we have calculated resonance parameters for the H(Ps-2), H(3s-1), H(3s-2), H(4s-1), and H(4s-2) states by using the complex-coordinate-rotation method together with highly correlated Hylleraas functions. The present results for two other states, H(2s-1) and Ps(2s-1), are in very good agreement with an earlier calculation that used the stabilization method. All the results reported here are determined by using basis functions including up to N=1140 terms, and they are well converged except for those of the H(3s-2) and H(4s-2) states. For these two states, we provide no conclusive evidence for their convergence as they are limited by the largest basis set used in the present work. Resonance widths for a higher member associated with a particular threshold decrease quite rapidly, and it becomes more challenging to obtain converged results for a resonance with an extremely narrow width. The use of more extensive basis sets for the wave functions may be of future interest, and it is outside the scope of our present investigation. To conclude, our findings will provide useful references to the communities in atomic physics, positron physics, plasma physics, and nuclear physics, as the present approach would be of interest in resonance investigations for nuclear systems interacting with Yukawa potentials. In addition, we hope that our work will stimulate others to further investigation of resonances with such screened Coulomb potentials.

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[1] F. J. Rogers, H. C. Graboske, Jr., and D. J. Harwood, Phys. Rev. A **1**, 1577 (1970).
[2] K. M. Roussel and R. F. O'Connell, Phys. Rev. A **9**, 52 (1974).
[3] S. Kar and Y. K. Ho, New J. Phys. **7**, 141 (2005); X. Lopez, C. Sarasola, and J. M. Ugalde, J. Phys. Chem. A **101**, 1804 (1997); P. K. Mukherjee, J. Karwowski, and G. H. F. Diercksen, Chem. Phys. Lett. **363**, 323 (2002); A. N. Sil and P. K. Mukherjee, Int. J. Quantum Chem. **102**, 1061 (2005); P. Winkler, Phys. Rev. E **53**, 5517 (1996); S. T. Dai, A. Solovyova, and P. Winkler, *ibid.* **64**, 016408 (2001).
[4] S. Kar and Y. K. Ho, Chem. Phys. Lett. **424**, 403 (2006).
[5] S. Kar and Y. K. Ho, Phys. Rev. E **70**, 066411 (2004).
[6] S. Kar and Y. K. Ho, Few-Body Syst. **40**, 13 (2006).
[7] S. Kar and Y. K. Ho, Phys. Rev. A **72**, 010703(R) (2005).
[8] S. Kar and Y. K. Ho, J. Phys. B **39**, 2445 (2006).
[9] S. Kar and Y. K. Ho, Phys. Rev. A **71**, 052503 (2005).
[10] S. Kar and Y. K. Ho, Phys. Rev. A **73**, 032502 (2006).
[11] S. Kar and Y. K. Ho, J. Phys. B **38**, 3299 (2005).
[12] Sumana Chakraborty and Y. K. Ho, Chem. Phys. Lett. **438**, 99 (2007).
[13] P. Debye and E. Hückel, Phys. Z. **24**, 185 (1923).
[14] Y. K. Ho and C. H. Greene, Phys. Rev. A **35**, 3169 (1987).
[15] Y. K. Ho, Phys. Rev. A **38**, 6424 (1988).
[16] Y. K. Ho and Z.-C. Yan, Phys. Rev. A **70**, 032716 (2004), and references therein.
[17] Y. K. Ho, Phys. Rep. **99**, 1 (1983).
[18] Y. D. Jung and O. K. Kim, Phys. Scr. **74**, 136 (2006).
[19] M. J. Lee and Y. D. Jung, J. Plasma Phys. **72**, 205 (2006).
[20] Y. D. Jung, Appl. Phys. Lett. **86**, 021502 (2005).
[21] B. L. Whitten, N. F. Lane, and J. C. Weisheit, Phys. Rev. A **29**, 945 (1984).
[22] Y. D. Jung, Phys. Fluids B **5**, 3432 (1993).
[23] G. J. Hatton, J. Phys. B **14**, 4879 (1983).
[24] C. Blanchard and J. Dubau, Laser Part. Beams **12**, 401 (1994).
[25] F. A. Gutierrez and J. Diazvaldes, J. Phys. B **27**, 593 (1994).
[26] Z. Q. Wu, G. X. Han, J. Yan, and J. Q. Pang, J. Phys. B **35**, 2305 (2002).
[27] Seungsuk Han and W. P. Reinhardt, J. Phys. B **28**, 3369 (1995).
[28] Miroslaw Bylicki, Artur Stachow, Jacek Karwowski, and Prasanta K. Mukherjee, Chem. Phys. **331**, 346 (2006).