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Resonances with unnatural parities in the positron-hydrogen system

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We present an investigation of resonances with unnatural parities in positron scattering with atomic hydrogen. The method of complex-coordinate rotation is used, together with Hylleraas wave functions to take care of the correlation effects among the three charged particles. States with angular momenta $L=1$ to $L=5$ and parity $(-1)^{L+1}$ are calculated. Resonance energies and widths for the states lying below the Ps ($N=2$), H ($N=3$), and H ($N=4$) thresholds are reported.

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I. INTRODUCTION

There has been continuous interest in the theoretical studies of resonances in positron-hydrogen scattering. In a related system, the electron hydrogen scattering, it is well known that the resonances below the H ($N=2$) threshold are the result of the $2s$-$2p$ degeneracy of the excited $N=2$ states of the target hydrogen atom [1]. Mittleman [2] pointed out that the attractive dipole potential that behaves similar to r^{-2} asymptotically in the e^+-H scattering is the same as that in the e^--H scattering. Therefore, resonances in the e^+-H scattering should also exist. The first accurate calculation for S-wave resonances in the e^+-H scattering below the H ($N=2$) threshold was carried out by Doolen *et al.* [3] using the method of complex-coordinate rotation [4] together with Pekeris functions that explicitly include the coordinates for the positronium. The method of complex-coordinate rotation has also been used to calculate S-wave, P-wave, and D-wave resonances in the e^+-H scattering associated with various thresholds of the hydrogen and positronium atoms [5–7]. We have recently extended the calculations to the angular-momentum states up to $L=6$ for the energy region below the Ps ($N=4$) threshold [8]. Other methods have also been used to calculate resonances in this system, including the close-coupling method [9], the use of hyperspherical functions [10], and the Harris-Nesbet variational method [11]. Several reviews have addressed the theoretical developments on this system [12].

While the aforementioned works deal with the resonances with the natural parity $\pi=(-1)^L$, the resonances with the unnatural parity $\pi=(-1)^{L+1}$ (see Ref. [13] for the definition of unnatural parity) have not been investigated for the e^+-H system, to the best of our knowledge. It is noted that recently Bromley *et al.* have reported a calculation of some unnatural parity bound states in positronic complexes [14]. We have noticed a related work for calculating the P^e states in the e^+-He system [15]. Here, we present an investigation of resonances with unnatural parities in the positron scattering with the atomic hydrogen. The method of complex-coordinate rotation is used in our work, together with Hylleraas wave functions to take care of the correlation effects among the three charged particles. States with angular momenta $L=1$ to $L=5$ and the parity $(-1)^{L+1}$ are calculated, which are the P^e, D^o, F^e, G^o, and H^e states. Resonance parameters (energies and widths) for states up to the H ($N=4$) threshold are reported. While such resonances cannot be reached by positron scattering with the ground-state hydrogen atom within the usual L-S coupling scheme, they can be accessed by the positron scattering with an excited-state hydrogen atom. Such resonances, in principle, are observable in perhaps a positron-hydrogen merged beam experiment. If somehow the hydrogen beam contains sufficient amount of hydrogen atoms in their excited states, the resonances predicted in the present work would manifest themselves as structures in the scattering cross sections.

Studies of the present positron-hydrogen system are part of the recent experimental and theoretical investigations on few-body exotic systems involving antimatter. For example, there has been renewed interest to carry out experimental studies on the positronium negative ion, a three-lepton system consisting of two electrons and a positron. Following the pioneer works by Mills [16], laboratories in Germany [17], in Denmark [18], and in Japan [19] have carried out investigations on the various properties of such a purely leptonic system. Also, with the improved technique for storing positrons [20], a related system, the positronium molecule Ps_2, has been recently produced in the laboratory [21].

II. HAMILTONIAN AND WAVE FUNCTIONS

The total Hamiltonian H for the e^+-H system, with the energy expressed in the Rydberg units, is given by

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

with

$$T = -\nabla_1^2 - \nabla_2^2 \tag{2}$$

and

$$V = -\frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}}, \tag{3}$$

where the indices 1 and 2 refer to the coordinates of the electron and the positron, respectively. Throughout this work

TABLE I. States with the total angular momentum L and the parity $(-1)^{L+1}$.

State	L	(l_1,l_2)	Ω	Total N
P^e	1	(1,1)	22	1771
D^o	2	(2,1); (1,2)	23	$2\times1771=3542$
F^e	3	(3,1);(2,2); (1,3)	23	$3\times1540=4620$
G^o	4	(4,1);(3,2);(2,3); (1,4)	23	$4\times1330=5320$
H^e	5	(5,1);(4,2);(3,3);(2,4);(1,5)	23	$5\times1140=5700$

the infinite nuclear mass is used. The basis set is constructed using Hylleraas coordinates

$$\{x_{ijk}(l_1,l_2;\alpha,\beta)=r_1^i r_2^j r_{12}^k e^{-\alpha r_1-\beta r_2} y_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2)\}, \quad (4)$$

where $y_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2)$ is the vector coupled product of solid spherical harmonics for the electron and the positron forming an eigenstate of total angular momentum L defined by

$$y_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2)=\sum_{m_1 m_2}\langle l_1 l_2 m_1 m_2|LM\rangle Y_{l_1 m_1}(\hat{r}_1)Y_{l_2 m_2}(\hat{r}_2), \quad (5)$$

and $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$ is the distance between the electron and the positron. The explicit form of the wave function is

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\sum_{l_1 l_2}\sum_{ijk} a_{ijk}x_{ijk}(l_1,l_2;\alpha,\beta), \quad (6)$$

where $i+j+k+l_1+l_2\le\Omega$ with i, j, and k being positive integers or zero [22].

III. CALCULATIONS AND RESULTS

Table I shows the total number of terms used for a given angular momentum state, as well as the individual (l_1,l_2) pairs for different angular momentum combinations. For the P^e states, both the electron and positron have the same angular momentum $l_i=1$ $(i=1,2)$, which couple to form the total angular momentum $L=1$. The higher harmonics are taken care of by the r_{ij} terms in the basis set. For the sum in Eq. (6), we use basis sets up to $\Omega=22$, leading to 1771 terms in the wave functions. For the states of $L=2$, the D^o states, the possible values for (l_1,l_2) are $(2,1)$ and $(1,2)$, and basis sets up to $\Omega=23$ are used, leading to a total of $2\times1771=3542$ terms. For the F^e states of $L=3$, we use $\Omega=23$, which corresponds to 1540 terms for each (l_1,l_2) pair with possible pairs being $(3,1)$, $(2,2)$, and $(1,3)$. The total number of terms is hence equal to $3\times1540=4620$. Similarly, for the G^o and H^e states, where $L=4$ and $L=5$, respectively, the total numbers of terms are $4\times1330=5320$ and $5\times1140=5700$, respectively. In the calculations of resonance energies and widths using the method of complex-coordinate rotation [4], the radial coordinate r (r stands for r_1, r_2 or r_{12}) is transformed into $re^{i\theta}$, where θ is the rotational angle. A complex eigenvalue is determined as a resonance eigenvalue when it exhibits stabilized character with respect to the changes of α and β in the wave functions [see Eq. (4)]. Furthermore, the resonance eigenvalue also shows convergence behavior when the size of the basis is increased.

TABLE II. Resonance energies and widths in the e^+-H system.

State		E_r (Ry)	$\Gamma/2$ (Ry)
P^e	$(L=1)$	−0.1273189	4.1×10^{-6}
		−0.11166322	1.16×10^{-6}
		−0.0711562	4.60×10^{-5}
		−0.0642955	1.91×10^{-5}
		−0.062905	7.0×10^{-6}
D^o	$(L=2)$	−0.11114	1.0×10^{-6}
		−0.0698375	2.96×10^{-5}
		−0.0637926	1.04×10^{-5}
		−0.0632305	2.15×10^{-5}
		−0.06275	5.0×10^{-6}
F^e	$(L=3)$	−0.0679131	2.12×10^{-5}
		−0.0631772	4.3×10^{-6}
G^o	$(L=4)$	−0.0654953	3.02×10^{-5}
		−0.062652	6.5×10^{-6}
H^e	$(L=5)$	−0.0629054	1.47×10^{-5}

Table II shows our numerical results. Figure 1 shows the resonance poles associated with the Ps $(N=2)$ and H $(N=3)$ thresholds, and Fig. 2 is for the H $(N=4)$ threshold. It is seen that we have located one P^e state lying slightly below the Ps $(N=2)$ threshold with the resonance parameters $(E_r,\Gamma/2)=(-0.1273189,4.1\times10^{-6})$ Ry. For the resonances below the H $(N=3)$ threshold, we have found one state each for the P^e and D^o states, with the parameters of $(-0.11166322,1.16\times10^{-6})$ Ry and $(-0.11114,1.0\times10^{-6})$ Ry, respectively. As for the resonances associated with the H $(N=4)$ threshold, we have calculated three P^e states, four D^o states, two states each for F^e and G^o, and one for the H^e state. We estimate that the uncertainties for the resonance energies and widths are within a few parts in the last quoted digits.

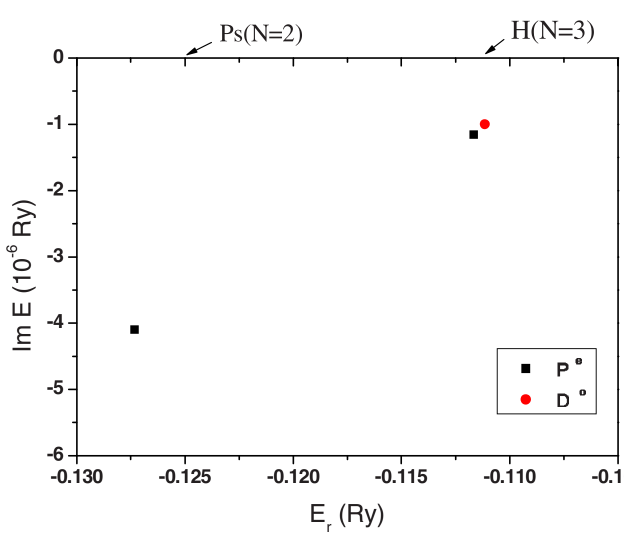

FIG. 1. (Color online) Resonances in the positron-hydrogen system below the Ps $(N=2)$ and H $(N=3)$ thresholds.

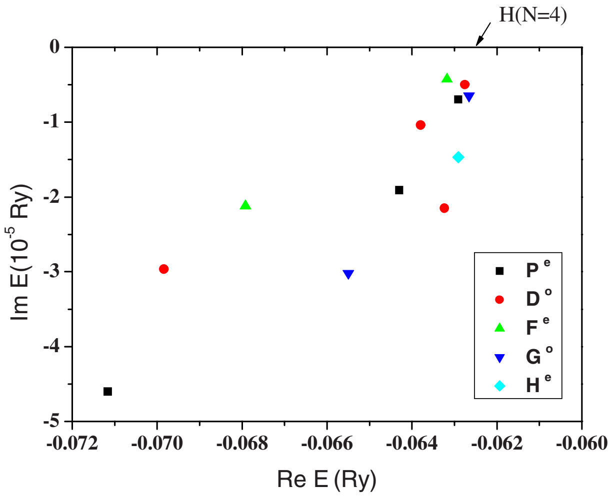

FIG. 2. (Color online) Resonances in the positron-hydrogen system below the H (N=4) threshold.

IV. DISCUSSION AND CONCLUSION

The resonances below the H (N=3) threshold are members of dipole series, a result of the positron attaching to the excited hydrogen atom due to the degenerate $3p$-$3d$ levels of the excited hydrogen. Here we should mention that the S-wave component does not contribute to the states with unnatural parities, since the ground state of the hydrogen atom is an S state. The quasibound dipole states interacting with the scattering continua will manifest themselves as resonances in the positron scattering with an excited hydrogen atom. Similarly, the resonances lying below the H (N=4) threshold are members of dipole series due to the degeneracy of the $4p$-$4d$-$4f$ hydrogen states. We have not tried to identify which resonance belongs to which series. It is possible that some of the higher-lying resonances near the H (N=4) threshold actually belong to some series converging on the higher-lying Ps (N=3) threshold. Also, we have not tried to calculate the higher members of the dipole series approaching the H (N=3) and H (N=4) thresholds. In principle, if more extensive basis sets for the wave functions were used, we might be able to determine the resonance parameters for the higher member of the resonance series to a desirable accuracy. But for practical reasons, the most extensive wave functions used in the present investigation are limited to those given in Table I. As for the P^e state lying below the Ps (N=2) threshold, we have been able to identify one resonance. We believe that it is not a result of dipole interaction due to the degenerate excited target states because the positronium $2S$ state does not contribute to this unnatural-parity state. In this case, it is most likely a result of the positronium in its $2P$ state moving with P-wave character interacting with the positively charged and infinitely massive proton. In the asymptotic region, the effective potential has an attractive polarization form of $-\alpha_d/(2r^4)$, where α_d is the dipole polarizability of the $2P$ positronium. Since the excited positronium has a dipole polarizability much larger than that of its hydrogen counterpart, and since the proton is a heavy particle, it is very likely that a P^e quasibound state could be formed which lies slightly below the Ps (N=2) threshold. Again, since there exists the lower-lying H (N=2) state, the quasibound P^e state will autoionize, and its interaction with the scattering continuum would manifest itself as a resonance in the positron scattering with an excited hydrogen atom.

In summary, we have reported resonances with unnatural parities in the positron-hydrogen system up to the H (N=4) threshold. To the best of our knowledge, there have been no such results available in the literature. Furthermore, resonances in e^+-H scattering have not been observed experimentally. We realize that the resonances predicted in the present work are extremely difficult to be detected experimentally, and observation of resonances in positron hydrogen would be a challenging task for experimentalists for some years to come. However, as intense positron beams with good resolution have recently become available [19,23], it is hoped that our accurate results on resonance energies would play a useful role for the experimental search of atomic resonances involving positrons.

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