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Positron-hydrogen resonances associated with the $N = 2$ positronium and $N = 3$ hydrogen thresholds

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Some lower-lying S-wave resonances in positron-hydrogen scattering associated with the positronium $N = 2$ and hydrogen $N = 3$ thresholds are investigated using the method of complex-coordinate rotation and using an adiabatic treatment in hyperspherical coordinates. Both calculations indicate that the lowest resonance associated with the positronium $N = 2$ threshold lies near $E = -0.150279$ Ry, in disagreement with Doolen's prediction that the lowest resonance occurs at $E = -0.222$ Ry. We also report for the first time resonance parameters associated with the hydrogen $N = 3$ threshold.

Several independent studies[1-4] have already demonstrated the existence of doubly excited state resonances in positron-hydrogen scattering just below the hydrogen $N = 2$ threshold. Comparatively little work has been carried out at higher energies. In a complex-rotation calculation with inverse iteration, Doolen[5] predicted four resonances below the positronium $N = 2$ threshold, of which the lowest was found at a total energy $E = -0.222$ Ry. The surprisingly large binding energy of this resonance [relative to the Ps($N = 2$) threshold] and the large uncertainties quoted by Ref. 5 have led us to carry out a study of the S-wave resonances below Ps($N = 2$) and H($N = 3$) using two independent methods. A complex-coordinate calculation gives the resonance features to high accuracy, while a hyperspherical-coordinate analysis shows the critical regions in energy and in configuration space despite somewhat poorer quantitative accuracy.

The first method starts from a complex-coordinate rotation, as described in detail elsewhere.[1] In rydberg units the Hamiltonian is $H = T + V$, where

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

and

$$V = -\frac{2}{r_{1p}} + \frac{2}{r_{2p}} - \frac{2}{r_{12}} \ . \tag{2}$$

Here (1) and (2) denote the electron and the positron, respectively, and p denotes the proton. Likewise, m_i is the mass of particle i and r_{ij} represents the distance between particles i and j. In the complex-coordinate calculation we use the true mass of the proton $m_p = 1836.151 m_1$. The kinetic-energy operator is expressed conveniently in terms of the interparticle separation coordinates as in Ref. 6. The approximate eigenfunctions of the resonant states are represented by a Hylleraas-type wave function:

$$\Psi = \sum_{k,l,m} C_{klm} r_{12}^k r_{1p}^l r_{2p}^m \exp[-\beta(r_{1p} + r_{2p})] \ , \tag{3}$$

with $k + l + m \leq \omega$ and ω a non-negative integer. Up to a total of $M = 969$ such terms have been included here, corresponding to $\omega = 16$. Moreover, to avoid potential problems associated with the ill-conditioned nature of Hylleraas-type wave functions, the calculations have been performed using quadruple precision arithmetic (about 30 significant digits) on an IBM 3084.

Theoretical details of the complex-coordinate rotation are given in Ref. 1, so we only summarize the main computational aspects of the method. Resonance parameters are determined from the conditions that the complex energy eigenvalues are stabilized with respect to changes of θ β, and M, where θ is the angle in the complex coordinate rotation $r \rightarrow r\exp(i\theta)$, β is the nonlinear parameter in the wave function (3), and M is the total number of terms included in the expansion (3). For a given set of θ and β, it takes about 8 h on the IBM 3084 to solve the complex eigenvalue problem for the most extensive $M = 969$-term basis wave functions.

Table I explores the convergence of the lowest resonance associated with the Ps($N = 2$) threshold. These results are given as a function of M with fixed values of β and θ ($\beta = 0.3$ and $\theta = 0.3$), showing that the results are converged quite well. Furthermore, results are also stabilized in ranges of θ from $\theta = 0.2$ to $\theta = 0.4$, and of β from $\beta = 0.2$

TABLE I. Convergence behavior for the lowest S-wave resonance below the positronium $N=2$ threshold ($\beta=0.30$, $\theta=0.30$).

M	ω	E(Ry)	$\frac{1}{2}\Gamma$(Ry)
455	12	−0.150 281 8	0.000 327 3
560	13	−0.150 278 8	0.000 332 8
680	14	−0.150 279 2	0.000 334 1
816	15	−0.150 279 4	0.000 334 6
969	16	−0.150 279 5	0.000 334 6

to $\beta=0.4$. Table II shows the complex-rotation results for three resonances associated with the Ps($N=2$) threshold, and for two resonances associated with the H($N=3$) threshold. Those associated with H($N=3$) are reported for the first time. In Table II we show Doolen's results, which were also obtained by a complex-coordinate rotation but through an inverse-iteration technique. In the inverse-iteration calculation, only one eigenvalue was calculated at a time. In the present calculation, however, the entire complex-eigenvalue spectrum is calculated as a function of θ, β, and M. This permits us to examine several resonant eigenvalues in a single diagonalization, and to distinguish the complex eigenvalues representing true resonances from those complex eigenvalues that represent "cuts," i.e., the nonresonant continua. In particular, we have found that Doolen's complex energy eigenvalue at $E=-0.222-0.010i$ Ry must be an artifact. No such eigenvalue shows stabilized character when θ, β, and M are changed. We now believe that this eigenvalue represents part of the cut that starts from the branch point of the hydrogen $N=2$ threshold at $E=-0.25$ Ry. The nonexistence of the resonance eigenvalue at $E=-0.222$ Ry is even clearer on qualitative grounds when studied using adiabatic hyperspherical potential curves.

These potential curves are eigenvalues of the adiabatic fixed-R Hamiltonian $H_{R=\text{const}}$, with the hyperspherical radius R defined as

$$R=(r_{1p}^2+r_{2p}^2)^{1/2} , \tag{4}$$

where for simplicity we now regard the proton as being infinitely massive. These eigenvalues then serve as adiabatic potential energy curves in the calculation of approximate energy eigenvalues.[7-9] In the adiabatic approximation these resonances appear to be true bound states, since their decay is a nonadiabatic transition between potential curves. Accordingly, no widths have been obtained in this study.

Adiabatic potential curves are normally found variationally by diagonalizing $H_{R=\text{const}}$ at each R in some convenient basis set. References 4 and 10 use very large basis sets consisting of hyperspherical harmonics, which are optimum for small values of R. In the present calculation we use instead a much smaller basis of only 15 functions optimized for large radii as in Refs. 11 and 12. These basis functions include all of the $N=1$, 2, and 3 wave functions of hydrogen and of positronium, augmented by the lowest three hyperspherical harmonics to improve convergence at small R.

Figure 1 shows the attractive potential curves converging to the Ps($N=2$) and H($N=3$) thresholds. These are the only potential curves in this energy range which contain resonances. The potential curves converging to lower thresholds are given by Pelikan and Klar.[4] Three entirely repulsive curves are not shown in Fig. 1 for clarity, since they show several sharp avoided crossings between $R=25$ and $R=30$ a.u. which have been allowed to cross diabatically. (Diagonal adiabatic correction terms have been neglected here as well.) The attractive curves in Fig. 1 have the following behavior at large R:

$$U_i(R) \xrightarrow[R\to\infty]{} E_i-\frac{a_i}{R^2} , \tag{5}$$

where in rydbergs $E_i=-\frac{1}{8}$ and $-\frac{1}{9}$ for Ps($N=2$) and H($N=3$), respectively, and where $a_i=23.02$ and 16.20 for these respective channels. The lowest resonance in each channel is drawn into the relevant potential curve of Fig. 1, and each is given in Table II, showing reasonable agreement with the more accurate complex-coordinate calculation discussed above. The presence of long-range dipole potentials in Eq. (5) requires (nonrelativistically) an infinite series of dipole levels to be present below each threshold. The binding energies E^b and decay widths Γ of successive levels r in each potential curve then scale ap-

TABLE II. S-wave resonances in $e^+-\text{H}$ scattering.

Complex rotation[a] (present work) E(Ry)	Complex rotation[a] (present work) $\frac{1}{2}\Gamma$(Ry)	Complex rotation (Doolen, Ref. 5) E(Ry)	Complex rotation (Doolen, Ref. 5) $\frac{1}{2}\Gamma$(Ry)	Hyperspherical (present work) E(Ry)
		Below Ps($N=2$) threshold		
−0.150 279(2)	0.000 335(2)	−0.150 318	0.000 334	−0.149 94
−0.131 659(2)	0.000 163(2)	−0.1316	0.000 087	−0.131 33
−0.126 774(5)	0.000 048(5)	−0.1267		−0.126 70
		Below H($N=3$) threshold		
−0.116 06(1)	0.000 62(1)			−0.116 71
−0.112 06(2)	0.000 14(2)			−0.112 27

[a]Numbers in parentheses represent the uncertainties in the last digits quoted.

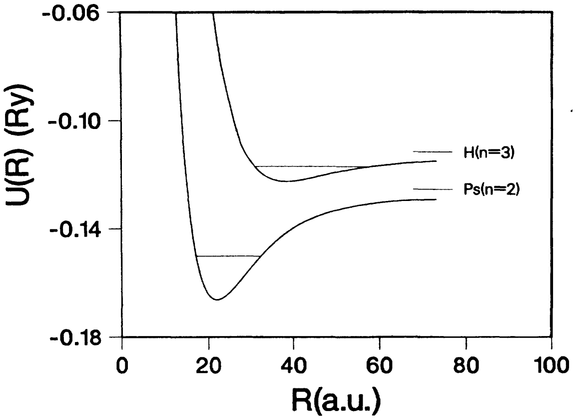

FIG. 1. Adiabatic hyperspherical potential curves for the $L=0$ positron-hydrogen system are shown as a function of the hyperspherical radius. Three other potential curves converging to Ps($N=2$) and H($N=3$) are not shown since they are entirely repulsive and support no resonances. The lowest resonance state in each potential is indicated by a horizontal line.

proximately[13] as

$$E^b_{r+1}=E^b_r\exp(-2\pi/\alpha),\ \ \Gamma_{r+1}=\Gamma_r\exp(-2\pi/\alpha)\ ,\qquad(6)$$

where $\alpha_i=(a_i-\frac{1}{4})^{1/2}$.

The most immediate conclusion which can be drawn from the potential curves shown in Fig. 1 is that the lowest resonance below the Ps($N=2$) threshold could not possibly lie at the energy given by Doolen, $E=-0.222$ Ry. This energy lies far below the minimum of the corresponding potential curve, and is thereby ruled out at once. Similarly, the potential curves of Ref. 4 rule out the possibility of an S-wave shape resonance just above the H($N=2$) threshold, which leads us to conclude again that there is no resonance feature whatsoever at $E=-0.222$ Ry.

We next compare the complex-coordinate calculation with other resonances reported by Doolen. The lowest resonance shown in Table II lies at $E=-0.150\,279$ Ry. This compares with Doolen's value of $-0.150\,318$ Ry. The difference is due to the fixed-nucleus (infinite-mass) approximation used in Ref. 5. The present complex-coordinate results shown in Table II are obtained using the finite proton mass, but it should be mentioned that we are able to reproduce Doolen's results for this resonance when we assume the proton to be infinitely massive. For the second resonance ($E=-0.131\,659$ Ry) below the Ps($N=2$) threshold, we find an appreciable difference between our width ($\frac{1}{2}\Gamma=0.000\,163$ Ry) and that given in Ref. 5 ($\frac{1}{2}\Gamma=0.000\,087$ Ry). This is presumably because more extensive wave functions ($M=969$, $\omega=16$) are employed in the present calculation than those of Ref. 5 ($M=680$, $\omega=14$). Furthermore, the use of more extensive basis functions enables us to determine the width for the third resonance, which was not obtained in Ref. 5.

In summary, we have used two independent methods (complex-coordinate rotation and adiabatic hyperspherical potential curves) to conclude that the lowest S-wave resonance associated with the Ps($N=2$) threshold lies at $E=-0.150\,279$ Ry, and not at $E=-0.222$ Ry as reported by Doolen.[5] Since more extensive wave functions have been used, the resonance parameters reported in this work improve over previous results in the literature. Finally, resonance parameters and potential curves for Feshbach resonances associated with the H($N=3$) threshold are reported for the first time.

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