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Positron-hydrogen resonances associated with the positronium $N=3$ and hydrogen $N=4$ thresholds

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Some lower-lying S-wave resonances in positron-hydrogen scattering associated with the $N=3$ positronium (Ps) and $N=4$ hydrogen thresholds are investigated by using the method of complex-coordinate rotation. Using Hylleraas-type wave functions with $M=969$ terms, several resonances in these energy regions are calculated for the first time. In particular, the lowest resonance associated with the Ps($N=3$) threshold is found to lie at $E=-0.077\,063$ Ry, and the lowest resonance associated with the H($N=4$) threshold is found to lie at $E=-0.067\,867$ Ry. In addition, we also locate a shape resonance lying just above the Ps($N=3$) threshold at $E=-0.055\,44$ Ry.

There has been considerable interest in investigating resonances in e^+-H scattering.[1] Several independent studies[2-4] have shown that resonances do exist associated with and below the hydrogen $N=2$ threshold. Resonances below the Ps($N=2$) threshold have been investigated by Doolen[5] and recently by Ho and Greene.[6] It was found in Ref. 6 that the lowest resonance associated with the Ps($N=2$) threshold would lie at $E=-0.150\,279$ Ry. Such a finding contradicts the result obtained by Doolen that it would lie at $E=-0.222$ Ry. Resonances below the $N=3$ hydrogen threshold were published in Ref. 6. Resonances in e^+-H scattering are also currently under investigation using a method of hyperspherical coordinates.[7] Here, we present new calculations of resonances associated with the $N=3$ positronium Ps and $N=4$ hydrogen thresholds. The method of complex-coordinate rotation is used in the present investigation.

In the method of complex-coordinate rotation, the Hamiltonian of the positron-hydrogen system is

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

where T and V are kinetic energy and potential energy operators, respectively, and

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

$$V=-\frac{2}{r_{1p}}+\frac{2}{r_{2p}}-\frac{2}{r_{12}}\,, \tag{3}$$

where 1 and 2 denote the electron and positron, respectively, and p the proton; m_i is the mass for particle i; and r_{ij} represents the distance between particles i and j. In this work we use the true mass value for the hydrogen nucleus, the proton, with $m_p=1836.151\,m_e$. Atomic units are used in this work, with energy expressed in *rydbergs*. The kinetic operator in Eq. (2) can be expressed in terms of distance coordinates (see Ref. 8, for example). Hylleraas-type wave functions of the form

$$\Psi=\sum_{k,l,m} C_{klm}\exp[-\alpha(r_{1p}+r_{2p})]r_{12}^k r_{1p}^l r_{2p}^m \tag{4}$$

are used, with $\omega \leq k+l+m$, and ω a positive integer or zero. In this work we employ up to a total of 969 terms ($\omega=16$). Also, to overcome possible ill-conditioned natures of the Hylleraas-type wave functions, calculations are performed in quadruple precision with an IBM 3084 computer. This gives us about 30-digit accuracy in calculations of matrix elements and in solving the eigenvalue problems.

The method of complex-coordinate rotation is used to calculate resonance parameters. The theoretical aspect of this method has been discussed in previous publications and will not be repeated. Here, we only briefly state the computational aspect of the method. Resonance parameters are determined from the conditions that the complex eigenvalues are stabilized with respect to changes of θ, α, and M, where θ is the so-called complex-rotation angle in the complex transformation $r \to r\exp(i\theta)$, where α is the nonlinear parameter in the wave function [Eq. (4)], and M the expansion length.

Figure 1 shows threshold energy levels for the e^+-H system. We use solid lines to represent the energy levels

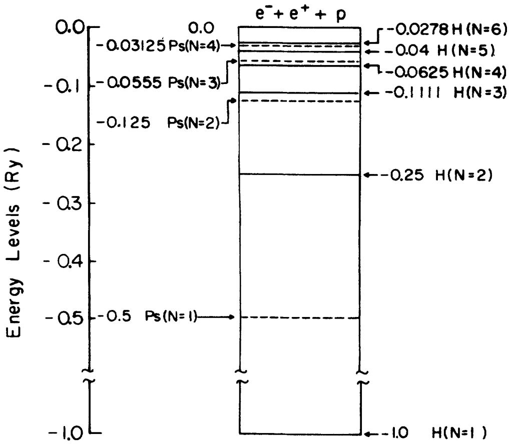

FIG. 1. Energy levels in the e^+-H system.

TABLE I. S-wave resonances in $e^{+}-\mathrm{H}$ scattering associated with the positronium $N=3$ and hydrogen $N=4$ thresholds. The asterisk represents a shape resonance lying above the Ps($N=3$) threshold of $E=-0.055\,556$ Ry.

E (Ry)	Γ (Ry)	Series
	Below H($N=4$) threshold	
−0.067 867	0.000 096	A1
−0.064 595	0.000 044	A2
−0.063 259	0.000 020	A3
−0.063 699	0.000 100	B1
	Below Ps($N=3$) threshold	
−0.077 063	0.000 095 2	A1
−0.0623	0.000 050	A2
−0.055 44*	0.000 08	B1

for hydrogen atoms and dashed lines for positronium atoms. This work reports resonances in energy regions associated with the H($N=4$) threshold ($E=-0.0625$ Ry) and Ps($N=3$) threshold ($E=-0.0555$ Ry).

For resonances associated with the $N=4$ hydrogen threshold, we show three members of one resonance series, as well as the lowest member for another series. For resonance associated with the $N=3$ positronium threshold, we have found two members for one series. In addition, a shape resonance lying just above the Ps($N=3$) threshold is located. The use of letters A and B in Table I is only for labeling purposes. The results for resonances associated with the Ps($N=3$) and H($N=4$) thresholds are shown in Fig. 2. In the figure we connect the resonances that are believed to belong to the same series and the threshold to which the series converge.

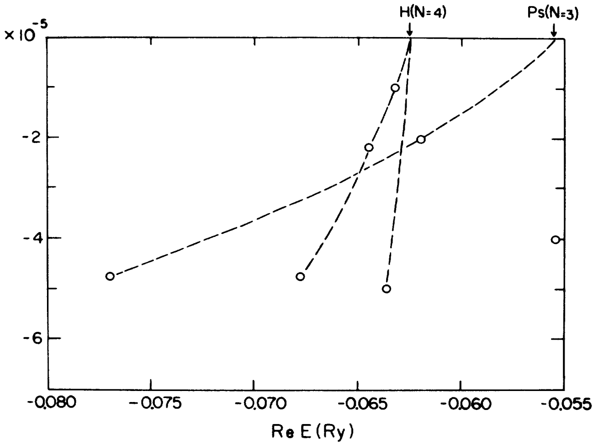

FIG. 2. S-wave resonances in $e^{+}-\mathrm{H}$ scattering associated with the positronium $N=3$ and hydrogen $N=4$ thresholds. The energy unit is rydbergs.

Table I summarizes the S-wave resonances in positron-hydrogen scattering in these energy regions.

In summary, we report here resonance parameters (both resonance positions and widths) in positron-hydrogen scattering associated with positronium $N=3$ and hydrogen $N=4$ thresholds. These results, reported for the first time in literature, are obtained from accurate calculations and should be useful for other theoretical and experimental work.

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[1] Y. K. Ho, Phys. Rep. **99**, 1 (1983).

[2] L. T. Choo, M. C. Crocker, and J. Nuttall, J. Phys. B **11**, 1313 (1978).

[3] G. D. Doolen, J. Nuttall, and C. Wherry, Phys. Rev. Lett. **40**, 313 (1978).

[4] E. Pelikan and H. Klar, Z. Phys. A **310**, 153 (1983).

[5] G. D. Doolen, Int. J. Quantum Chem. **14**, 523 (1978).

[6] Y. K. Ho and C. H. Greene, Phys. Rev. A **35**, 3169 (1987).

[7] B. J. Archer, G. A. Parker, and P. T. Packs, Bull. Am. Phys. Soc. **33**, 936 (1988).

[8] Y. K. Ho, Phys. Rev. A **19**, 2347 (1979).