Comparative Studies of Excitations and Resonances in H^-, Ps^-, and $e^+ + H$ Systems

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The hyperspherical close coupling method for general Coulomb three-body systems is used to examine e^- + H, e^+ + Ps, and e^+ + H collisions to investigate how the excitation cross sections and resonances depend on the masses, the charges, and the quantum statistics of the system. Hyperspherical potential curves are used to help unravel the nature of Feshbach resonances, shape resonances, and overlapping resonances in these systems.

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In nonrelativistic quantum mechanics, the solution of the Schrödinger equation for a Coulomb two-body system is well known. However, much less is understood for Coulomb three-body systems. While many theoretical approaches have been successful for treating special subsets of Coulomb three-body systems, there is no well-established method for addressing the general problems.

In this Letter we compare the inelastic scattering cross sections and analyze resonances in e^- + H, e^+ + H, and e^- + Ps collisions to illustrate how the properties of these systems vary with the charges and the masses. Among the three systems, the first and the third each contains two identical fermions, while the second consists of three distinguishable particles. For H^- and Ps^-, we note that the two-body systems, H and Ps, differ only in the reduced mass where the energy levels and lengths can be appropriately scaled. Furthermore, the calculated ground state energy of H^- is $-1.055\,50$ Ry (assuming the mass of the proton is infinity), and of Ps^- is $-0.524\,01$ Ry. By removing the reduced mass factor 0.5 for the latter, the total ground state energies of the two systems differ by about 0.7%.

In view that the experimental data for these systems are incomplete, we perform the analysis based on results obtained using the hyperspherical close coupling method (HSCC) which can be applied to any Coulomb three-body systems [1–5]. When comparison is possible, it is shown that numerical results obtained using the HSCC method are in good agreement with variational calculations. Thus results from the HSCC method for different systems are believed to be accurate enough to address even the small differences found in the calculations.

The basic idea of the hyperspherical close coupling method is very simple. Denote the three-body system as ABC. From the two vectors, $\vec{r}_{AB}$ and $\vec{r}_{AB,C}$, where the former is from A to B, and the latter is from the center of mass of A and B to C, one can define a hyperspherical radius R and a hyperangle ϕ. In the HSCC method, the total wave function is expanded in the form

$$\Psi(R,\Omega) = \sum_\mu F_\mu(R)\Phi_\mu(R;\Omega), \qquad (1)$$

where Ω denotes $(\phi, \hat{r}_{AB}, \hat{r}_{AB,C})$ collectively and $\Phi_\mu(R;\Omega)$ is the adiabatic "channel" function obtained by solving the three-body Schrödinger equation at fixed values of R

$$H|_{R=\text{const}}\Phi_\mu(R;\Omega) = U_\mu(R)\Phi_\mu(R;\Omega). \qquad (2)$$

The potential curves $U_\mu(R)$ obtained in (2) are used to identify different channels in each collision system. In the asymptotic limit, each potential curve $U_\mu(R)$ approaches one of the well-known two-body excitation thresholds.

In actual calculations the adiabatic approach outlined above is slightly modified. The more accurate HSCC calculation employs the so-called diabatic-by-sector method where in the inner region the hyperradius is divided into many small sectors. Within each sector, the basis functions are fixed, and are chosen to be the adiabatic functions (2) calculated at the midpoint of the sector. The resulting set of hyperradial equations is integrated over the sector until the boundary where it is expanded in terms of basis functions of the next sector. This procedure is continued until it reaches a large hyperradius where the resulting solutions in hyperspherical coordinates are matched to the solutions in the asymptotic region expressed in independent particle coordinates. The matching provides the K matrix which is used to obtain scattering cross sections. The detailed method is described in Ref. [4], although some numerical procedures have been modified in the present calculation in order to obtain accurate potential curves at large R. Furthermore, the independent particle wave functions in the outer region used are dipole states to account for the long-range interaction when the core is in the hydrogenlike excited states. The outer matching radius was chosen to be at 250 a.u. in the calculation. We used about 20–40 channels in the close coupling calculation and the results are very stable against variation of the matching radius.

In this Letter we show results for $L = 0$ states only, emphasizing the comparison among the three systems mentioned above. The results for nonzero angular momentum states will be presented in the future.

At first, the ground state energies for H^- and Ps^- from the present restricted calculation were found to be $-0.527\,79$ and $-0.262\,05$ a.u., respectively, in good agreement with the well-known data $-0.527\,75$ and

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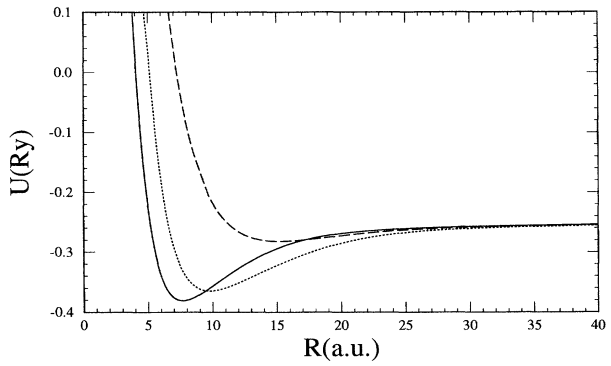

FIG. 1. Comparison of attractive adiabatic potentials vs hyperradius below the $N = 2$ threshold. The solid line is for $^1S^eH^-$. The dashed line is for $L = 0$ states of the $e^+ + H$ system converging to the $H(N = 2)$ threshold. The dotted line is for $^1S^e$ states of Ps^- where the potential has been multiplied by 2 and the hyperradius reduced by a factor of $\sqrt{2}$ in order to account for the smaller reduced mass for Ps.

$-0.262\,00$ a.u. There is no stable ground state for the $e^+ + H$ system. We then proceed to analyze the three systems at energies near and above the $N = 2$ excitation threshold. In order to compare Ps^- with the other two systems on an equal footing, we remove the reduced mass factor by multiplying the energy scale by 2 and reduce the hyperradius by a factor of $\sqrt{2}$.

(i) Resonances below the N=2 threshold.—The lowest $L = 0$ potential curves from each system that converge to the $N = 2$ threshold are shown in Fig. 1. For H^- and Ps^-, these curves support singlet S states. Because of the $2s$-$2p$ degeneracy for two-body Coulomb systems, each curve approaches the limit following a dipole potential $-\alpha/R^2$ where α is the permanent dipole moment. On the other hand, the potential at small R is drastically different if the system has two identical particles, as shown by the deep attractive potential wells for H^- and Ps^-. Also note that the potential curves for these two systems are very similar after being rescaled by the reduced mass.

The potential curves in Fig. 1 allow for an estimate of the positions of resonances. However, more accurate calculations can be carried out using the HSCC method. The results for the first two Feshbach resonances in each of the three systems are shown and compared to those from other methods in Table I [6,7]. It is clear that the positions and widths obtained using the HSCC and those from the variational methods [6] are in good agreement. In Table I we also show results from the other earlier hyperspherical calculation performed by Sadeghpour [8]. His approach differs from ours in that he used adiabatic hyperspherical basis functions for the inner region and that his method is applicable only to one-centered atomic systems such as H^-. His calculations using a smaller basis set are also in reasonable agreement with ours for the two states shown. In Table I, it is also clear that the lowest states of H^- and Ps^- have much lower energies, reflecting the effect of Pauli exclusion principle. For these states, the two electrons tend to stay on opposite sides of the positive charge and at about the same distances from it, resulting in a smaller Coulomb repulsion between the two electrons and thus lower binding energies. (This is also reflected in that there is always at least one stable bound state for a three-body Coulomb system if it contains two identical particles [9]. If all the particles are different, there is a restricted range of masses where bound states can exist [10].) For the $e^+ + H$ system, the positron in the lowest Feshbach resonance state tends to stay far away from the proton; it is bound essentially only by the attractive dipole field of the excited H atom.

The HSCC method solves the three-body Schrödinger equation directly. Unlike the complex coordinate rotation method [6] which is very useful primarily for studying resonances, the HSCC approach gives full details of inelastic scattering cross sections over the whole energy

TABLE I. Comparison of $^1S^e$ resonances in H^-, Ps^-, and in $L = 0$ states in $e^+ + H$ below the $N = 2$ threshold [for $e^+ + H$, below $H(2)$]. Each resonance is expressed as $(-E_R, \Gamma/2)$ where E_R is the resonance energy and Γ is the width in Rydberg units. For Ps^-, both the energies and widths have been multiplied by 2 to account for the scaling due to the reduced mass in Ps. The results from the present calculations are shown without the superscript in each entry.

	H^-	Ps^-	$e^+ + H$
1	$(0.29743, 1.73^{-3})$	$(0.30416, 8.70^{-5})$	$(0.25731, 6.64^{-5})$
	$(0.29755, 1.73^{-3})$[a]	$(0.30412, 8.60^{-5})$[b]	$(0.25725, 6.66^{-5})$[c]
	$(0.29743, 1.75^{-3})$[e]		
2	$(0.25203, 9.16^{-5})$	$(0.25470, 1.75^{-5})$	$(0.25030, 3.91^{-6})$
	$(0.25201, 9.55^{-5})$[d]	$(0.25460, 2.00^{-5})$[b]	$(0.25017, < 1.00^{-5})$[c]
	$(0.2509, 11.4^{-5})$[e]		

[a]Ho [6(a)].
[b]Ho [6(b)].
[c]Ho [6(c)].
[d]Pathak, Kingston, and Berrington [7].
[e]Sadeghpour [8].

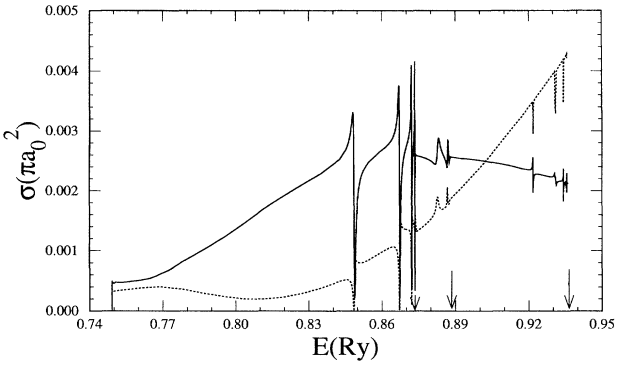

FIG. 2. $L = 0$ partial wave contribution to $H(2s)$ and $H(2p)$ excitation cross sections in $e^+ + H$ scattering. The solid line is for $H(2s)$ and the dashed line is for $H(2p)$. The arrows along the horizontal axis indicate the inelastic thresholds. The thresholds are $Ps(N = 2)$, $H(N = 3)$, and $H(N = 4)$ in the order of increasing energies.

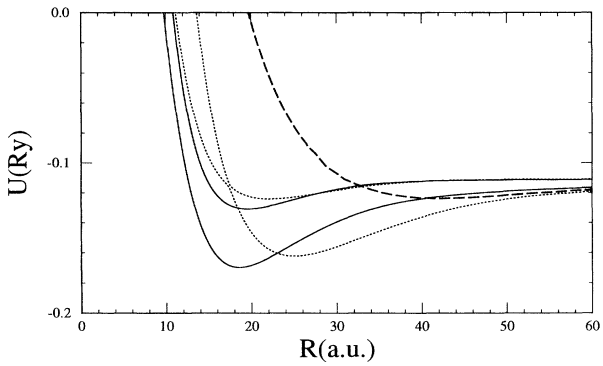

FIG. 3. Comparison of attractive potential curves vs hyperradius below the $N = 3$ threshold. The two solid lines are for $^1S^e$ states of H^-. The two dotted lines are for $^1S^e$ states of Ps^-, with the scaling as explained in Fig. 1. The avoided crossing near $R = 17$ should be treated diabatically. The only dashed curve is for the $L = 0$ states of $e^+ + H$. Other belonging to this manifold are repulsive and are not shown.

region. In Fig. 2 we show the cross sections for excitation to $2s$ and $2p$ states of H in $e^+ + H$ collisions. The cross sections are quite small and rise rapidly with energies. They are also marked by numerous Feshbach resonances below each higher threshold (see below). These thresholds are indicated by arrows in Fig. 2; they are Ps(2), H(3), and H(4), respectively, in the order of increasing energies. Another calculation for these excitation cross sections used the close coupling method in momentum space [11]. Although their cross sections are very close to ours, the resonance positions are about 30% higher than ours as measured from the threshold. The HSCC method has also been used to calculate $^1S^e$ excitation cross sections to the $N = 2$ states for the other two systems. For $e^- + H$, both $2s$ and $2p$ excitation cross sections calculated are relatively energy independent and are in agreement with other calculations and with the recent results of Wang and Callaway [12] where the Schrödinger equation was solved in a numerical grid. For excitation to the $2s$ and $2p$ states of Ps in $e^- + Ps$ collisions, the cross sections are also relatively energy independent.

(ii) Resonances near the N=3 threshold.—In Fig. 3 we show the two lowest potential curves for $^1S^e$ states of H^- and of Ps^-, and the lowest curve for $L = 0$ states of $e^+ + H$. The lowest curve of each system has a similar shape as the corresponding one below the $N = 2$ threshold. On the other hand, each of the upper curves of H^- and Ps^- has an attractive well at small R and a repulsive potential barrier at large R. Depending on the strength of the potential well, resonances associated with such a curve can lie either below or above the threshold.

We have performed HSCC calculations to locate resonances in the energy region near the $N = 3$ threshold. The results are listed together with those from other calculations in Table II. For H^-, we have found that the energy positions of the first, second, and fourth resonances follow reasonably well the scaling relation expected from a dipole potential, namely, that successive resonances follow the relation $\epsilon_{n+1}/\epsilon_n = e^{-2\pi/\beta}$ where $\beta = \sqrt{\alpha - 0.25}$, with α being the permanent dipole moment from the lowest curve and that energy ϵ is measured from the threshold. The third resonance does not follow the scaling pattern and it is attributed to be associated with the second H^- curve in Fig. 3. The same analysis for the first four resonances for Ps^- indicates that they follow the relation expected from the dipole potential of the lowest curve. By carrying out a scattering calculation for $e^- + Ps$ collisions above the $N = 3$ threshold, there a shape resonance was found and we interpret it to be associated with the second potential curve of Ps^-. Table II also shows that resonance parameters obtained using HSCC are in good agreement with variational results [6].

(iii) The overlapping resonances near the H(N=4) and Ps(N=3) thresholds.—For the $e^+ + H$ system, the $H(N = 4)$ and the $Ps(N = 3)$ thresholds lie at 0.9375 and 0.9444 Ry from the ground state of H, respectively. The two thresholds are so close that resonances associated with the two limits may interact with each other. In Fig. 4 we show the two lowest curves from each threshold and we note that the lowest curve from $Ps(N = 3)$ indeed lies below the $H(N = 4)$ threshold in the region where the potential curve is near the minimum. More importantly, Fig. 4 indicates that the lowest curve from each threshold interacts with each other strongly, showing a pronounced avoided crossing at $R \simeq 100$ a.u. Such an avoided crossing may modify the spectral behaviors from those expected out of a single isolated potential curve.

We have carried out HSCC calculations in the energy region below the $H(N = 4)$ threshold and identified four resonances. The positions and half-widths $(-E_r, \Gamma/2)$ (in rydbergs) of the lowest four resonances obtained are $(0.077\,100, 4.76^{-5})$, $(0.067\,902, 4.78^{-5})$, $(0.064\,625, 1.63^{-5})$ and $(0.063\,725, 4.88^{-5})$, in good agreement with the variational results of Ho [6]. By

TABLE II. Camparison of $^1S^e$ resonance in H^-, Ps^-, and in $L = 0$ states in $e^+ + H$ below the $N = 3$ threshold [for $e^+ + H$, below $H(3)$]. Format is the same as in Table I.

	H^-	Ps^-	$e^+ + H$
1	(0.13798, 1.42^{-3})	(0.14142, 1.48^{-4})	(0.11610, 6.16^{-4})
	(0.13801, 1.42^{-3})[d]	(0.14137, 1.5^{-4})[a]	(0.11606, 6.2^{-4})[b]
2	(0.115593, 3.07^{-4})	(0.11945, 1.04^{-4})	(0.11210, 1.30^{-4})
	(0.115563, 3.08^{-4})[d]	(0.11938, 1.1^{-4})[a]	(0.11206, 1.4^{-4})[b]
3	(0.112262, 9.13^{-5})	(0.11322, 2.50^{-5})	
	(0.112277, 8.20^{-5})[d]		
4	(0.112012, 5.06^{-5})	(0.11162, 1.07^{-5})	
	(0.112013, 4.50^{-5})[d]		
Shape		(0.11102, 1.00^{-4})	
		(0.1109, 8.4^{-5})[c]	

[a]Ho [6(b)].
[b]Ho [6(c)].
[c]Ho [6(e)].
[d]Ho [6(f)].

analyzing the relative resonance positions, $\epsilon_{n+1}/\epsilon_n$, we found that they do not follow the expected scaling from a single dipole potential. The relative widths, which are to scale like the relative energy positions for a dipole potential, also display no simple regularity among the four resonances. We interpret this irregular sequence as the result of channel coupling between resonances associated with two different thresholds. Such interchannel coupling can result in modulation in the spectral intensity, as seen experimentally in He above the $N = 5$ threshold [13]. In the present $e^+ + H$ system, the coupling is between resonances associated with channels from two different dissociation arrangements.

In summary, we have shown that the hyperspherical close coupling method can be used to obtain accurate results for any Coulomb three-body systems. From the adiabatic potential curves, the nature of resonances and inelastic scattering cross sections for the three elementary systems, H^-, Ps^-, and $e^- + H$, has been analyzed simultaneously. The analysis reveals that the existence of two identical particles tends to make the three-body Coulomb systems more bound. We further examine the fine dependence of resonance positions on the masses in the system, and show that the HSCC method is a powerful approach for studying reactive scattering in three-body Coulomb systems. It is worthwhile also to mention that the hyperspherical approach can be applied to non-Coulombic three-body systems, as demonstrated recently in the study of the role of three-body collisions in Bose-Einstein condensation [14].

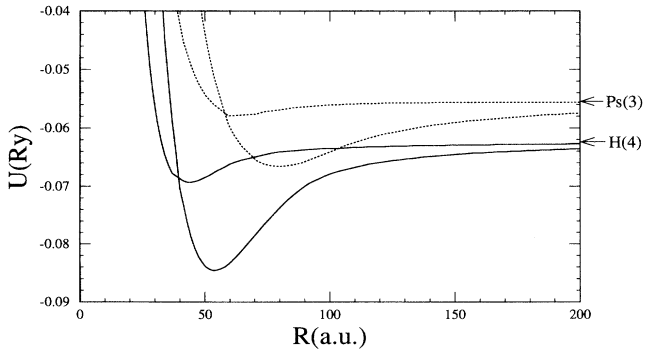

FIG. 4. Attractive potential curves that converge to the $H(N = 4)$ and $Ps(N = 3)$ thresholds for the $L = 0$ states in $e^+ + H$ system.

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