S-wave resonances in positron scattering by He^+

Akinori Igarashi and Isao Shimamura
The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama 351-01, Japan
(Received 2 July 1997)

S-wave $e^+ + He^+$ scattering is calculated using the hyperspherical close-coupling method. The two resonances found at about -0.73 Ry and -0.39 Ry by Bhatia and Drachman [Phys. Rev. A **42**, 5117 (1990)] and reproduced by Ho [Phys. Rev. A **53**, 3165 (1996)] do not occur in the present results. An argument against these proposed resonances is presented on the basis of the adiabatic hyperspherical potentials. Instead of these resonances, we have found narrow Feshbach resonances just below the thresholds (-0.25 a.u. and -0.0625 a.u.) of the formation of Ps($n=1$) and Ps($n=2$) and an extremely narrow shape resonance just above the threshold -0.08 a.u. of $He^+(n=5)$. They would be hardly detected since (i) the resonance widths are of the order of 10^{-4}–10^{-5} a.u. or less, (ii) the resonance is weak in the elastic cross section, (iii) the magnitudes of the inelastic and Ps-formation cross sections are small, and (iv) the smooth cross sections due to higher partial waves should still be added to the *S*-wave cross section. [S1050-2947(97)04212-1]

PACS number(s): 34.80.Kw, 31.15.Ja, 36.10.Dr

I. INTRODUCTION

Resonance calculations can sometimes be quite subtle. In particular, the question of the occurrence of resonances in positron scattering by positive ions is of interest because of the asymptotic repulsive Coulomb potential in the initial arrangement channel and the attractive long-range potentials in the positronium (Ps) channels, namely, the polarization potential in the ground-state Ps channel and the dipole potentials in excited-state Ps channels.

Bhatia and Drachman [1] applied the stabilization method to $e^+ + He^+$ scattering and found two *S*-wave resonances lying at energies -0.73 Ry and -0.39 Ry of the total scattering system $e^+ He^+$. The calculations by Ho [2] using the method of complex-coordinate rotation reproduced these resonances; the resonance energies E_r and the widths Γ are $(E_r, \Gamma) = (-0.371,\ 0.125)$ and $(-0.186,\ 0.039)$ in a.u. Ho noted the possibility of the detection of these resonances, the widths being 3.4 eV and 1.1 eV. Ho [2] also found broad *P*-wave resonances in this system. Both the stabilization and the complex-coordinate-rotation methods are of bound-state type.

Here we report the results of detailed scattering calculations for the *S*-wave $e^+ + He^+$ collision system using the hyperspherical close-coupling (HSCC) method and reexamine resonance structures in the cross sections. The power of the HSCC method in the study of continuum processes involving a positron has been demonstrated in the literature [3,4]. The recent development of the hyperspherical approach is reviewed by Lin [5]. One of the advantages of the HSCC method is that nonlocal potentials are completely absent in the scattering equations even for the system for which rearrangement channels (or Ps-formation channels in the present case) must be considered. This allows one to use the visual information on the adiabatic hyperspherical potentials for associating bound states and resonances with particular adiabatic states and for classifying resonances into Feshbach and shape resonances. Examination of the adiabatic hyperspherical potentials may also lead to a persuasive argument that no resonances occur in a certain energy region.

II. THE HYPERSPHERICAL CLOSE-COUPLING METHOD

The formalism of the present HSCC method is outlined here; further details may be found in a previous paper [3]. Let $\mathbf{r}_+$ and $\mathbf{r}_-$ denote the position vectors of the positron and the electron relative to the nucleus He^{2+}. The hyperradius $\rho \equiv \sqrt{r_+^2 + r_-^2}$ and the hyperangle $\phi \equiv \tan^{-1}(r_-/r_+)$ replace the pair of the radial coordinates r_+ and r_- and Ω denotes the five angular variables $(\phi, \hat{r}_+, \hat{r}_-)$ collectively. An adiabatic Hamiltonian $h_{\rm ad}$ is defined by writing the total Hamiltonian H as

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2} + \frac{5}{\rho}\frac{\partial}{\partial\rho}\right) + h_{\rm ad}(\rho;\Omega). \tag{1}$$

In other words, $h_{\rm ad}$ is the Hamiltonian obtained by fixing the value of ρ. Then the adiabatic channel functions φ_μ of the angular variables Ω and the corresponding adiabatic hyperspherical potentials $U_\mu(\rho)$ are defined as the eigenfunctions and eigenvalues of the adiabatic Schrödinger equation

$$h_{\rm ad}(\rho;\Omega)\varphi_\mu(\rho;\Omega) = \left(U_\mu(\rho) - \frac{15}{8\rho^2}\right)\varphi_\mu(\rho;\Omega) \tag{2}$$

for fixed values of ρ. As $\rho \to \infty$, each of the potentials U_μ approaches a hydrogenic energy of either the He^+ ion or the positronium Ps.

The wave function Ψ of the total scattering system is expanded in terms of the complete set of adiabatic wave functions as

$$\Psi(\rho,\Omega) = \sum_\mu \rho^{-5/2} F_\mu(\rho)\varphi_\mu(\rho;\Omega). \tag{3}$$

Substitution of this form into the Schrödinger equation for the total system leads to coupled radial equations for $F_\mu(\rho)$, namely,

$$\left(-\frac{1}{2}\frac{d^2}{d\rho^2} + U_\mu(\rho) - E \right) F_\mu(\rho) + \sum_\nu V_{\mu\nu} F_\nu(\rho) = 0, \quad (4)$$

the coupling potentials $V_{\mu\nu}$ stemming from the kinetic-energy operator or from the nonadiabatic effect. These coupled equations are referred to as the HSCC equations.

In fact, a slight modification in this formalism is made for computational convenience since $V_{\mu\nu}$ can be sharply peaked in the vicinity of avoided crossings between adiabatic potentials $U_\mu(\rho)$. First, the entire region of ρ is divided into a large number of small sectors. If an avoided crossing between adiabatic potentials $U_\mu(\rho)$ and $U_{\mu'}(\rho)$ occurs, the corresponding adiabatic channel functions $\varphi_\mu(\rho;\Omega)$ and $\varphi_{\mu'}(\rho;\Omega)$ in Eq. (3) in each sector k in the vicinity of the avoided crossing are replaced by $\varphi_\mu(\rho_k;\Omega)$ and $\varphi_{\mu'}(\rho_k;\Omega)$ at the midpoint $\rho=\rho_k$ of that sector. These functions are referred to as piecewise diabatic functions since they are independent of ρ in each sector. Those adiabatic channel functions unassociated with the avoided crossing are used as they are. Thus our expansion is a hybrid of adiabatic and diabatic channel functions.

In solving the HSCC equations, the wave function is matched smoothly from sector to sector so that the value and derivative are continuous over the boundary between adjacent sectors. The solutions are thus propagated up to a large enough value $\rho_{\max}$ of ρ. There, they are matched to the proper scattering boundary condition in Jacobi coordinates and the scattering matrix is extracted. For hydrogenic excited states, we use dipole states, which are such linear combinations of hydrogenic states with a common principal quantum number n that diagonalize the sum of the dipole operator and the angular-momentum operator [6]. The Coulomb (for the $e^+ + \mathrm{He}^+$ channels) or Bessel (for the $\mathrm{He}^{2+} + \mathrm{Ps}$ channels) functions of complex order, instead of integral angular momentum, are employed for the radial asymptotic scattering functions. Two choices of the matching radius $\rho_{\max}$, namely, 450 a.u. and 600 a.u., have led to results differing by less than 0.1% from each other. The channel functions φ_μ in Eq. (2) are calculated by means of a variational method with Slater-type orbitals as discussed in Ref. [3]; the variational trial function includes 35 s, 25 p, 20 d, 15 f, 15 g, and 15 h orbitals centered on He^{2+} and 20 s, 15 p, and 10 d orbitals as functions of $\mathbf{r}_- - \mathbf{r}_+$. In the close-coupling expansion (3), we coupled 24 channels describing fragmentation into $e^+ + \mathrm{He}^+(n=1\text{–}6)$ and $\mathrm{He}^{2+} + \mathrm{Ps}(n=1,2)$ in the asymptotic region.

III. RESULTS AND DISCUSSION

The calculated S-wave adiabatic hyperspherical potential curves are shown in Figs. 1 and 2. The potential curves that lead to the arrangement $e^+ + \mathrm{He}^+(n)$ in the asymptotic region decay as $1/\rho$ owing to the repulsive Coulomb force between e^+ and He^+. No potential curves are seen in Fig. 1 that have an attractive well strong enough to support a resonance around an energy of -0.37 a.u. or -0.19 a.u., around which resonances were found by Bhatia and Drachman [1] and Ho [2]. Since any Feshbach-type or shape resonances are considered to appear as bound or resonance states supported by an adiabatic hyperspherical potential, we expect no resonances near the energies where these authors located resonances. Indeed, the 24-channel HSCC calculation revealed no resonance structure in this energy region; note that the resonance widths quoted by Ho are so large that we could not have missed them if these resonances really existed.

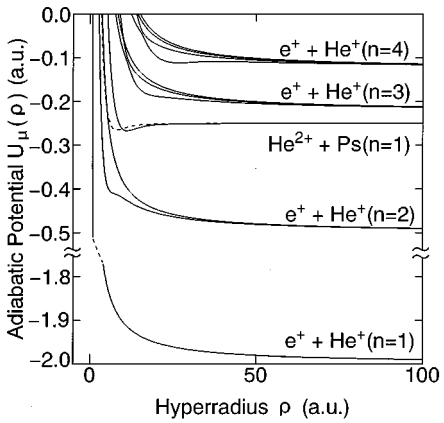

FIG. 1. S-wave hyperspherical adiabatic potential-energy curves of the system $e^+\mathrm{He}^+$. In the asymptotic limit, each potential-energy curve approaches the energy of either $\mathrm{He}^+(n)$ or $\mathrm{Ps}(n)$. Their asymptotic arrangements are indicated as $e^+ + \mathrm{He}^+(n)$ or $\mathrm{He}^{2+} + \mathrm{Ps}(n)$. The adiabatic potential for the system $e^+\mathrm{H}$ that dissociates into $\mathrm{H}^+ + \mathrm{Ps}(n=1)$ is also shown by the dashed curve for comparison.

The potential curve that converges to $\mathrm{He}^{2+} + \mathrm{Ps}(n=1)$ has an attractive dipole polarization potential, which behaves asymptotically proportional to $-\rho^{-4}$ and connects to a short-range potential well. The HSCC calculation with fine energy-mesh points just below the threshold of -0.25 a.u. for $\mathrm{Ps}(n=1)$ produced a resonance supported by this potential well. A fit of the eigenphase sum to the Breit-Wigner one-level formula yielded a resonance position of $E_r = -0.250\,012$ a.u. and a width of $\Gamma = 7.7\times10^{-6}$ a.u. This resonance is much narrower than the one that was calculated by Ho [2] at ~ -0.37 a.u. and that was not found in the present calculation. Furthermore, the bottom of the potential well is -0.27 a.u. and is much higher than -0.37 a.u. Thus the resonance found in the present calculation is quite differ-

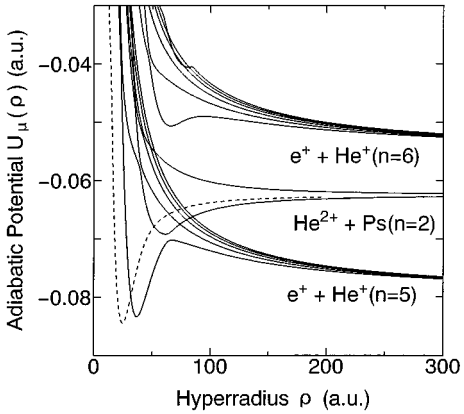

FIG. 2. S-wave hyperspherical adiabatic potential curves of the system $e^+\mathrm{He}^+$ near the $\mathrm{Ps}(n=2)$ threshold. The adiabatic potential for the system $e^+\mathrm{H}$ that dissociates into $\mathrm{H}^+ + \mathrm{Ps}(n=2)$ is also shown by the dashed curve for comparison.

TABLE I. *S*-wave resonances in the system $e^+e^-He^{2+}$ below the thresholds $He^{2+}+Ps(n=1)$ and $He^{2+}+Ps(n=2)$. Each resonance is expressed as (E_r,Γ), where E_r is the resonance energy and Γ is the width, both in atomic units. $a[b]=a\times10^b$.

Present	Bhatia and Drachman [1]	Ho [2]
	below the $Ps(n=1)$ threshold	
	(−0.365, —)	(−0.370 50, 0.1294)
(−0.250 012, 7.7[−6])		
	below the $Ps(n=2)$ threshold	
	(−0.195, —)	(−0.1856, 0.0393)
(−0.075 595, 1[−13])		
(−0.067 42, 6.8[−4])		
(−0.064 32, 3.6[−4])		

ent from the one located by Ho at −0.37 a.u., and Ho's conjecture that the latter might be supported by the polarization potential is excluded. Note that no resonance was found for the e^++H collisions just below the $Ps(n=1)$ threshold [4] because of the weaker polarization potential between H^+ and $Ps(n=1)$ than between He^{2+} and $Ps(n=1)$ by a factor of 1/4; see the potential-energy curve for the system H^+Ps, shown by the dashed curve in Fig. 1 for comparison, that dissociates into $H^++Ps(n=1)$.

One of the potential curves near the $Ps(n=2)$ threshold, shown in Fig. 2, has an asymptotic attractive dipole potential due to the degenerate $Ps(n=2)$ states. This adiabatic potential supports an infinite series of bound states just below the $Ps(n=2)$ threshold, the two lowest of which lie at −0.0669 a.u. and −0.0642 a.u. These bound states turn into Feshbach resonances when coupled with open channels [6]. We first solved HSCC equations retaining only the seven channels dissociating into either $e^++He^+(n=5)$ or $He^{2+}+Ps(n=2)$, for energies between −0.09 a.u. and −0.0625 a.u. with a step of 1.0×10^{-4} a.u. This test calculation revealed several resonances, of which the two lowest have resonance parameters $E_r=-0.066\,72$ a.u., $\Gamma=4.8\times10^{-4}$ a.u. and $E_r=-0.064\,37$ a.u., $\Gamma=2.2\times10^{-4}$ a.u. With a 24-channel calculation, they changed into $E_r=-0.067\,42$ a.u., $\Gamma=6.8\times10^{-4}$ a.u. and $E_r=-0.064\,32$ a.u., $\Gamma=3.6\times10^{-4}$ a.u. Similar values found in the 7-channel and 24-channel calculations imply weak coupling of these resonances with channels augmented in the latter calculation.

The adiabatic potential curve supporting these two resonances (and many other) has an avoided crossing with the lowest potential curve shown in Fig. 2. If these two adiabatic potential curves are connected smoothly over the avoided crossing, one of the two resultant diabatic curves looks much like the potential curve for H^+Ps, shown by the dashed curve in Fig. 2 for comparison, that dissociates into $H^++Ps(n=2)$. Because of this attractive potential, the system H^+Ps has resonances $(E_r,\Gamma)=(-0.0751, 1.7\times10^{-4})$ and $(-0.0658, 8.1\times10^{-5})$ in a.u. [4,7]. Similarly, an attractive diabatic potential calculated for the present system $He^{2+}Ps$ by somewhat arbitrary smooth connection of adiabatic curves supports bound states, of which the two lowest are found to lie at −0.0771 a.u. and −0.0686 a.u. A HSCC calculation coupling the two channels washes away the second state completely since this level lies in the energy region of the avoided crossing. On the other hand, the lowest state

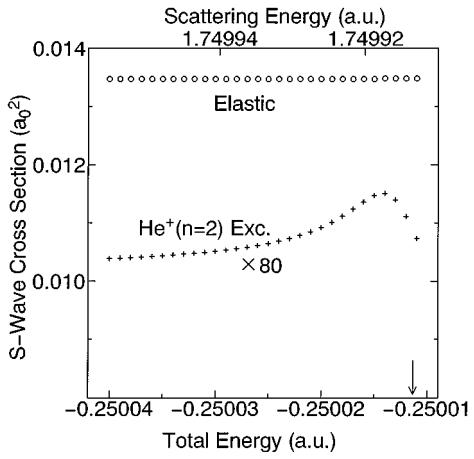

FIG. 3. *S*-wave cross sections for e^++He^+ scattering below the $Ps(n=1)$ threshold. Circles, elastic; pluses, excitation of $He(n=2)$. The positron energy is indicated on the upper scale and the energy of the total system e^+He^+ on the lower scale. The resonance position is indicated by an arrow.

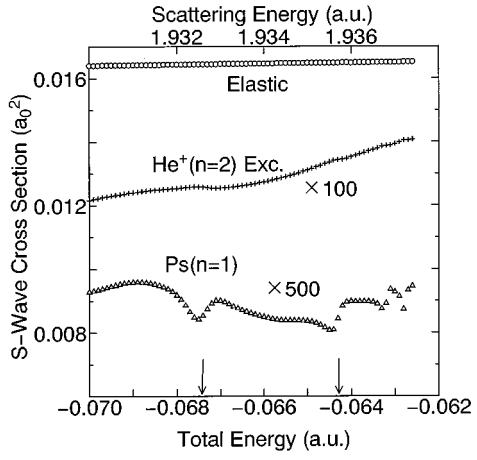

FIG. 4. *S*-wave cross sections for e^++He^+ scattering below the $Ps(n=2)$ threshold. Circles, elastic; pluses, excitation of $He(n=2)$; triangles, formation of $Ps(n=1)$. The positron energy is indicated on the upper scale and the energy of the total system e^+He^+ on the lower scale. The positions of two resonances are indicated by arrows.

changes into a very narrow resonance since this level lies far below the maximum of the lower adiabatic potential of the two and yet above the threshold of -0.08 a.u. for $e^+ + \mathrm{He}^+(n=5)$. In fact, this resonance is observed at $E_r = -0.075\,46$ a.u. as a shape resonance with $\Gamma = 9\times10^{-13}$ a.u., already in a single-channel calculation with the lowest adiabatic potential in Fig. 2 together with the adiabatic correction on it. The resonance parameters change slightly into $(E_r,\Gamma) = (-0.075\,598,\ 1\times10^{-13})$ in the two-channel calculation and into $(-0.075\,595,\ 1\times10^{-13})$ in a seven-channel calculation.

The resonance parameters determined in this work are summarized in Table I together with the results of Bhatia and Drachman [1] and Ho [2]. The present values are very different from the results of these previous authors, implying different origins.

Figure 3 shows the calculated S-wave elastic and inelastic cross sections for $e^+ + \mathrm{He}^+(n=1)$ scattering below the $\mathrm{Ps}(n=1)$ threshold. The S-wave elastic, inelastic, and Ps-formation cross sections for energies below the $\mathrm{Ps}(n=2)$ threshold are shown in Fig. 4. In both figures, the elastic cross section is much larger than the inelastic and rearrangement cross sections. The effect of S-wave resonances on the elastic cross section is weak. The resonance effect appears clearly in the cross section (in Fig. 3) for excitation of $\mathrm{He}^{2+}(n=2)$ just below the $\mathrm{Ps}(n=1)$ threshold and in the Ps formation cross section (in Fig. 4) just below the $\mathrm{Ps}(n=2)$ threshold. Experimental verification, however, must be difficult because of the small magnitude of the cross sections, the small resonance widths, and the smooth cross sections due to higher partial waves, which should be added to the S-wave cross section.

IV. CONCLUSION

We have calculated resonance parameters and cross sections for S-wave $e^+ + \mathrm{He}^+$ scattering using the hyperspherical close-coupling method. The resonancelike phenomenon calculated by Bhatia and Drachman [1] and confirmed by Ho [2] does not appear in the present calculation. Instead, we have found narrow Feshbach resonances with widths of the order of 10^{-4}–10^{-5} a.u. just below the threshold of $\mathrm{Ps}(n=1)$ and just below the threshold of $\mathrm{Ps}(n=2)$. We have also found an extremely narrow shape resonance just above the threshold of $e^+ + \mathrm{He}^+(n=5)$. These resonances may be difficult to detect experimentally. Generalization of this work for higher partial waves would be of interest in two ways: On one hand, the contributions from higher partial waves to the cross sections may be far from negligible in the resonance region and, on the other hand, possible resonances in higher partial waves for which the adiabatic potentials look different from the S-wave potentials would be worth studying.

[1] A. K. Bhatia and R. J. Drachman, Phys. Rev. A **42**, 5117 (1990).
[2] Y. K. Ho, Phys. Rev. A **53**, 3165 (1996).
[3] A. Igarashi and N. Toshima, Phys. Rev. A **50**, 232 (1994).
[4] Y. Zhou and C. D. Lin, J. Phys. B **27**, 5065 (1994); **28**, 4907 (1995).
[5] C. D. Lin, Phys. Rep. **257**, 1 (1995).
[6] M. Gailitis and R. Damburg, Proc. Phys. Soc. London **82**, 192 (1963).
[7] Y. K. Ho, Hyperfine Interact. **73**, 109 (1992).