

Resonances in positronium hydride

Joseph Di Rienzi, College of Notre Dame of Maryland, Baltimore, MD 21210

Richard J. Drachman, NASA Goddard Space Flight Center, Greenbelt, MD 20771

We re-examine the problem of calculating the positions and widths of the lowest-lying resonances in the $\text{Ps} + \text{H}$ scattering system which consists of two electrons, one positron and one proton. The first of these resonances, for $L=0$, was found by the methods of complex rotation and stabilization, and later described as a Feshbach resonance lying close to a bound state in the closed-channel $e^+ + \text{H}^-$ system. Recently, results for the $L=1$ and 2 scattering states were published, and it was found, surprisingly, that there is a large shift in the positions of these resonances. In this work we repeat the analysis for $L=1$ and find an unexpected explanation for the shift.

I. INTRODUCTION AND HISTORY

The first evidence for the existence of at least one resonance in the low-energy scattering of positronium (Ps) on hydrogen atoms came from a stabilization calculation [1] followed by complex rotation computations [2]. At the time it was not clear what the mechanism of the resonance might be, but the authors suggested that it was connected with the degenerate $2s$ - $2p$ threshold in the Ps atom that lies nearby. Because of the neutrality of the systems this was not likely.

A better suggestion was that there should be resonances generated by the Rydberg bound states in the closed, re-arranged $e^+ + \text{H}^-$ channel. There should be an infinite number of such states, and they should lie fairly close to the levels of hydrogen, although perturbed by the extended charge distribution of the hydrogen negative ion. We can also expect that the L degeneracy of the hydrogen

levels should be broken by the short-range repulsive potential of the H^- ion so as to raise the low- L states more than the higher ones, since the low-lying states are more penetrating. Furthermore, these resonances should be found only in the electronic singlet state, since the hydrogen ion is in a singlet state. It should be possible to carry out a fairly simple calculation based on this picture in order to obtain values for the resonant energies (presumably shifted somewhat from the Rydberg positions due to coupling with the open channel) and the widths.

This program was carried out [3] using a simple form of scattering trial function, but one that included a reasonable representation of both the open and closed channels. In that calculation it was found that there was only a very small shift of the first two s-wave resonances away from the Rydberg energies, and the width of the first of these was in fairly good agreement with earlier calculations. This encouraging result made it seem that the mechanism of resonant scattering in the $Ps+H$ system was well understood and that no surprises would be found in the higher angular momentum states.

Recent results [4] of a very extensive complex-rotation calculation for $L=1$ and 2 have turned out to be quite different. There is a large shift upward of the lowest-lying p-state resonance from its expected location near the 2p Rydberg energy, and a corresponding, but smaller, upward shift of the lowest-lying d-state resonance. The position of the p-state resonance is actually higher than the first s-wave resonance, reversing our qualitative expectation based on the picture discussed above. The authors of Ref. [4] suggested that this result could be explained by assuming that there is a very large coupling shift in these higher angular momentum states, although its cause remained unknown.

This Paper is the result of an investigation into this puzzling situation, again using the methods of Ref. [3] extended to higher angular momentum. We are not trying to improve on the very

accurate values obtained in [4]. Rather, we are trying to understand those somewhat counterintuitive results. First, we will formulate the scattering method used and will re-calculate the s-wave results, verifying the earlier work. Then the p-wave problem will be examined, and an interesting qualitative conclusion will be reached. The d-state problem will be relegated to a future report.

II. FORMULATION OF THE METHOD

To describe both the open channel $[F(\vec{R})]$ in the conventional way and the closed channel $[G(\vec{x})]$ in terms of bound states of the positron in the field of the hydrogen ion we write the Ps-H scattering function in the following form:

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{x}) = F(\vec{R}_1) \phi(\rho_1) \psi(r_2) + F(\vec{R}_2) \phi(\rho_2) \psi(r_1) + G(\vec{x}) \Phi(r_1, r_2). \quad (1)$$

In this expression \vec{r}_1 and \vec{r}_2 are the position vectors of the two electrons relative to the proton taken as fixed at the origin, and \vec{x} is the position vector of the positron. The relative coordinates describing the position of the center of mass of the Ps atom and its internal coordinate are $\vec{R}_j = (\vec{r}_j + \vec{x})/2$ and $\vec{\rho}_j = \vec{x} - \vec{r}_j$, respectively. The internal wave functions of the H atom and the Ps atom are, of course, known exactly:

$$\psi(r) = \frac{e^{-r}}{\sqrt{\pi}} \text{ and } \phi(\rho) = \frac{e^{-\frac{\rho}{2}}}{\sqrt{8\pi}}. \quad (2)$$

The nonrelativistic Hamiltonian for the interacting system (in atomic units with energies in Rydbergs) is

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_x^2 + \frac{2}{x} + \frac{2}{r_{12}} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{\rho_1} - \frac{2}{\rho_2}. \quad (3)$$

It is convenient to break up the Hamiltonian in different ways corresponding to each of the channels in the trial function. When considering the open channel the following breakup is useful:

$$H = -\frac{1}{2}\nabla_{R_{1,2}}^2 + H_{Ps}^{1,2} + H_H^{2,1} + \bar{V}_A^{1,2}, \text{ where} \quad (4)$$

$$H_{Ps}^j = -2\nabla_{\rho_j}^2 - \frac{2}{\rho_j}, \quad H_H^j = -\nabla_{r_j}^2 - \frac{2}{r_j}, \quad \bar{V}_A^{1,2} = \frac{2}{r_{12}} + \frac{2}{x} - \frac{2}{r_{1,2}} - \frac{2}{\rho_{2,1}}.$$

For the closed channel we break the Hamiltonian as follows:

$$H = H_{H^-} - \nabla_x^2 + \bar{V}_B \quad (5)$$

$$\text{where } H_{H^-} = -\nabla_1^2 - \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}}, \quad \bar{V}_B = \frac{2}{x} - \frac{2}{\rho_1} - \frac{2}{\rho_2}.$$

We could treat both F and G in the trial function as completely free to be determined variationally [5], but in the spirit of the earlier calculation we will represent G as a finite sum of bound-state functions:

$$G(\vec{x}) = \sum_n C_n G_n(\vec{x}), \text{ where } \int \int \int d\vec{r}_1 d\vec{r}_2 dx G_n(\vec{x}) \Phi(r_1, r_2) H \Phi(r_1, r_2) G_n(\vec{x}) = \epsilon_n + E_{H^-}. \quad (6)$$

Since Φ is the wavefunction of the negative hydrogen ion, it is an eigenfunction of H_H (defined in Eq. (5)) with eigenvalue $E_H = -1.0555$, and Eq.(6) becomes

$$\epsilon_n = \int d\vec{x} G_n(\vec{x}) \left[-\nabla_x^2 + U(x) \right] G_n(\vec{x}), \text{ where } U(x) = \int \int d\vec{r}_1 d\vec{r}_2 \Phi(r_1, r_2) \bar{V}_B \Phi(r_1, r_2). \quad (7)$$

We can solve for these energies and wave functions both variationally in the form

$$G_n(\vec{x}) = x^L e^{-\alpha x} P_L(\hat{x}) \sum_{k=0} d_k^{(n)} x^k, \quad (8)$$

and by solving the variational differential equation numerically:

$$-\nabla_x^2 G_n(\vec{x}) + U(x) G_n(\vec{x}) = \epsilon_n G_n(\vec{x}). \quad (9)$$

(Later we will discuss the details of this part of the program, including approximate forms for Φ and hence $U(x)$ and the low-lying eigenvalues ϵ_n .)

Without loss of generality and for simplicity we will next derive the optical-potential scattering equation with only one term in the expansion for G . We begin with the usual functional

$$I = \int \int \int d\vec{R}_1 d\vec{p}_1 d\vec{r}_2 \Psi(H-E)\Psi. \quad (10)$$

Using the wave function from Eq. (1) with $G(\vec{x}) = C_n G_n(\vec{x})$, where n refers to a particular eigenstate supposed to be the main component of the resonance of interest, we can write the compact form

$$\Psi = P + C_n Q, \text{ and } I = A + B C_n + D C_n^2, \quad (11)$$

where $A = \langle P | H - E | P \rangle$, $B = \langle Q | H - E | P \rangle + \langle P | H - E | Q \rangle$, $D = \langle Q | H - E | Q \rangle$.

We first set the variation on the coefficient C_n to zero, obtaining the result $C_n = -B/2D$. But from Eqs.(6) and (11) we see that $D=E_{H^-}+\epsilon_n-E$; this has the form of a resonant denominator. After having accounted for the coefficient C_n we can write I in the following form:

$$I = \langle P|H-E|P \rangle + \frac{\langle P|H-E|Q \rangle \langle Q|H-E|P \rangle}{E-E_{H^-}-\epsilon_n}. \quad (12)$$

Varying in the usual way on the function F we obtain the following scattering equation:

$$-\frac{1}{2}[\nabla^2 + k^2]F(\vec{R}) + \int d\vec{R}' K(\vec{R}, \vec{R}') F(\vec{R}') + 2 \sum_n \frac{V_n(\vec{R}) \int d\vec{R}' V_n(\vec{R}') F(\vec{R}')}{E-E_{H^-}-\epsilon_n} = 0, \quad (13)$$

$$\text{where } E_H = -1 \text{ Ry, } E_{Ps} = -\frac{1}{2} \text{ Ry, } k^2 = 2(E - E_{Ps} - E_H) = (2E+3) \text{ Ry}$$

(Here we have restored the sum over bound states.) The kernel K comes from exchange of the two electrons; it is a very complicated expression and was evaluated long ago by Fraser [6]. The potentials V_n appearing in the separable integral terms are defined as follows:

$$\begin{aligned} V_n(\vec{R}_1) &= \int \int d\vec{p}_1 d\vec{r}_2 \phi(\rho_1) \psi(r_2) [H-E] G_n(\vec{x}) \Phi(r_1, r_2) \\ &= \int \int d\vec{p}_1 d\vec{r}_2 \phi(\rho_1) \psi(r_2) [V_B - U + \epsilon_n + E_{H^-} - E] G_n(\vec{x}) \Phi(r_1, r_2), \end{aligned} \quad (14)$$

where we have used the separation of the Hamiltonian from Eq. (5) and the differential equation of Eq. (9) in the second form of V_n appearing in Eq. (14). Eq. (13) has exactly the form of the well-known Feshbach optical-potential equation [7] with one important exception: We have not made use of projection operators in our derivation, so the open- and closed-channel parts of the wave function

of Eq. (1) are not orthogonal. For that reason, the coupling potentials V_n contain explicit energy dependence, not present in the strict Feshbach formalism, as can be seen from Eq. (14).

In the next Section, we will discuss simplified forms of the kernel K and the hydrogen ion wave function Φ , and we will construct and display the coupling potentials.

III. EXPLICIT FORM OF THE SCATTERING EQUATION

A. The static-exchange approximation

Consistent with our program of continuing the type of calculation introduced in [3] we will not try to use the exact form of the kernel K given by Fraser [6], but instead will replace it by a *separable* kernel of the following simple form (for $L=0$ and 1):

$$K_L(\vec{R}, \vec{R}') = g_L P_L(\hat{R}) P_L(\hat{R}') e^{-\alpha_L(R+R')}. \quad (15)$$

The static-exchange approximation corresponds to the first two terms of Eq. (13), and it has been numerically solved [8] with the exact exchange kernel K for $L=0,1,2$. For each partial wave we can solve the corresponding scattering equation with our separable kernel analytically and will adjust the constants α and g to give good agreement with the results of Ref. [8]. The idea is that the adjusted kernel can then be used unchanged in the full optical equation. For $L=0$ and 1 we make the usual substitution $F_L(\vec{R}) = \frac{u_L(R)}{R} P_L(\hat{R})$ and find the following integro-differential equation to be solved:

$$-u_L''(R) - k^2 u_L(R) + \frac{L(L+1)}{R^2} u_L(R) + \lambda_L R e^{-\alpha_L R} \int_0^\infty dR' R' e^{-\alpha_L R'} u_L(R'), \quad \text{where } \lambda_L \equiv \frac{8\pi g_L}{2L+1}. \quad (16)$$

Solutions for $L=0$ and 1 can be easily obtained, and they have the following forms. For $L=0$:

$$u_0(R) = \sin(kR) + \tan(\eta_0) \left[\cos(kR) - e^{-\alpha_0 R} \left(1 + \frac{(\alpha^2 + k^2)R}{2\alpha} \right) \right],$$

$$\text{and } k \cot(\eta_0) = -\frac{(\alpha_0^2 + k^2)^4}{4\lambda_0 \alpha_0^2} + \frac{k^6 + 5k^4 \alpha_0^2 + 15k^2 \alpha_0^4 - 5\alpha_0^6}{16\alpha_0^5}. \quad (17)$$

For $L=1$:

$$u_1(R) = \bar{j}_1(kR) - \tan(\eta_1) \left[\bar{n}_1(kR) + e^{-\alpha_1 R} \left(\frac{1}{kR} + \frac{\alpha}{k} + \frac{\alpha^2 + k^2}{2k} R \right) \right],$$

$$\text{where } \bar{j}_1(z) = \frac{\sin(z)}{z} - \cos(z) \text{ and } \bar{n}_1(z) = -\frac{\cos(z)}{z} - \sin(z), \quad (18)$$

$$\text{and } k^3 \cot(\eta_1) = -\frac{(\alpha_1^2 + k^2)^4}{4\lambda_1} + \frac{(k^2 - \alpha_1^2)(\alpha_1^4 + 10\alpha_1^2 k^2 + k^4)}{16\alpha_1^3}.$$

When we fit these analytic expressions to the numerical values given in [8] we obtain the following values of the constants λ_L and α_L : $\lambda_0 = -2.18372$, $\alpha_0 = 1.10432$, $\lambda_1 = -2.31168$, and $\alpha_1 = 1.08183$. It is interesting that these constants are almost the same for both values of L .

B. Constructing the e^+H^- bound states

Next we must choose a reasonable form for the function Φ appearing in the definition of the potentials V_n [Eq. (14)] that represents the hydrogen negative ion. It would, of course, be best to use some sophisticated expression, perhaps in the Hylleraas form with many linear parameters. Following the simple ideas of Ref.[3], however, we continue to use the single-term, closed-shell wave function $\Phi(r_1, r_2) = \frac{Z^3}{\pi} e^{-Z(r_1 + r_2)}$, which leads to simplified mathematics. This function is not a very accurate one for the H^- system, since it actually does not even give rise to a bound ion, but

it does mimic the distribution of charge density fairly well. In any case, it is the first function that one should try; later other simple forms may be worth exploring. (We have already made use of the correct binding energy of the ion, $E_H = -1.0555$, regardless of the actual variational energy corresponding to this form of Φ .)

The potential U in which the positron moves then has the following form [Eq. (7)]:

$$U(x) = \frac{Z^6}{\pi^2} \int \int d\vec{r}_1 d\vec{r}_2 e^{-2Z(r_1+r_2)} \left(\frac{2}{x} - \frac{2}{\rho_1} - \frac{2}{\rho_2} \right) = -\frac{2}{x} + 4e^{-2Zx} \left(\frac{1}{x} + Z \right). \quad (19)$$

(We let $Z=11/16$, the best variational value.) Notice that this potential has the correct asymptotic form, becoming $-2/x$ for large x values (giving the infinite set of hydrogenic states discussed above) and becoming $+2/x$ for small x values (the repulsive short-range potential that should raise the low- L states more than the higher- L ones.) In Ref. [3] a table of the first few energies obtained by solving Eq. (9) are given for $L=0,1$, and 2 . Four of those energies are of interest here: $\epsilon_{1s} = -0.3653$, $\epsilon_{2s} = -0.1449$, $\epsilon_{2p} = -0.2121$, and $\epsilon_{3p} = -0.0990$. These correspond to Ps scattering energies ($k^2/2 = 0.4445 + \epsilon_D$) of 0.0792 , 0.2996 , 0.2324 , and 0.3455 , respectively.

It has always been understood that the $1s$ bound state should not be associated with a resonance but is just a contribution to the non-resonant scattering and also lowers the energy of the PsH bound state. The $2s$ scattering energy should be compared with the value 0.2944 obtained by Yan and Ho [9]; the agreement is quite close. But the $2p$ scattering energy given above is not at all close to the first scattering resonance energy 0.3149 given in Ref. [4]. Actually, our $3p$ value is closer.

C. The resonant separable potentials.

We are interested in solving Eq. (13) for p-wave scattering with the separable form of the kernel K given in Eq. (15) and with the potentials V_{2p} and V_{3p} calculated using the simple product form for the hydrogen ion wave function. By using this function in Eq. (14) we can carry out the integration over $d\vec{r}_2$ analytically:

$$\int d\vec{r}_2 \frac{e^{-(Z+1)r_2}}{\sqrt{\pi}} \left[f(x, \rho_1) - \frac{2}{\rho_2} \right] = \frac{8\sqrt{\pi}}{(1+Z)^3} \left[f(x, \rho_1) - \frac{2}{x} + e^{-(1+Z)x} \left(\frac{2}{x} + 1 + Z \right) \right], \quad (20)$$

where $f(x, \rho_1) = \frac{2}{x} - \frac{2}{\rho_1} - U(x) + \epsilon_{Np} + 1.5 - \frac{k^2}{2}$.

The remaining integral over $d\vec{\rho}_1$ can be done by numerical integration over the magnitude of ρ_1 and $\mu = \hat{R}_1 \cdot \hat{\rho}_1$, after we re-write the positron bound-state function as follows:

$$G_{Np}(\vec{x}) = g(x) \hat{x} \cdot \hat{z} = \frac{g(x)}{x} \left(\vec{R}_1 \cdot \hat{z} + \frac{1}{2} \vec{\rho}_1 \cdot \hat{z} \right). \quad (21)$$

Here \hat{z} refers to the fixed external coordinate system. Since both x and r_1 depend on μ , it is convenient to make the change of variables

$$\vec{\rho}_1 \cdot \hat{z} = \rho_1 \frac{4\pi}{3} \sum_{m=-1}^1 Y_1^m(\hat{R}_1 \cdot \hat{z}) Y_1^{m*}(\hat{R}_1 \cdot \hat{\rho}_1) - \rho_1 \mu \hat{R}_1 \cdot \hat{z}. \quad (22)$$

(The expression beyond the arrow can be used in our integral because the terms in the summation with $m \neq 0$ will vanish since the rest of the integrand involves only $m=0$.) Finally, we have two terms in the potential, one of which depends on the scattering energy:

$$V_{Np}(\vec{R}) = \Delta_{Np}(k) V_{Np}^{(1)}(\vec{R}) + V_{Np}^{(2)}(\vec{R}), \text{ where } \Delta_{Np}(k) = 0.4445 + \epsilon_{Np} - \frac{k^2}{2},$$

$$V_{Np}^{(1,2)} = \sqrt{\frac{24}{\pi}} \left(\frac{Z}{Z+1} \right)^3 \hat{R} \cdot \hat{z} \int_0^\infty d\rho \int_{-1}^1 d\mu e^{-\frac{\rho}{2} \left(R + \frac{\rho\mu}{2} \right)} e^{-Zr \frac{g(x)}{x}} \left\{ \frac{1}{q(x)\rho^2 - 2\rho} \right\}, \quad (24)$$

$$\text{and } q(x) = e^{-(Z+1)x} \left(\frac{2}{x} + Z + 1 \right) + \frac{2}{x} - 4e^{-2Zx} \left(\frac{1}{x} + Z \right).$$

In carrying out the two numerical integrals, one must substitute the explicit forms of x and r in terms of R , ρ , and μ :

$$\left\{ \begin{array}{c} x \\ r \end{array} \right\} = \sqrt{R^2 + \frac{\rho^2}{4} \pm R\rho\mu}. \quad (25)$$

Then, for a set of values of R (up to the reasonable upper limit of 15) we carry out the indicated double integration, after which we interpolate to obtain smooth forms of the potentials for use in solving the separable integro-differential equation (13).

IV. SOLUTION OF THE SCATTERING EQUATION

The complete equation we must solve is an extension of Eq. (16), including both the term involving the exchange kernel K and as many "resonant" terms as desired:

$$-\frac{d^2 u(R)}{dR^2} - k^2 u(R) + \frac{2u(R)}{R^2} + \lambda_1 R e^{-\alpha_1 R} I_{1p} + \frac{16\pi R}{3} \sum_{N=2} \frac{V_{Np}(R) I_{Np}}{\Delta_{Np}}, \quad (26)$$

In this equation the integrals I_{Np} are defined in terms of the function $u(R)$ as follows:

$$I_{1p} = \int_0^{\infty} dR R e^{-\alpha_1 R} u(R), \text{ and } I_{Np} = \int_0^{\infty} dR R V_{Np}(R) u(R), \text{ for } N > 1, \quad (27)$$

and $\Delta_{Np} = \frac{k^2}{2} - \epsilon_{Np} - 0.4445$. The non-iterative method of solution of such equations works by first making the following decomposition of the solution:

$$u(R) = u_{0p}(R) + I_{1p} u_{1p}(R) + \frac{16\pi}{3} \sum_N \frac{I_{Np} u_{Np}(R)}{\Delta_{Np}}. \quad (28)$$

Then the complete solution $u(R)$ is obtained from the partial functions $u_{Np}(R)$ that satisfy the following equations:

$$\begin{aligned} \Omega u_{0p}(R) &= 0 \\ \Omega u_{1p}(R) + \lambda_1 R e^{-\alpha_1 R} &= 0 \\ \Omega u_{Np}(R) + R V_{Np}(R) &= 0, [N=2,3,\dots], \end{aligned} \quad (29)$$

where $\Omega = -\frac{d^2}{dR^2} - k^2 + \frac{2}{R^2}$.

Two of these equations have simple analytic solutions:

$$u_{0p}(R) = \bar{j}_1(kR) \text{ and } u_{1p}(R) = \frac{2k\lambda_1}{(\alpha_1^2 + k^2)^2} \left[\bar{n}_1(kR) + e^{-\alpha_1 R} \left(\frac{1}{kR} + \frac{\alpha_1}{k} + \frac{\alpha_1^2 + k^2}{2k} R \right) \right]. \quad (30)$$

(These are obviously related to the solution of the static-exchange approximation.) The other inhomogeneous differential equations must be solved numerically. When $u(R)$ is inserted in the definitions of the integrals I_{np} a set of inhomogeneous linear algebraic equation for the quantities I_{np} is obtained and is easily solved. This finally gives the scattering function explicitly, from whose asymptotic form the phase shift is read off.

V. RESULTS AND DISCUSSION

We began our investigation of the p-wave scattering by including only the lowest "resonant" term obtained from the 2p state. The results are shown in Fig.1, where it is clear that there is no sign of any resonant behavior at all. We searched quite thoroughly near the expected position of the resonance ($k=0.6818$) and also near the position found for the lowest resonance in Ref. [4] ($k=0.7936$) without finding anything but smooth behavior of the phase shift. On this figure we have also plotted the static-exchange results, and it is clear that adding the 2p term has raised the non-resonant phase shifts quite considerably. As a last resort we reduced the coupling potential by various factors as small as 0.1 and were able to produce a narrow, almost unshifted resonance of the expected kind. Our tentative conclusion at this stage was that the coupling between the closed and open channels had broadened the expected resonance so radically that it could no longer be identified; for all practical purposes the resonance had disappeared.

We then replaced the 2p term by the 3p term and recalculated the phase shifts. These are shown in Fig. 2, where clear resonant behavior is seen. A least-squares fit was made to the standard resonant formula

$$\eta(E) = A + BE + \arctan \left[\frac{\Gamma}{2(E_R - E)} \right], \quad (31)$$

and this gave an excellent fit to the computed phase shifts. The resonance we obtain ($E_R=0.3648$ Ry and $\Gamma=0.0339$ Ry), however, is wider and higher in energy than that calculated in Ref. [4]: $E_R=0.3149$ Ry and $\Gamma=0.0032$ Ry. (In this case the coupling with the open channel has raised the resonance position by 0.0193 Ry, and its width is about 10 times as wide as in Ref. [4].) Finally, we included both 2p and 3p terms and obtained the results also shown in Fig. 2; the 3p resonance remains but is now shifted downward in energy and narrowed. The best fit was obtained with the following values of the resonance parameters: $E_R=0.3287$ Ry, and $\Gamma=0.0060$ Ry, which compare more favorably with the values reported in Ref. [4] than those determined from the 3p state alone. (The non-resonant parts of the 2p-3p curve are essentially unchanged from the curve with 2p alone.)

Our final conclusion from this is the following: The lowest-lying p-wave Ps+H scattering resonance is not generated by the lowest-lying bound hydrogenic p-state in the e^+H re-arranged channel, as had been assumed in Ref. [3]. In fact, it is the first excited p-state [3p] that produces the lowest resonance, while the 2p term is effective only in increasing the non-resonant scattering phase shift. So the apparent large shift between the closed-channel bound-state energy and the position of the lowest true resonance is spurious; the character of the resonance was just not correctly identified. (There is no reason to believe, however, that there should not be an infinite number of higher resonances corresponding to the infinite set of higher Rydberg states.)

We have referred to this result as unexpected, as indeed it is. But perhaps (in hindsight) the result should not have been quite so surprising. After all, exactly the same phenomenon occurs in the s-wave case: the 1s Rydberg state does not produce a resonance either, and the 2s term generates the lowest-lying s-wave resonance. In that case, the existence of the true bound PsH state may have confused the issue, leading us not to expect a 1s resonance (In the Appendix we briefly re-examine the s-wave calculation.) We see now, however, that this phenomenon may be more widespread. In particular, we will soon be extending the present work to the $L=3$ case, where there is a corresponding, but smaller, discrepancy [4]; perhaps the same explanation will be applicable there as well.

ACKNOWLEDGMENTS

Part of this work was done while one of us (J. D.) held a 2001 NASA-ASEE Summer Faculty Fellowship at Goddard Space Flight Center. Most of the numerical work reported here was carried out using *Mathematica*, developed by Wolfram Research Inc.

APPENDIX

Before beginning the p-wave calculations described in this Paper, we wished to review the s-wave problem that had been treated in [3]. The intent was to try to verify the results found there-- that the coupling between the closed-channel 2s wavefunction and the open-channel scattering function shifted and broadened the resonance by a small amount. This would justify the reliance on the energies of these bound states as good approximations to the resonance energies, at least for s-waves, and perhaps also for higher angular momenta. It was not that we doubted the old results, but

we planned to use the coordinate-space integro-differential equation method described here, rather than the momentum-space integral-equation technique employed previously, and it seemed worthwhile to check the two methods against one another.

The new results are essentially in agreement with those of Ref. [3]. In addition, by a minor modification of the scattering calculation we obtained the binding energy of the PsH state. With the inclusion of the 1s and 2s terms the binding energy is increased from 0.01686 Ry in the static-exchange approximation to 0.03007 Ry. (This should be compared with the accurate PsH binding energy of 0.078393 Ry [9].) Again we find no resonance near the position of the 1s closed-channel bound state. A least-squares fit of the present s-wave phase shift gives the following values of the resonant parameters: $E_R=0.2955$ Ry and $\Gamma=0.0019$, compared with the values in [3] of $E_R=0.2954$ Ry and $\Gamma=0.0022$ Ry and the precision results in [9] of $E_R=0.2944$ Ry and $\Gamma=0.0070$ Ry. The agreement between the various values of the resonant energy is quite satisfactory, while the resonant width is not as good. The main point, however, that the lowest bound state does not produce a resonance, is still supported by our new calculation. (As in the 2p case, we tried reducing the amplitude of the 1s potential and recovered an almost unshifted resonance.)

REFERENCES

- [1].S. K. Houston and R. J. Drachman, *Electronic and Atomic Collisions*, edited by B. C. Čobić and M. V. Kurepa (Institute of Physics, Belgrade, 1973) p. 495.
- [2].R. J. Drachman and S. K. Houston, Phys. Rev. **12**, 885 (1975); Y. K. Ho, Phys. Rev. A **17**, 1675 (1978).
- [3].R. J. Drachman, Phys. Rev. A **19**, 1900 (1979).
- [4].Z.-C. Yan and Y. K. Ho, Phys. Rev. A **57**, R2270 (1998); Y. K. Ho and Z.-C. Yan, J. Phys. B **31**, L877 (1998).
- [5].H. R. J. Walters, J. E. Blackwood, and M. T. McAlinden, (unpublished, 2001).
- [6].P. A. Fraser, Proc. Phys. Soc. London **78**, 329 (1961).
- [7].H. Feshbach, Ann. Phys. (N. Y.) **19**, 287 (1962).
- [8].S. Hara and P. A. Fraser, J. Phys. B **8**, L472 (1975); H. Ray and A. S. Ghosh, J. Phys. B **29**, 5505 (1996); **30**, 3745 (1997).
- [9].Z.-C. Yan and Y. K. Ho, Phys. Rev. A **59**, 2697 (1999).

FIGURE CAPTIONS

Figure 1. P-wave phase shifts as functions of the Ps scattering energy. The solid line gives the static-exchange results [7] fitted according to Eq. (18). The points (+) are the results when only the 2p closed-channel function is included; there is no resonant behavior seen.

Figure 2. Resonant behavior of the P-wave phase shifts as functions of the Ps scattering energy. The solid points (■) are the results when only the 3p closed-channel function is included. The other points (+) give the results when both 2p and 3p functions are included; the resonance is lowered and narrowed. The curves are least-squares fits to the analytic form given in Eq. (31).





