D-wave resonances in positronium hydride

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Abstract

In a previous paper [Phys. Rev. A **65**, 032721 (2002)] we re-examined a model describing the structure of the low-energy Ps-H resonances as being due to quasi-bound states of the positron in the perturbed Coulomb potential of the H^- ion appearing in the closed, rearranged channel. In particular, we wished to understand why the lowest p-state resonance was so far away from the lowest quasi-bound $(2p)$ state. We found that the lowest resonance actually corresponds to the first excited $[3p]$ state, while the lowest state is not recognizable as a resonance. In the present work we repeat our analysis, but this time for the lowest d state. We find that the lowest $[3d]$ state does correspond to a resonance shifted moderately.

There has been much recent theoretical interest in the positronium-hydrogen [Ps-H] scattering system [1], and special interest has focused on the properties of elastic scattering resonances that have been predicted by a variety of theoretical techniques [2, 3]. In particular, the model of resonances due to hydrogenic bound states in the re-arranged [e$^+$-H$^-$] channel predicts the existence of an infinite sequence of resonances in all angular-momentum states [4]. We may expect these resonances to lie fairly close to the levels of hydrogen although perturbed by the non-Coulomb parts of the negative hydrogen ion's potential. In addition, the L-degeneracy of the hydrogen levels should be broken by this short-range repulsive potential so as to raise the low-L states more than the higher ones, since they are more penetrating. A simple S-wave calculation based on this idea was carried out long ago [4], including the coupling between the hydrogenic bound states and the scattering continuum. The lowest S-state was not expected to correspond to a resonance, since there is a single S-wave bound state in Ps-H, but the $2s$ state did generate a resonance that agreed well with other calculations [2]. Based on this success, it was assumed that the correspondence between hydrogenic bound states and resonances would carry over trivially to higher values of the angular momentum.

Therefore it was a surprise when the lowest P and D resonances were found [3] to be radically shifted from their expected positions, based on the hydrogenic model. That was our motivation for re-examining that model, including P-states in our analysis. We were again surprised to find [5] that the $2p$ state was broadened out of all recognition, and that it was actually the $3p$ state that produced the lowest P resonance, at a position in good agreement with the results of Ref.[3]. Since we now know that the lowest state in both S- and P-waves is ineffective at producing scattering resonances, we wish to find out whether this situation is true for higher-L waves too. In this Brief Report we outline the corresponding calculation for L=2. In this case, we find that the lowest state does in fact correspond to the lowest resonance, in contrast to the lower-L cases.

The method described in Ref.[4, 5] is essentially a two-state approximation:

$$\Psi(\vec{x}, \vec{r}_1, \vec{r}_2) = F(\vec{R}_1)\phi(\rho_1)\psi(r_2) + \{1 \leftrightarrow 2\} + G(\vec{x})\Phi(r_1, r_2) \tag{1}$$

where

$$G(\vec{x}) = \frac{g(x)}{x} P_2(\hat{x} \cdot \hat{z}) \tag{2}$$

and the ground states of Ps and H atoms have the following forms:

$$\phi(\rho) = \frac{e^{-\rho/2}}{\sqrt{8\pi}}, \ \psi(r) = \frac{e^{-r}}{\sqrt{\pi}}. \tag{3}$$

The function $F(\vec{R})$ represents the Ps-H scattering, both atoms being unexcited, while $G(\vec{x})$ is the wave function of the positron bound in a d-state to the negative hydrogen ion. The system is in the singlet electronic spin state (corresponding to the symmetry of the ionic bound state $\Phi(r_1, r_2)$) and is explicitly antisymmetrized.

In Ref.[5] the details of the variational derivation of an integro-differential equation for $F(\vec{R})$ are described. This has the following form:

$$-\frac{1}{2}[\nabla^2 + k^2]F(\vec{R}) + \int d\vec{R}' K(\vec{R}, \vec{R}')F(\vec{R}') + 2\sum_N \frac{V_{Nd}(\vec{R}) \int d\vec{R}' V_{Nd}(\vec{R}')F(\vec{R}')}{E - E_{H-} - \epsilon_{Nd}} = 0. \tag{4}$$

Two major simplifications are then made: First, the integral kernel coming from the exchange of the two electrons is replaced by an effective separable form

$$K(\vec{R}, \vec{R}') = be^{-\alpha(R+R')}RR'P_2(\hat{R} \cdot \hat{z})P_2(\hat{R}' \cdot \hat{z}) \tag{5}$$

and second, the hydrogen ion wave function is replaced by its simplest approximation

$$\Phi(\hat{r}_1, \hat{r}_2) = \frac{Z^3}{\pi}e^{-Z(r_1+r_2)}, \ Z = \frac{11}{16}. \tag{6}$$

The first step is to omit the closed-channel function $G(\vec{x})$ which removes the optical potential terms from Eq.(4) and solve the resulting static-exchange equation:

$$-u''(R) - k^2 u(R) + \frac{6u(R)}{r^2} + \lambda e^{-\alpha R}R^2 \int_0^\infty dR' R'^2 e^{-\alpha R'} u(R') = 0, \tag{7}$$

where $\lambda = 8\pi b/5$ and $F(\vec{R}) = u(R)P_2(\hat{R} \cdot \hat{z})/R$. This equation has the following solution:

$$u(R) = \bar{j}(kR) - \tan\eta\left[\bar{n}(kR) + e^{-\alpha R}\sum_{n=0}^4 C_n R^{n-2}\right], \tag{8}$$

where

$$C_0 = \frac{3}{k^2}, \ C_1 = \frac{3\alpha}{k^2}, \ C_2 = \frac{3\alpha^2 + k^2}{2k^2}, \ C_3 = \frac{\alpha(\alpha^2 + k^2)}{2k^2}, \ C_4 = \frac{(\alpha^2 + k^2)^2}{8k^2}, \tag{9}$$

and

$$\bar{j}(z) = \frac{3\sin z}{z^2} - \frac{3\cos z}{z} - \sin z$$

$$\bar{n}(z) = -\frac{3\cos z}{z^2} - \frac{3\sin z}{z} + \cos z.$$

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The effective range formula takes the form

$$k^5 \cot \eta = -\frac{(\alpha^2 + k^2)^6}{64\lambda} + \frac{(k^2 - \alpha^2)}{256\alpha^5} \left[3\alpha^8 + 28\alpha^6 k^2 + 178\alpha^4 k^4 + 28\alpha^2 k^6 + 3k^8 \right]. \tag{10}$$

By fitting this expression to the $L = 2$ phase shifts calculated in the static-exchange approximation Ref.[6] we find a best fit for $\alpha = 1.30244$ and $\lambda = -1.02029$, and we will assume that the separable form of the exchange kernel shown in Eq.(5) is appropriate even when we add the correlated terms coming from the closed-channel hydrogen-ion parts of the wave function of Eq.(1).

The virtual bound state wave function $G(\vec{x})$ can consist of one or more D-state eigenfunctions of the differential equation

$$-g_{Nd}''(x) + \frac{6}{x^2} g_{Nd}(x) + U(x) g_{Nd}(x) = \epsilon_{Nd} g_{Nd}(x), \tag{11}$$

where $U(x)$ is the potential due to the simple form of Φ shown in Eq.(6):

$$U(x) = -\frac{2}{x} + 4e^{-2Zx} \left(\frac{1}{x} + Z \right). \tag{12}$$

The two lowest eigenvalues are $\epsilon_{3d} = -0.1097 Ry$ and $\epsilon_{4d} = -0.0618 Ry$, which lie very close to the unperturbed hydrogenic values of $-1/9$ and $-1/16$. We are interested in finding how close to these positions the corresponding scattering resonances lie. (Note that the second of these lies above the inelastic threshold of the Ps atom at $\epsilon = -3/8 - E_{H^-} + E_H + E_{Ps} = -0.0695$.)

We follow the same procedure in calculating the separable potentials $V_{Nd}(\vec{R})$ as for the earlier S- and P-wave calculations of Ref.[5]:

$$V_{Nd}(\vec{R}_1) = \int \int d\vec{\rho}_1 d\vec{r}_2 \phi(\rho_1) \psi(r_2) \frac{g_{Nd}(x)}{x} P_2(\hat{x} \cdot \hat{z}) \Phi(r_1, r_2) \left[\Delta_{Nd} + \frac{2}{x} - U(x) - \frac{2}{\rho_1} - \frac{2}{\rho_2} \right]. \tag{13}$$

Here $\Delta_{Nd} = E_{H^-} + \epsilon_{Nd} - E_H - E_{Ps} - k^2/2$, so that for the lowest resonance $\Delta_{3d} = 0.3348 - k^2/2$. Once the potentials have been evaluated the numerical solution of the scattering equation by the noniterative method is quite straightforward.

The potential $V_{Nd}(\vec{R}_1)$ is the result of an integration over the two remaining independent Jacobi coordinates describing the system, $\vec{\rho}_1$ and $\vec{r}_2$. But there are additional coordinates involved in the integration, especially the argument of the Legendre polynomial giving the angular dependence of the bound state function $G(\vec{x})$. We expect the angular dependence

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of the optical potential to involve only D-states of the variable $\mu_R = \hat{R}_1 \cdot \hat{z}$, so the variables in the integrand must be appropriately transformed. (The integration over $d\vec{r}_2$ is trivial.)

Since $\vec{x} = \vec{R}_1 + \vec{\rho}_1/2$ we can write

$$\hat{x} \cdot \hat{z} = \frac{1}{x}\left(R_1\mu_R + \frac{1}{2}\rho_1\mu_\rho\right) \tag{14}$$

where we define $\mu_\rho = \hat{\rho}_1 \cdot \hat{z}$ and $\mu = \hat{\rho}_1 \cdot \hat{R}_1$. The first term in Eq.(14) has the desired form, and we can write the second in terms of

$$\mu_\rho = \frac{4\pi}{3}\sum_{m=-1}^{1}Y_1^m(\mu_R,\phi_R)Y_1^{-m}(\mu,\phi) = \mu_R\mu - \sqrt{(1-\mu_R^2)(1-\mu^2)}\cos(\phi_R - \phi) \tag{15}$$

In our previous work on P-states, at this point we could neglect the ϕ-dependent terms which would vanish after integration over $d\phi$. But in the present case we must construct $P_2(\hat{x} \cdot \hat{z})$ which is quadratic in its argument, and the quadratic ϕ-dependent terms do not vanish after integration. After some algebra we obtain the transformed expression

$$P_2(\hat{x} \cdot \hat{z}) = \frac{P_2(\mu_R)}{x^2}\left[R_1^2 + R_1\rho_1\mu + \frac{\rho_1^2}{4}P_2(\mu)\right]. \tag{16}$$

Finally, we can now write the potential explicitly in terms of a double integral:

$$V_{Nd}(\vec{R}) = 4\sqrt{2}\left(\frac{Z}{Z+1}\right)^3 P_2(\mu_R)\int_0^\infty d\rho\rho^2 e^{-\frac{\rho}{2}}\int_{-1}^{1}d\mu e^{-Zr}\frac{g(x)}{x^3}Q\left(\Delta_{Nd} + P\right). \tag{17}$$

Here we have used the definitions

$$Q = R^2 + R\rho\nu + \frac{1}{4}\rho^2 P_2(\mu)$$

which comes obviously from Eq.(16), and

$$P = e^{-(1+Z)x}\left(\frac{2}{x} + 1 + Z\right) - U(x) - \frac{2}{\rho}.$$

Everything has now been re-written in terms of the three variables R, ρ, and μ, keeping in mind that $[x, r] = \sqrt{R^2 + \rho^2/4 \pm R\rho\mu}$. In practice we separate $V_{Nd}(\vec{R})$ into two parts, one independent of energy and one proportional to Δ_{Nd}, carry out the double integrals numerically for a range of values of R, and then fit the results smoothly by interpolation. The resulting potentials are then used in the scattering equation (4), after expansion in partial waves, to compute the D-wave phase shift as a function of energy.

The results are not as surprising as were those presented in Ref.[5]. In Fig.1 we show the phase shift when only the $3d$ closed-channel state is included in $G(\vec{x})$. In this case a single,
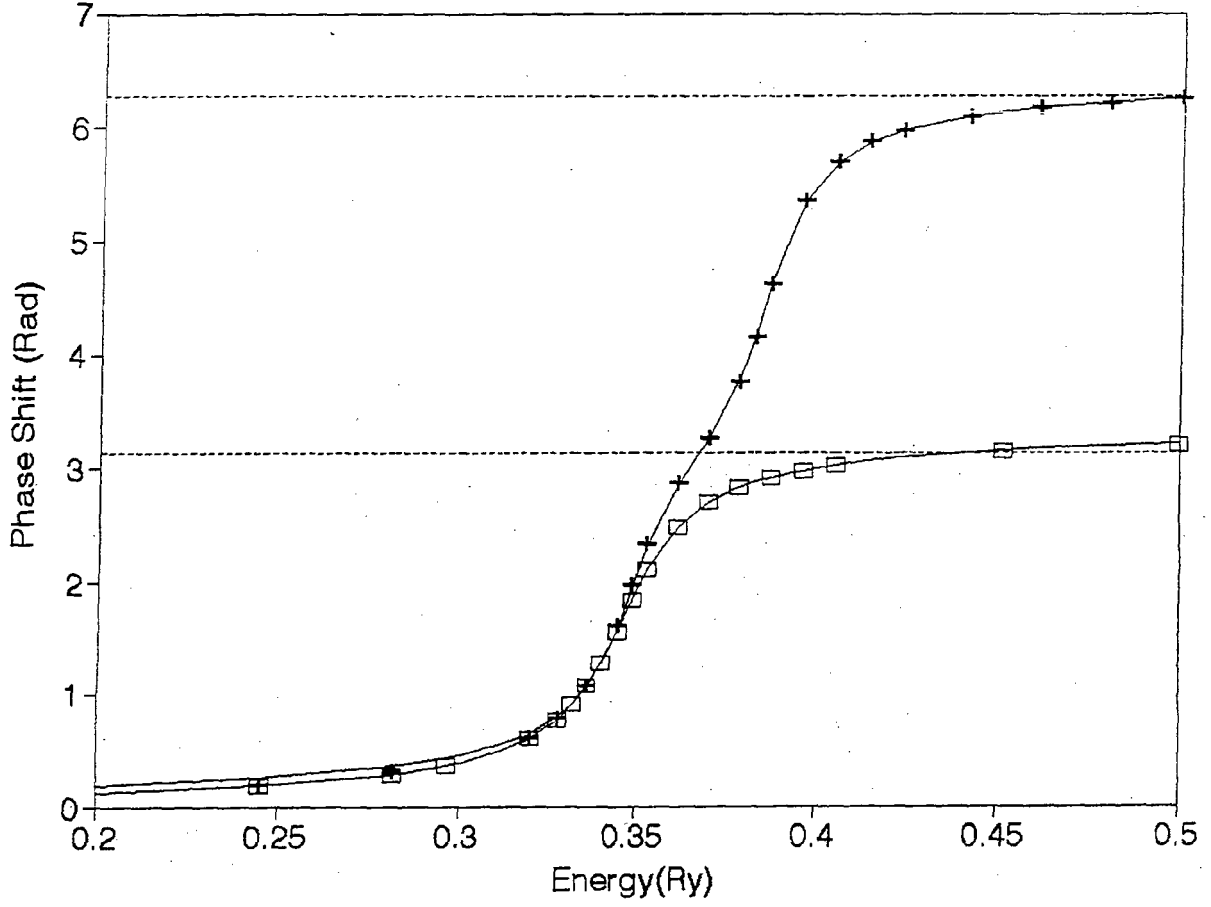
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FIG. 1: Ps-H D-wave phase shifts. The squares are the result when only the 3d state is included, and the crosses are the result when the 4d state is added. The curves are best-fit analytical functions of the standard form [Eq.(18)]. The two horizontal lines are at π and 2π, respectively, to guide the eye.

fairly narrow resonant feature is seen, and when it is fitted with the standard resonance formula

$$\eta(E) = A + BE + \arctan\left[\frac{\Gamma}{2(E_R - E)}\right] \qquad (18)$$

we find the results shown in Table I. (The energies there are the Ps-H scattering energies $k^2/2$, not energies measured relative to H$^-$). You can see that the resonance energy obtained this way is very close to the result in [4], although the width is too large.

Also in Fig.1 we plot the phase shift when we add the 4d state. Here we find two resonances, which lie quite close together. The results of a two-term fit are also shown in Table I, although the higher one is perhaps not too significant since it lies above the Ps

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TABLE I: D-wave resonances in various approximations. The energies ϵ_{Nd} do not include coupling to the continuum. The lowest resonance is labeled 1 and the second is 2.

Method	Ps scattering energy (eV)	Width (eV)
ϵ_{3d}	4.555	
ϵ_{4d}	5.207	
E_1(1 term)	4.708	0.394
E_1(2 term)	4.729	0.327
E_1[4]	4.710±0.0027	0.0925±0.0054
E_2(2 term)	5.253	0.266

inelastic threshold of 0.375 Ry and has not been previously calculated. With the inclusion of this second state the position of the first resonance rises slightly and is in somewhat poorer agreement with Ref.[4], while its narrower width is a slight improvement.

We conclude from these calculations that the D-wave resonances behave almost exactly as we would have expected before the problem with the P-wave scattering arose. That is, coupling with the continuum shifts the position of the lowest resonance, but only by a modest amount. There is no sign of the phenomenon that startled us in the P-wave work, where the lowest potential resonance disappeared due to that coupling. We now feel confident that calculations of higher-L resonances (which we do not intend to carry out) will continue to act normally, although their positions above the inelastic threshold would necessitate multi-channel formulations.

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