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Using a wave function including the 1s-2s-2p eigenstates of hydrogen and the $\overline{1s}$ ground state of positronium, we have calculated the position and width of the lowest Feshbach resonance in the e^+-H system, which lies between the positronium rearrangement threshold and the n = 2 hydrogen threshold. The method differs from the usual close-coupling method, resembling in its formulation the projection operator technique, although orthogonality of closed-channel and open-channel functions is not demanded. The resonance lies 9.8281 eV above the ground state of hydrogen and has a width of 0.029 eV in this approximation.

I. Introduction

In the past few years the theory of non-resonant positron-hydrogen scattering has been throughly investigated.[1] For S-waves, the situation below the positronium formation threshold is very clear,[2] while recent work[3,4,5] seems to be leading rapidly to a solution of the two-channel problem above threshold.

A number of investigations into possible structure in the S-wave problem have also been carried out with negative results. Attempts to find a three-body bound state by variational methods[6,7] were not successful and it was finally proven[8] that no such state exists. An indication of a scattering resonance[9] below the positronium formation threshold is probably an artifact.[7,10]

The usual method of searching for such compound-atom resonances is with the aid of Feshbach projection operators.[11] The idea is to remove the open-channel parts of the scattering problem, leaving a residual Hamiltonian possessing a discrete spectrum. Resonances of the scattering problem can be shown[12] to lie in the vicinity of the eigenvalues of the residual Hamiltonian, and in practice such resonances are really extremely close.[13] For this reason, it has usually been assumed that resonances exist whenever eigenvalues of the residual Hamiltonian appear; the shifts Δ due to coupling between closed and open channels have never yet been large enough to alter the qualitative situation. Several attempts to find eigenvalues below the positronium formation threshold gave negative results[2,7,14] and it is now believed that no resonances exist in this region.

It is natural to consider next the possible existence of resonances just below the n = 2 threshold in hydrogen. One might be optimistic about finding such resonances in the positron-hydrogen case since it is well known that the 2s-2p degeneracy produces an infinite sequence of resonances in the electron-hydrogen case.[15] Not only do the eigenvalues of the residual Hamiltonian form a clear-cut infinite sequence lying wholly below the threshold,[15] but scattering calculations[16] imply very small values of Δ, at least for the low-lying resonances.

Mittleman[17] has examined the analogous problem for positrons. Here the situation differs because a second (positronium) channel is open and it is more difficult to handle the non-orthogonal functions representing the two open channels. Nevertheless, he showed that the potential is the same asymptotically as in the electron case, falling off as the inverse square of the positron coordinate. Hence, the same conclusion follows: there must be an infinite set of eigenvalues here also. No information on the actual energies was obtained, however, since that depends on the short-range behavior of the potential as well.

Also important, however, is the fact that Mittleman's paper[17] gives no information about Δ, the energy shift, which in this case involves coupling with both open channels and might be large enough to move the resonances far away from the positions of the eigenvalues. Although this phenomenon has never been observed before, it must not be overlooked as a possibility. This is especially true since a fairly close search[5] has failed to find any resonances in a two-channel lower bound calculation, while a close-coupling calculation[18] omitting the positronium channel gave the first three S-wave resonances explicitly.

It is the purpose of this Article to clarify the situation with regard to the two-channel resonances. In Section II we formulate an approximate two-channel scattering equation, from which the lowest resonance position and width can be obtained by a modification of the Feshbach operator formalism. In section III we discuss an explicit form for the correlation function describing the resonant state. Section IV gives our conclusions and a discussion, while some mathematical details are in an Appendix.

II. Formulation of the Approximation

Let us assume for the moment that some normalized function Φ exists and describes well the long-lived three-particle state responsible for the resonance. (Later on a particular form for Φ will be selected). A two-channel scattering function can be constructed in the following form:

$$\Psi = \chi(\underset{\sim}{x})\phi_{1s}(\underset{\sim}{r}) + F(\underset{\sim}{R})\phi_{\overline{1s}}(\underset{\sim}{\rho}) + C\Phi. \tag{1}$$

Here the ground state of hydrogen is designated 1s and that of positronium is $\overline{1s}$, $\underset{\sim}{x}$ and $\underset{\sim}{r}$ are the positron and electron coordinates respectively, while the two coordinates

$$\underset{\sim}{R} = \frac{1}{2}(\underset{\sim}{x}+\underset{\sim}{r}) \, , \quad \underset{\sim}{\rho} = \underset{\sim}{x}-\underset{\sim}{r} \tag{1a}$$

describe the center of mass position and relative coordinate of the positronium. The two functions χ and F and the constant C are to be determined; the last is large when the energy is near resonance.

Coupled equations for these three unknowns are derived by standard variational methods. The resulting set is as follows:

$$\int d\underset{\sim}{r}\, \phi_{1s}(r)\,[H-E]\,\Psi = 0 \tag{2a}$$

$$\int d\underset{\sim}{\rho}\, \phi_{\overline{1s}}(\rho)\,[H-E]\,\Psi = 0 \tag{2b}$$

$$\iint d\underset{\sim}{r}\, d\underset{\sim}{x}\, \Phi\,[H-E]\,\Psi = 0. \tag{2c}$$

(Here

$$H = -\nabla_r^2 - \nabla_x^2 + 2\left(\frac{1}{x} - \frac{1}{r} - \frac{1}{\rho}\right)$$

and

$$E = E_{1s} + k^2 = E_{\overline{1s}} + \frac{1}{2} q^2.)$$

From Eq. (2c) we can obtain an expression for C in terms of χ and F as

$$C = (E-\mathcal{E})^{-1}\Big[\iint d\underset{\sim}{r}\, d\underset{\sim}{x}\, \Phi\,(H-E)\,\phi_{1s}\,\chi + \iint d\underset{\sim}{\rho}\, d\underset{\sim}{R}\, \Phi\,(H-E)\,\phi_{\overline{1s}}\,F\Big], \tag{3}$$

where we have defined

$$\mathcal{E} \equiv \iint d\underset{\sim}{r}\, d\underset{\sim}{x}\, \Phi\, H\, \Phi, \tag{4}$$

and have re-written the volume element in the second integral. The energy $\mathcal{E}$ should lie near the resonance represented by Φ. It is convenient to define two new functions

$$S(x) \equiv \int d\underset{\sim}{r}\, \phi_{1s} (H-E)\, \Phi \tag{5a}$$

and

$$T(R) \equiv \int d\underset{\sim}{\rho}\, \phi_{\overline{1s}} (H-E)\, \Phi , \tag{5b}$$

and to rewrite Eq. (3) (after integration by parts) as

$$C = (E-\mathcal{E})^{-1} \left[\int dx\, \chi S + \int d\underset{\sim}{R}\, F T \right] . \tag{6}$$

Inserting this expression into Eqs. (2a, 2b) we derive the coupled equations in the optical potential form

$$\mathcal{L} \underset{\sim}{\psi} + \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi} \rangle (E-\mathcal{E})^{-1} \underset{\sim}{V} = 0 , \tag{7}$$

where $\underset{\sim}{\Psi}$ and $\underset{\sim}{V}$ are column vectors defined as

$$\begin{aligned} \underset{\sim}{\psi} &\equiv \begin{pmatrix} \chi \\ F \end{pmatrix} \\ \underset{\sim}{V} &\equiv \begin{pmatrix} S \\ T \end{pmatrix} , \end{aligned} \tag{8}$$

$\langle \underset{\sim}{V} \cdot \underset{\sim}{\Psi} \rangle$ is the quantity in square brackets in Eq. (6), and $\mathcal{L}$ is the 2 × 2 matrix whose elements are as follows:

$$\mathcal{L}_{ij} = \int d\underset{\sim}{z}_i \, \phi_i(z_i)\left[H-E\right]\phi_j(z_j), \quad (i,j=1,2) \tag{9}$$

where

$$\underset{\sim}{z}_1 \equiv \underset{\sim}{r}, \quad \underset{\sim}{z}_2 \equiv \underset{\sim}{\rho}, \quad \phi_1 \equiv \phi_{1s}, \quad \phi_2 \equiv \phi_{\overline{1s}}.$$

(The diagonal elements of $\mathcal{L}$ are no more complex than differential operators, while the two off-diagonal elements are integral operators understood to operate on F and χ respectively. Details are given in the Appendix.) Eq. (7) is thus a set of coupled homogeneous integro-differential equations, whose possible resonant behavior is due to the second (optical potential) term. The similarity to the usual optical potential methods is clear.

Following Chen and Chung[19] we solve Eq. (7) by a non-iterative method. Letting

$$\underset{\sim}{\psi}^{j} = \underset{\sim}{\psi}_0^{j} + \langle \underset{\sim}{V}\cdot\underset{\sim}{\psi}^{j}\rangle (E-\mathcal{E})^{-1}\, \underset{\sim}{\psi}_1, \tag{10}$$

where j = 1, 2 refers to two regular, linearly independent solutions of Eq. (7), we must solve

$$\mathcal{L}\, \underset{\sim}{\psi}_0^{j} = 0 \tag{11a}$$

$$\mathcal{L}\, \underset{\sim}{\psi}_1 + \underset{\sim}{V} = 0. \tag{11b}$$

Only one particular solution of the inhomogeneous equation (11b) is needed. Using the definitions given in Eqs. (8) and (10) one finds

$$\langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}^{j} \rangle (E-\mathcal{E})^{-1} = \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}_0^{j} \rangle \left[E - \mathcal{E} - \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}_1 \rangle \right]^{-1} \tag{12}$$

where the bracket notation is an obvious extension of that defined in Eq. (8). Thus from two solutions of the homogeneous equation (11a) one can construct the "coupled static" approximation, while through Eqs. (10) and (12) the solution of the inhomogeneous equation (11b) leads to two solutions incorporating the effect of coupling to the "resonant" state Φ.

The most convenient way to represent the scattering parameters, for coupled and uncoupled cases alike, is in terms of the K-matrix. For any two regular, linearly independent solutions (either $\underset{\sim}{\Psi}^{j}$ or $\underset{\sim}{\Psi}_0^{j}$) one obtains the following asymptotic form

$$\begin{pmatrix} \frac{1}{x\sqrt{k}} \left[A_{1j} \sin kx + B_{1j} \cos kx \right] \\ \frac{1}{R}\sqrt{\frac{2}{q}} \left[A_{2j} \sin qR + B_{2j} \cos qR \right] \end{pmatrix}. \tag{13}$$

For i, j = 1, 2 the quantities A_{ij} and B_{ij} form 2 × 2 matrices and the K-matrix is defined as

$$K \equiv B A^{-1} \tag{14}$$

and is related to the S-matrix by

$$S = (1 + iK)(1 - iK)^{-1}. \tag{15}$$

Let us now choose a special set of solutions to the homogeneous equation (11a) with the matrix A equal to the identity matrix and hence $B = K^{\circ}$, the coupled static K-matrix. Noting the fact that the off-diagonal elements of K are very small compared with the diagonal elements[3,4,5] [see Table I], we simplify the analysis by setting $K^{\circ}_{12} = K^{\circ}_{21} = 0$. This approximation is equivalent to treating the two physical channels (e^{+} + H and Ps + p) as eigenchannels in the coupled static approximation. It does not imply that the coupling between these two channels is unimportant, and in our numerical solutions we have not neglected the off-diagonal elements of $\mathcal{L}$. (See Sec. IV.) Only in the asymptotic region are the two physical channels assumed to be uncoupled.

With the above simplification it will be convenient to choose the asymptotic forms of $\underset{\sim}{\Psi}_0$ and $\underset{\sim}{\Psi}$ as follows:

$$\underset{\sim}{\psi}{}_0^1 \sim \begin{pmatrix} \frac{1}{x\sqrt{k}}\left[\sin kx + K^{\circ}_{11}\cos kx\right] \\ 0 \end{pmatrix} \tag{16a}$$

$$\underset{\sim}{\psi}{}_0^2 \sim \begin{pmatrix} 0 \\ \frac{1}{R}\sqrt{\frac{2}{q}}\left[\sin qR + K^{\circ}_{22}\cos qR\right] \end{pmatrix} \tag{16b}$$

$$\underset{\sim}{\psi}{}_1 \sim \begin{pmatrix} C_1/x\sqrt{k}\left[\cos kx - K^{\circ}_{11}\sin kx\right] \\ C_2\sqrt{2}/R\sqrt{q}\left[\cos qR - K^{\circ}_{22}\sin qR\right] \end{pmatrix}. \tag{16c}$$

From the expressions in Eqs. (10 - 14) we can now construct the K-matrix including the coupling to the resonant state as follows:

$$K_{ij} = K^\circ_{ij} + \frac{f_{ij}}{G}\left[1+\left(K^\circ_{i\ell}\right)^2\right], \tag{17}$$

where

$$f_{ij} = C_i \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}{}^j_0 \rangle \left[E - \mathcal{E} - \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}_1 \right]^{-1}$$

and

$$G = 1 - f_{11} K^\circ_{11} - f_{22} K^\circ_{22} \, .$$

To relate the various quantities appearing in Eq. (17) to the resonance position and width, we note that the eigenphase sum exhibits typical Breit-wigner behaviour. That is,

$$\eta_1 + \eta_2 = \eta^\circ_1 + \eta^\circ_2 + \tan^{-1} \frac{\Gamma}{2(E_R - E)} , \tag{18}$$

where η_j and η_j^0 are the resonant and non-resonant (static exchange) eigenphases, Γ is the width and E_R is the position of the resonance. (The individual eigenphases may or may not exhibit such behavior). Using trigonometric identities we can show that

$$\frac{P}{1-Q} = \left[\frac{P^\circ}{1-Q^\circ} + \frac{\Gamma}{2(E_R-E)}\right]\left[1 - \frac{P^\circ}{1-Q^\circ}\,\frac{\Gamma}{2(E_R-E)}\right]^{-1}, \tag{19}$$

where

$$P \equiv \mathrm{Tr}\, K, \; P^0 \equiv \mathrm{Tr}\, K^0, \; Q \equiv \det K, \; Q^0 \equiv \det K^0, \tag{20}$$

and we recall that the eigenvalues of K are tan η_1 and tan η_2. Using Eq. (17) we find that

$$\begin{aligned} P &= G^{-1}\left[P^0 + (f_{11} + f_{22})(Q^0 - 1)\right], \\ Q &= G^{-1}\left[Q^0 + f_{11} K^0_{22} + f_{22} K^0_{11}\right]. \end{aligned} \tag{21}$$

Inserting these expressions for P and Q into the left side of Eq. (19), we can make the following identification

$$f_{11} + f_{22} = \frac{\Gamma}{2(E_R - E)} \tag{22}$$

and hence (from Eq. (17))

$$\begin{aligned} E_R &= \mathcal{E} + \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}_1 \rangle \equiv \mathcal{E} + \Delta \\ \Gamma &= -2 . \sum_{j=1}^{2} c_j \langle \underset{\sim}{V} \cdot \underset{\sim}{\psi}_0^j \rangle . \end{aligned} \tag{23}$$

These relations are the principal results of this section of the paper, and are correct provided (as usual) that η_j^0, E_R and Γ can be treated as constant across the resonance, and that Δ is not too large. We have essentially re-derived the results of Chen and Chung[19] for the two-channel special case being examined here with special emphasis on the asymptotic forms of $\underset{\sim}{\Psi}_0^{i}$ and $\underset{\sim}{\Psi}_1$. In addition, we have not required that the resonant part of the trial function be orthogonal to the rest of the function as is usually done.[20]

III. The Close-Coupling Correlation Function

Since we know that the degeneracy between the 2s and 2p levels of hydrogen produces the infinite series of Feshbach resonances[15,17], it is natural to choose the resonant term in our trial function to include those two states:

$$\Phi = N x^{-1}\left[u(x)\,\phi_{2s}(r) + v(x)\,\phi_{2p}(r)\,\hat{x}\cdot\hat{r}\right] \tag{24}$$

where

$$\phi_{2s}(r) = (32\pi)^{-\frac{1}{2}}\,e^{-\frac{1}{2}r}\,(2-r)$$

and

$$\phi_{2p}(r) = (32\pi)^{-\frac{1}{2}}\,e^{-\frac{1}{2}r}\,r\,.$$

The normalization constant is given by

$$N = \left[4\pi\int_0^\infty dx\,(u^2+v^2)\right]^{-\frac{1}{2}}. \tag{25}$$

By minimizing $\mathcal{E}$ with respect to u and v in Eq. (4) we obtain the equations

$$(\mathcal{H}+\epsilon)\underset{\sim}{M}=0 \tag{26}$$

where

$$\underset{\sim}{M} \equiv \begin{pmatrix} u \\ v \end{pmatrix},$$

$$\mathcal{H}_{ij} \equiv -\delta_{ij}\frac{d^2}{dx^2}+V_{ij}\,, \quad j=1,2$$

and

$$\epsilon \equiv E_{2s,2p}-\mathcal{E}\,.$$

The potentials are easily obtained:[21]

$$\begin{aligned} V_{11} &= 2e^{-x}\left(\frac{1}{x}+\frac{3}{4}+\frac{x}{4}+\frac{x^2}{8}\right)\\ V_{22} &= \frac{2}{x^2}-24\left[\frac{1}{x^3}-e^{-x}\left(\frac{1}{x^3}+\frac{1}{x^2}+\frac{7}{12x}+\frac{11}{48}+\frac{x}{16}+\frac{x^2}{96}\right)\right] \qquad (27)\\ V_{12}=V_{21} &= \frac{6}{x^2}-6e^{-x}\left[\frac{1}{x^2}+\frac{1}{x}+\frac{1}{2}+\frac{x}{6}+\frac{x^2}{24}\right]. \end{aligned}$$

Assuming a value for the eigenvalue ϵ, the two coupled second-order differential equations (26) were solved numerically: two regular, linearly independent solutions were obtained by integration outward from the origin and two others by integration inward from some large radius x_0. Admissable solutions are those for which $\underset{\sim}{M}$ and $d\underset{\sim}{M}/dx$ are continuous at the matching point $\bar{x}$; the continuity condition is equivalent to the determinantal condition

$$\det a_{ij}(\bar{x}) = 0. \tag{28}$$

The index i varies from 1 to 4 to specify the four linearly independent solutions, while j varies from 1 to 4 to denote a = u, v, du/dx and dv/dx, respectively. We were able to obtain the first two eigenvalues accurately (with $x_0 \lesssim 100$) using Eq. (28). They are

$$\begin{aligned} \epsilon_1 &= 3.1267 \times 10^{-2}\ \mathrm{Ry}, \\ \epsilon_2 &= 1.916 \times 10^{-3}\ \mathrm{Ry}. \end{aligned} \tag{29}$$

In the next section we will discuss these results, comparing them with previous work.[18] For the moment, let us just note that the ratio of the two eigenvalues $\epsilon_2/\epsilon_1 = 0.0613$; this is to be compared with the ratio 0.0583 based on the x^{-2} potential alone.[15]

We can now proceed to the calculation of $\underset{\sim}{V}$ [Eqs. (5) and (8)], required for obtaining the resonance parameters. Its two components are [from Eqs. (5) and (24)]

$$S(x) = N x^{-1} \int d\underset{\sim}{r}\, \phi_{1s}(r) \left(\frac{2}{x} - \frac{2}{\rho}\right) \left[\phi_{2s}(r)\, u(x) + \phi_{2p}(r)\, (\hat{x}\cdot\hat{r})\, v(x)\right], \tag{30a}$$

$$T(R)=N\int d\underset{\sim}{\rho}\,\phi_{1s}(\rho)\,x^{-1}\Big\{u(x)\Big[\Big(\frac{2}{x}-\frac{2}{\rho}-V_{11}\Big)\phi_{2s}(r) - V_{21}\,\hat{x}\cdot\hat{r}\,\phi_{2p}(r)\Big] + v(x)\Big[\Big(\frac{2}{x}-\frac{2}{\rho}+\frac{2}{x^2}-V_{22}\Big)\hat{x}\cdot\hat{r}\,\phi_{2p}(r) - V_{12}\,\phi_{2s}(r)\Big]\Big\} \tag{30b}$$

Equation (30a) is simple because of orthogonality while Eq. (30b) has been simplified somewhat by removing any derivatives that appear through the use of Eq. (26). We can re-write Eq. (30a) as

$$S(x) = N x^{-1}\left[V_s(x)\,u(x) + V_p(x)\,v(x)\right], \tag{31}$$

where

$$V_s(x) = -\frac{4\sqrt{2}}{9}\,e^{-\frac{3}{2}x}\left(\frac{2}{3}+x\right)$$
$$V_p(x) = \frac{256\sqrt{2}}{243}\left[e^{-\frac{3}{2}x}\left(\frac{1}{x^2}+\frac{3}{2x}+\frac{9}{8}+\frac{27x}{64}\right)-\frac{1}{x^2}\right], \tag{32}$$

while Eq. (30b) requires double numerical integration. In Fig. 1 we plot $\bar{S} = 2\pi^{1/2}$ x S and $\bar{T} = 4\sqrt{\pi}$ RT to give an idea of their range and form; only the first resonance, corresponding to ϵ_1, will be discussed from now on.

IV. Results and Discussion

Once the coupling term $\underset{\sim}{V}$ [Eqs. (8) and (30)] and the operator $\mathcal{C}$ [Eq. (9) and Appendix] are in hand we need only to solve the two sets of coupled equations (11), as discussed above, to obtain the position and width of the lowest e^+ - H resonance. These parameters constitute the main results of this work and will be discussed below.

In Table I we list the non-resonant scattering parameters, obtained from the homogeneous equations (11a), and compare them with the results of Ref. 5. These depend on the accuracy of our integration technique and our representation of the integral operator $\mathcal{L}$, as discussed in the Appendix. We used a simple, less accurate method than that in Ref. 5, truncating the coupled equations at $x = 20$ and $R = 12$, and it is reassuring that only small errors were thus introduced. The two off-diagonal elements of K° should be equal; our truncation results in significant inequality, although the average of the off-diagonal terms is in almost exact agreement with Ref. 5. Note, however, that these off-diagonal elements are small, as we have assumed; the two eigentangents are almost indistinguishable from the corresponding diagonal elements of K°. We also show results of the uncoupled approximation resulting from the omission of the off-diagonal parts of $\mathcal{L}$. It is interesting to note that this omission hardly affects the e^+ - H channel,[4] while the Ps - P channel is modified radically.

In Table II we give the properties of the lowest resonance. (Details of the numerical calculation are in the Appendix.) The main conclusion is that the resonance is quite far below the n = 2 threshold (0.3763 eV) and narrow enough to be well defined, with a width only 8% of the distance to threshold. Several other points should be noted:

1. When we drop the off-diagonal parts of $\mathcal{L}$ the widths and shifts of the two channels separate, and one in effect is calculating with the two distinct wave functions (1s, 2s, 2p) and (1s, 2s, 2p). Since the decay of the resonant state (2s, 2p) can occur through either open channel the total width and shift are sums over the two distinct cases. The first of these (e^+ - H) should correspond to the case treated by Seiler et al.[18] Comparing the first two lines in Table II we see that the resonance positions are in quite good agreement, while the width is not in agreement at all. We do not understand this discrepancy, but have noticed that the ratio of the two results is close to the numerical value of the rydberg in eV. It may be that an error was made in Ref. 18 in expressing Γ in eV. Assuming that, we divide their value for Γ by R_∞ and obtain a value of 8.305×10^{-5} eV, differing from our result by only 1.3%.

2. The second (Ps - P) channel has a much larger effect on both width and shift than the first. In the uncoupled approximation this amounts to a factor of about 7 in Δ and about 35 in Γ. This is expected for Δ, since only the sum $\mathcal{E} + \Delta$ has physical meaning and $\mathcal{E}$ itself depends on the separation between "open" and "closed" parts of the wave function. In channel 1 we have used an open-channel function orthogonal to the (2s, 2p) closed-channel function, but not in channel 2. We expect $E_R = \mathcal{E} + \Delta$ to be fairly reliable and probably an upper bound to the true resonance energy. On the other hand, Γ is an observable itself, and its sensitivity to the several approximations shown perhaps implies that even our best result may be unreliable: our best Γ is about 10 times

larger than our uncoupled width, while our best Δ is only 1.4 times smaller than our uncoupled shift.

3. In order to compare our non-resonant results with previous work,[5] we solved the scattering equations at $k = 0.85$ instead of $k = 0.847781$ which corresponds to the exact value of $\mathcal{E}$. This is certainly an insignificant error. An improvement would be to calculate Δ again at the value of k corresponding to E_R, continuing to recompute Δ until convergence is attained. This correction is also expected to be small. In fact, the value at our E_R is $k = 0.8499$; by accident we have evaluated Δ and Γ at very nearly the best possible k.

4. The resonance described here may be compared with the lowest resonance in e^- - H scattering, as treated in the 1s-2s-2p approximation[18] as follows:

$$\left(E_{Re^+} - E_{2s,2p}\right) / \left(E_{Re^-} - E_{2s,2p}\right) = 0.60$$

$$\Gamma_{e^+H} / \Gamma_{e^-H} = 0.54 .$$

Thus, the two two types of resonances are not qualitatively different. The long-range potentials are the same and the positronium channel is similar to the exchange channel, while the change in sign of the short-range static potential raises the e^+ - H energy and lowers the e^- - H energy.

APPENDIX

A. Evaluation of the operator $\mathcal{L}$

In order to solve Eq. (7) [or its equivalent, Eq. (11)] we must evaluate the integro-differential operator $\mathcal{L}$ [Eq. (9)]. Its diagonal elements are very easy to obtain:

$$\mathcal{L}_{11} = \int d\underset{\sim}{r}\, \phi_{1s}(r)\left[H_c(r) - \nabla_x^2 + \frac{2}{x} - \frac{2}{|\underset{\sim}{x}-\underset{\sim}{r}|} - E_{1s} - k^2\right]\phi_{1s}(r) \tag{A1}$$

$$= -\nabla_x^2 - k^2 + V_{1s}(x),$$

$$\mathcal{L}_{22} = \int d\underset{\sim}{\rho}\, \phi_{\overline{1s}}(\rho)\left[H_c(\rho) - \frac{1}{2}\nabla_R^2 + \frac{2}{|\underset{\sim}{R}+\frac{1}{2}\underset{\sim}{\rho}|} - \frac{2}{|\underset{\sim}{R}-\frac{1}{2}\underset{\sim}{\rho}|} - E_{\overline{1s}} - \frac{1}{2}q^2\right]\phi_{\overline{1s}}(\rho) \tag{A2}$$

$$= -\frac{1}{2}\nabla_R^2 - \frac{1}{2}q^2.$$

Here we have used either ($\underset{\sim}{x}$, $\underset{\sim}{r}$) or ($\underset{\sim}{R}$, $\underset{\sim}{\rho}$) variables as convenient and have made the definitions

$$H_c(r) \equiv -\nabla_r^2 - \frac{2}{r}\ , \quad H_c(\rho) \equiv -2\nabla_\rho^2 - \frac{2}{\rho}\ ; \tag{A3}$$

also note that ϕ_{1s} and $\phi_{\overline{1s}}$ are eigenfunctions of these Hamiltonians with eigenvalues $E_{1s} = -1$ and $E_{\overline{1s}} = -1/2$ respectively. The potential in Eq. (A1) is

$$V_{1s}(x) = 2e^{-2x}\left(1 + \frac{1}{x}\right), \tag{A4}$$

the static or Hartree potential felt by the positron in the field of an undistorted hydrogen atom. (The corresponding potential in the positronium channel vanishes due to antisymmetry and is absent from Eq. (A2). That is why $K^{\circ}_{22} = 0$ in the uncoupled approximation in Table II).

The off-diagonal elements are discussed in Chan's thesis [Ref. 5] and will be briefly reviewed here. The (21) element can be written as

$$\mathcal{L}_{21}\chi = \int d\underset{\sim}{\rho}\, \phi_{\overline{1s}}(\rho)\,\phi_{1s}(r)\left[-\nabla_x^2 + \frac{2}{x} - \frac{2}{|\underset{\sim}{x}-\underset{\sim}{r}|} - k^2\right]\chi(x), \qquad \text{(A5)}$$

where we have used the fact that ϕ_{1s} is an eigenfunction of $H_0(r)$ and have commuted it to the left side. By changing variables from $\underset{\sim}{R}, \underset{\sim}{\rho}$ to $\underset{\sim}{R}$, $\underset{\sim}{x}$ and integrating by parts we obtain the form

$$\begin{aligned}\mathcal{L}_{21}\chi &= 8\int d\underset{\sim}{x}\, \chi(\underset{\sim}{x})\left[-\nabla_x^2 + \frac{2}{x} - \frac{1}{|\underset{\sim}{R}-\underset{\sim}{x}|} - k^2\right]\phi_{1s}(|2\underset{\sim}{R}-\underset{\sim}{x}|)\,\phi_{\overline{1s}}(2|\underset{\sim}{R}-\underset{\sim}{x}|) \\ &\equiv \int d\underset{\sim}{x}\, G(\underset{\sim}{R},\underset{\sim}{x})\,\chi(\underset{\sim}{x})\end{aligned} \qquad \text{(A6)}$$

where the factor of 8 is the Jacobian of the transformation. In analogous fashion we can write

$$\begin{aligned}\mathcal{L}_{12}F &= 8\int d\underset{\sim}{R}\, F(\underset{\sim}{R})\left[-\frac{1}{2}\nabla_R^2 - \frac{1}{2}q^2 + \frac{2}{x} - \frac{1}{|\underset{\sim}{R}-\frac{1}{2}\underset{\sim}{x}|}\right]\phi_{1s}(|2\underset{\sim}{R}-\underset{\sim}{x}|)\,\phi_{\overline{1s}}(2|\underset{\sim}{R}-\underset{\sim}{x}|) \\ &\equiv \int d\underset{\sim}{R}\, \bar{G}(\underset{\sim}{x},\underset{\sim}{R})\,F(\underset{\sim}{R}).\end{aligned} \qquad \text{(A7)}$$

We can show that $\overline{G}(\underset{\sim}{x}, \underset{\sim}{R}) = G(\underset{\sim}{R}, \underset{\sim}{x})$ by changing variables from $\underset{\sim}{x}$, $\underset{\sim}{R}$ to $\underset{\sim}{r}$, $\underset{\sim}{\rho}$ and writing

$$\overline{G}(\underset{\sim}{x},\underset{\sim}{R}) - G(\underset{\sim}{R},\underset{\sim}{x}) = \left[H_0(r) - E_{1s} - H_0(\rho) + E_{\overline{1s}}\right]\phi_{1s}(r)\,\phi_{\overline{1s}}(\rho) = 0. \tag{A8}$$

Then we can evaluate the kernel itself most conveniently as

$$\begin{aligned} G = \tfrac{1}{2}(G+\overline{G}) = 4\Big[-3\nabla_r^2 - 6\nabla_\rho^2 - 8\,\underset{\sim}{\nabla}_r\cdot\underset{\sim}{\nabla}_\rho - k^2 - \tfrac{1}{2}q^2 \\ + \frac{4}{x} - \frac{2}{r} - \frac{2}{\rho}\Big]\phi_{1s}(r)\,\phi_{\overline{1s}}(\rho) \qquad \text{(A9)} \\ = 4\Big[3H_0(r) + 3H_0(\rho) - 8\,\underset{\sim}{\nabla}_r\cdot\underset{\sim}{\nabla}_\rho + \frac{4}{x} + \frac{4}{r} + \frac{4}{\rho} - k^2 - \tfrac{1}{2}q^2\Big]\phi_{1s}\,\phi_{\overline{1s}}. \end{aligned}$$

The cross-term is done explicitly and we use the relations between the energies [Eq. (2)]. Finally, we obtain the result

$$G(\underset{\sim}{R},\underset{\sim}{x}) = 16\left[\frac{1}{x} + \frac{1}{r} + \frac{1}{\rho} - \hat{r}\cdot\hat{\rho} - 1 - \tfrac{1}{2}k^2\right]\phi_{1s}(r)\,\phi_{\overline{1s}}(\rho), \tag{A10}$$

where $\underset{\sim}{r} = 2\underset{\sim}{R} - \underset{\sim}{x}$ and $\underset{\sim}{\rho} = 2(\underset{\sim}{R} - \underset{\sim}{x})$.

Since we are interested only in total S-wave scattering, we allow X and F to depend only on the magnitudes x and R. This allows us to carry out the angular integrations in Eqs. (A6) and (A7) over $\mu = \hat{X}\cdot\hat{R}$ by numerical Gaussian quadrature. The final expression of Eqs. (11) involving the operator $\mathcal{L}$ is then

$$\frac{d^2f}{dx^2} + k^2 f = V_{1s} f + \int_0^\infty dR\, K(R,x)\, g(R) + \left[0, \bar{S}(x)\right]$$
$$\frac{d^2g}{dR^2} + q^2 g = \quad 2\int_0^\infty dx\, K(R,x)\, f(x) + \left[0, \bar{T}(R)\right], \qquad \text{(A11)}$$

where

$$f(x) = \chi(x)/x\sqrt{4\pi}, \quad g(R) = F(R)/R\sqrt{4\pi},$$

and $\bar{S}$, $\bar{T}$ are defined following Eq. (32) and shown in Fig. 1. The S-wave kernel is

$$K(R,x) = 8\sqrt{2}\, Rx \int_{-1}^{1} d\mu \left[A^{-1} + \tfrac{1}{2}B^{-1} + x^{-1} - C A^{-1} B^{-1} - 1 - \tfrac{1}{2}k^2\right] e^{-(A+B)} \qquad \text{(A12)}$$

where

$$A = \left(4R^2 + x^2 - 4Rx\mu\right)^{1/2},$$
$$B = \left(R^2 + x^2 - 2Rx\mu\right)^{1/2},$$
$$C = 2R^2 + x^2 - 3Rx\mu.$$

It is easily shown that for small x, $K(R,x)\alpha e^{-3R}$ while for small R, $K(R,x)\alpha e^{-2x}$. From these results it appears that K extends further in x than in R. A troublesome ridge occurs for $x \approx R$, along which K decreases very slowly. Following Chan[5] we have evaluated K(R,x) separately in the four regions bounded by the straight lines x = 0, x = R, $x = 2^{1/2}R$, x = 2R and R = 0, using simple transformations to avoid singularities and employing numerical Gaussian quadrature.

We chose to solve the integro-differential equations by converting them to a set of linear algebraic equations which is numerically inverted. Specifically, we used a three-point central-difference formula to approximate the second derivative and the trapezoid rule for integration. A considerable improvement in accuracy is obtained by a simple modification; for example, the first homogeneous equation of (A11) becomes

$$f_{n+1}\left[1-\frac{h^2}{12}\left(V_{n+1}-k^2\right)\right]+f_n\left[-2+\frac{10}{12}h^2\left(V_n-k^2\right)\right]+f_{n-1}\left[1-\frac{h^2}{12}\left(V_{n-1}-k^2\right)\right]$$
$$=\frac{h^3}{12}\sum_m\left[K_{m,n+1}+10K_{m,n}+K_{m,n-1}\right]g_m \qquad \text{(A13)}$$

where

$$f_n \equiv f(x_n),\ g_m \equiv g(R_m),\ V_n \equiv V_{1s}(x_n),\ K_{m,n} \equiv K(R_m,x_n),$$

and h is the appropriate lattice interval Δx or ΔR. We obtained sufficient accuracy for the homogeneous equations using the following set of intervals:

$\Delta x = 0.1$ for $0 < x \leq 4$, $\Delta x = 0.2$ for $4 < x \leq 12$, $\Delta x = 0.4$ for $12 < x \leq 20$; $\Delta R = 0.06$ for $0 < R \leq 2.4$, $\Delta R = 0.12$ for $2.4 < R \leq 7.2$, $\Delta R = 0.24$ for $7.2 < R \leq 12$.

This gives a total of 100 values each for f_n and g_m and a set of 200 linear equations to invert. Beyond this region, the equations (A11) effectively uncouple since $K \approx 0$, but the inhomogeneous terms are not negligible. The inhomogeneous equations were continued out to x, R = 50 as ordinary differential equations, and all the integrals needed to obtain Δ and Γ were also carried out that far.

On the other hand, Chan and Fraser[5] chose to solve the homogeneous Eqs. (A11) by first converting them to integral equations. This involves some addition work, but enables one to use Gauss-Laguerre integration which can represent the unknown functions on an optimal lattice of points. Judging from their results and ours, it would seem that the integral equation method has some real advantages in accuracy and economy.

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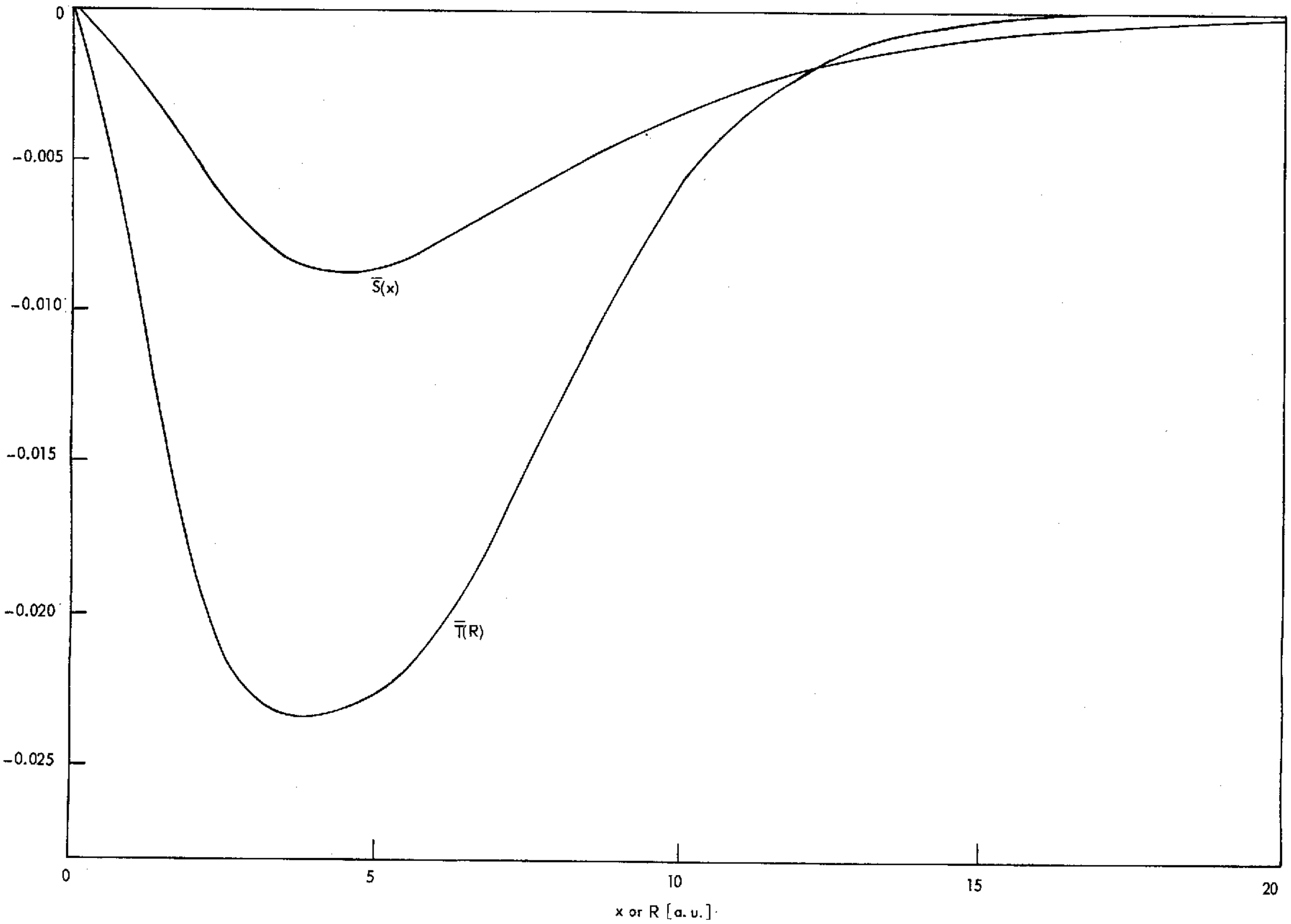
Table I. Non-Resonant (1s - $\overline{1s}$) Scattering Results at k = 0.85

	Ref. 5	Present Work	
	Coupled	Coupled	Uncoupled
K°_{11}	-0.3674	-0.3672	-0.4058
K°_{21}	0.1035	0.0943	0
K°_{12}	0.1035	0.1078	0
$1/2\ (K^{\circ}_{12} + K^{\circ}_{21})$	(0.1035)	(0.101)	(0)
K°_{22}	10.196	10.207	0
tan η°_{1}	-0.3684	-0.3682	-0.4058
tan η°_{2}	10.197	10.208	0

Table II. Properties of the lowest resonance. Our results are in eV, using $R_\infty = 13.60583$ eV [Ref. 22]. (The results in Ref. 18 were reported in eV; but the value of the rydberg used was not stated). The unshifted energy $\mathcal{E} = 9.77896$ eV. Our best result is given on the last line.

	Width Γ	Shift Δ	Resonance position $E_R = \mathcal{E} + \Delta$
e^+ - H channel only	8.20 (-5)	8.94 (-3)	9.7879
Ref. 18.	1.130 (-3)	–	9.7845
Both channels (uncoupled)	3.03 (-3)	6.88 (-2)	9.8478
Both channels (coupled)	2.94 (-2)	4.91 (-2)	9.8281

Figure 1. The resonant coupling functions $\bar{S} = 2\pi^{1/2}\ x\,S(x)$ and $\tilde{T} = 4\pi^{1/2}\ RT(R)$, plotted against x and R respectively.


0
-0.005
-0.010
-0.015
-0.020
-0.025
$\overline{S}(x)$
$\overline{T}(R)$
0
5
10
15
20
x or R [a.u.]