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POSSIBLE RESONANCE IN POSITRON-HYDROGEN SCATTERING

Richard J. Drachman

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GODDARD SPACE FLIGHT CENTER
Greenbelt, Maryland

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Richard J. Drachman
Lab for Theoretical Studies
National Aeronautics and Space Administration
Goddard Space Flight Center
Greenbelt, Maryland

The positron-hydrogen system is considered, with the view to determining whether a scattering resonance below the positronium threshold is likely to occur, as has been suggested by Bransden and Jundi. The likeliest mechanism for producing such a resonance would be the existence of a virtual bound state in the positronium-proton channel, brought about by the large dipole polarizability and mass of the positronium atom. A modification of Holøien's technique enables one to reject spurious solutions without the use of the projection operator technique. A non-variational adiabatic calculation seems to indicate that a resonance does exist, lying at 0.1 eV below the threshold. When, however, a variational treatment is employed, certain essential non-adiabatic terms appear. The resultant reduction in attraction serves to eliminate the apparent resonance. It is concluded that the previously reported resonance is probably an artifact.

I. INTRODUCTION

Bransden and Jundi[1] have recently examined the positron-hydrogen system above the threshold for positronium formation (6.8 eV). With the aid of the M-Matrix method[2] they have extrapolated their results below the threshold, and have presented evidence that a resonance occurs in the e^+-H elastic channel. Their estimate of the position of this resonance corresponds to a state of the positronium-proton system, bound by about 0.02 eV (1.6×10^{-3} Rydberg). The present work is intended to examine the evidence for the existence of such a resonance.

The simplest method of locating such a resonance would be the projection operator technique,[3] which has been very satisfactory in finding e^--H resonances below degenerate thresholds.[4] This technique effectively decouples the open and closed channel parts of the scattering wave function, and reduces the problem of resonances to that of bound states. The most likely physical mechanism which could produce binding is the electric polarization of the positronium atom in its ground state by the proton. Thus a wave function including this polarizability will be the basis of the present work.

If we construct an appropriate scattering trial function ψ including polarizability, the projection operator prescription for computing the resonant energies is as follows:

(1) Construct a projection operator Q which removes the hydrogen ground-state component from ψ, and

(2) Carry out a Rayleigh-Ritz variational energy calculation using $Q\psi$ as the trial function.

Using the simple form $Q = 1 - |H\rangle\langle H|$, where $|H\rangle$ represents the hydrogen ground state $\phi_H(r)$, $\mathbf{x}$ is the positron coordinate, and the trial function has the form

$$\psi(\mathbf{r}, \mathbf{x}) = f(\mathbf{x})\,\phi_H(r) + \Phi(\mathbf{x}, \mathbf{r}), \tag{1}$$

one can write the closed-channel part of ψ as

$$Q\psi = \psi(\mathbf{r}, \mathbf{x}) - \phi_H(r)\int d^3r'\,\phi_H(r')\,\psi(\mathbf{r}, \mathbf{x}), \tag{1a}$$

$$Q\psi = \Phi(\mathbf{x}, \mathbf{r}) - \phi_H(r)\int d^3r'\,\phi_H(r')\,\Phi(\mathbf{x}, \mathbf{r}'). \tag{1b}$$

If, for example, Φ were a close-coupling expansion in excited states of the target, then $Q\psi = \Phi$. We wish, however, to write Φ in terms of the positronium atom in the field of a proton, so the second term in Eq. (1b) does not necessarily vanish.

Holøien[5] has used a simplification of the projection operator method in searching for electron-atom resonances, and we will here apply a form of his approach to the positron problem. To do this, we first neglect the second term in Eq. (1b), and use Φ itself for the energy calculation. Some of the resulting energies will correspond to functions Φ for which the integral in Eq. (1b) is very small; i.e., for which the projection onto the hydrogen ground state is very small. We follow Holøien in considering such states to be genuine resonances, although the energies thus obtained have no necessary upper bound character.

II. THE SCATTERING WAVE FUNCTION

Let us consider the motion of a positronium atom (Ps) in the field of a fixed proton (P). We will use a trial function of the following form

$$\Phi = [\chi(\mathbf{R}) + F(\mathbf{R})\, G(R, \zeta, \cos\theta)]\, \phi(\zeta), \tag{2}$$

where $\phi(\zeta) = (8\pi)^{-1/2}\, e^{-1/2\,\zeta}$ is the positronium ground-state wave function, while $\mathbf{R} = 1/2\,[\mathbf{x} + \mathbf{r}]$, $\boldsymbol{\zeta} = \mathbf{x} - \mathbf{r}$ and $\cos\theta = (\mathbf{R}\cdot\boldsymbol{\zeta})/R\zeta$. The functions χ and F will be determined later, while G is to represent the adiabatic distortion of the positronium atom.

The Hamiltonian can be written in atomic units, with energies in Rydbergs as

$$H = H_\zeta + V - \frac{1}{2}\nabla_R^2, \tag{3}$$

where

$$H_\zeta = -2\left(\nabla_\zeta^2 + \frac{1}{\zeta}\right), \quad \left[H_\zeta + \frac{1}{2}\right]\phi(\zeta) = 0,$$

$$V = 2\left[\frac{1}{|\vec{R} + \frac{1}{2}\vec{\zeta}|} - \frac{1}{|\vec{R} - \frac{1}{2}\vec{\zeta}|}\right] = \sum_{\ell\,(\mathrm{odd})} v(R, \zeta)\, P_\ell(\cos\theta).$$

The first-order (in V) adiabatic form for G is obtained by solving the equation^6

$$[G, H_\zeta]\,\phi = V\phi, \tag{4}$$

and since by symmetry only odd multipoles are retained in the expansion for the potential, it is a good approximation to keep only the dipole $[\ell = 1]$ term. Then, $G = g(R,\zeta)P_1$ $(\cos\theta)$ and Eq. (4) becomes

$$\frac{d^2g}{d\zeta^2} + \left(\frac{2}{\zeta} - 1\right)\frac{dg}{d\zeta} - \frac{2}{\zeta^2}\, g = f, \tag{5}$$

where $f = -\zeta/R^2$ for $\zeta \leq 2R$ and $f = -8R/\zeta^2$ for $\zeta \geq 2R$. The properly continuous, regular solution of Eq. (5) with continuous first derivative is found to be

$$\begin{aligned} g(\zeta \leq 2R) &= \frac{1}{8R^2}\left[\zeta + \frac{1}{4}\zeta^2\right] - \frac{3}{8}e^{-2R}\left(1 + \frac{1}{R}\right)^2\left[\frac{2}{\zeta^2}e^{\zeta} - \left(1 + \frac{2}{\zeta} + \frac{2}{\zeta^2}\right)\right] \\ g(\zeta \geq 2R) &= -\frac{R}{2}\left[\frac{1}{\zeta} + \frac{1}{\zeta^2}\right] + \frac{3}{8}\left[1 - \frac{1}{R^2} + e^{-2R}\left(1 + \frac{1}{R}\right)^2\right] \cdot \left[1 + \frac{2}{\zeta} + \frac{2}{\zeta^2}\right]. \end{aligned} \tag{6}$$

III. THE ADIABATIC NON-VARIATIONAL METHOD

Our first evaluation of χ and F will be non-variational, and resembles the polarized-orbital method[7] used previously for positron-hydrogen scattering.[8] We assume that $F = \chi$ in Eq. (2) and require χ to satisfy the equation

$$\langle [H - E]\ [1 + G] \rangle\ \chi = 0, \tag{7}$$

where $E = -1/2 + \epsilon$, and the bracket is defined as

$$\langle q(\mathbf{R}, \zeta) \rangle \equiv \int d^3\zeta\ \phi(\zeta)\ q(\mathbf{R}, \zeta)\ \phi(\zeta). \tag{8}$$

A bound state in the Ps - P channel would occur if a normalizable solution of Eq. (7) can be found with $\epsilon < 0$, and it would represent a resonance in the elastic e^+-H channel near a positron energy $1/2 + \epsilon$. Since $\langle G \rangle = 0$, Eq. (7) can be written explicitly as

$$\left[-\frac{1}{2}\nabla^2_R + V_2\right] \chi = \epsilon \chi, \tag{9}$$

where $V_2 \equiv \langle GV \rangle$ is the adiabatic dipole potential, listed in Table I. Before solving the eigenvalue problem of Eq. (9), one can check whether any bound states exist by solving the S-Wave, zero-energy $[\epsilon = 0]$ scattering problem. The number of nodes in the radial wave function will give the number of bound states. This radial function $U = R\chi$ is obtained by numerically integrating the equation

$$-\frac{1}{2}U'' + [V_2 - \epsilon]\ U = 0 \tag{9a}$$

outward from the origin in the usual way. The result for $\epsilon = 0$ is plotted in Fig. 1, and one sees that two bound states occur. The more compact of these is spurious, and results from the omission of the second term in Eq. (1b), but the state giving the second node may represent the resonance found in Ref. (1).

The eigenvalues are then obtained numerically from Eq. (9a), by integrating outward from the origin and inward from the asymptotic region. Continuity of the logarithmic derivative determines ϵ. The lower eigenvalue is $\epsilon \approx -0.6$ Ry; this energy is close to that of the 1S state of hydrogen, and the corresponding eigenfunction peaks at $R \approx 1.5$, so this clearly is one of the spurious states which would have been eliminated by the Q operator technique. The second eigenvalue is $\epsilon = -7.5 \times 10^{-3}$ Ry, and represents a resonance lying 0.1 eV below the positronium threshold.[9] In Fig. 2 the low-lying e^{+} -e^{-} -P states are shown on a level diagram in order to clarify the situation. The two bound states just discussed are in the closed channel below the ground state of positronium [Ps(1s) + P]. The spurious state is seen to be in the vicinity of the ground state of hydrogen [H (1s) + e^{+}], while the second state corresponds to a resonance in the open channel. In Section V we will discuss the relation between this resonance and that found in Ref. 1.

IV. THE VARIATIONAL METHOD

The assumptions made in Section III [that $F = \chi$ and that Eq. (7) holds] depend on the ability of the positronium atom to adjust adiabatically to the polarization induced by the electric field of the proton.[10] This in turn depends roughly on the smallness of the velocity of the positronium center of mass. The very tightly bound (spurious) lower state probably has too much kinetic energy to satisfy the adiabatic conditions, but the resonance state may satisfy them.

The variational method relaxes the above condition on F and determines both functions by free variation. Eq. (7) is replaced by the following two equations:

$$\begin{aligned} &\langle [H - E]\ [\chi + FG] \rangle = 0 \\ &\langle G\,[H - E]\ [\chi + FG] \rangle = 0, \end{aligned} \tag{10}$$

whose solution corresponds to solving the Schrödinger equation in the restricted subspace spanned by the orthogonal vectors ϕ and $G\phi$. Explicitly, these result in the following system of differential equations:[11]

$$\begin{aligned} &\left[\frac{1}{2}\nabla_R^2 + \epsilon\right] \chi - V_2 F = 0 \\ &\left[N\left(\frac{1}{2}\nabla_R^2 + \epsilon\right) + V_2 - W - V_N \frac{d}{dR}\right] F - V_2 \chi = 0, \end{aligned} \tag{11}$$

where

$$N \equiv \langle G^2 \rangle, \quad W \equiv -\frac{1}{2} \langle G\, \nabla_R^2 G \rangle, \quad V_N \equiv -\frac{1}{2}\frac{dN}{dR}, \quad V_2 \equiv \langle GV \rangle .$$

[These functions were evaluated numerically and are given in Table I.] Except for $R \to \infty$, the relation $F = \chi$ does not satisfy Eq. (11). Interesting features of Eq. (11) are the short-range potential W and the velocity-dependent term involving V_N.

Letting $\chi = R^{-1}U$ and $F = R^{-1}g$ one can write the S-wave, $\epsilon = 0$ form of Eq. (11) as follows:

$$\frac{1}{2}U'' = V_2 g$$

$$\frac{N}{2}g'' - V_N g' + [V_2 - W + V_N/R]\, g = V_2 U. \tag{12}$$

These equations resemble those of a two-state close-coupling calculation, and to treat them similar techniques are used.[12] Two linearly independent regular solutions of Eq. (12) exist for small R; their leading terms are

$$U_1 = R, \quad g_1 = 0$$

and

$$U_2 = 0, \quad g_2 = R. \tag{13}$$

Each of these solutions is integrated numerically from the origin out to a convenient intermediate point $\bar{R}$, at which point a linear combination

$$U_<(\bar{R}) = A U_1(\bar{R}) + B U_2(\bar{R}) \tag{14}$$

with undetermined coefficients represents the numerical value of U. A similar combination is formed for g. Three linearly independent regular solutions of Eq. (12) exist for large R. To find them, we use the asymptotic forms of the potentials given in Table I. Eq. (12) becomes

$$\frac{1}{2}U'' = -36R^{-4}g$$

$$\frac{1}{2}g'' - 2R^{-1}g' - \frac{18}{43}g = -\frac{18}{43}U, \tag{15}$$

where terms of order R^{-2} were neglected in the second line. The three solutions required for large R are

$$U_3 = 1 - 6/R^2 , \; g_3 = U_3 ,$$

$$U_4 = R - 18/R , \; g_4 = U_4 - 43/9R , \tag{16}$$

$$U_5 = 0 , \; g_5 = e^{-\beta R} \left[1 + \beta R + \frac{1}{3} (\beta R)^2 \right] , \; (\beta^2 = 36/43) .$$

[Solutions 3 and 4 contain the first two terms of a series in inverse powers of R]. Each of these solutions is integrated numerically inward from an asymptotic point R_0 (= 20 in the present work) to the intermediate point $\bar{R}$ where the linear combination

$$U_> (\bar{R}) = U_3 (\bar{R}) + C U_4 (\bar{R}) + D U_5 (\bar{R}) \tag{17}$$

represents the numerical value of U, and similarly for g. (The coefficient of U_3 is taken equal to unity, and U has the conventional normalization to unit slope at $R \to \infty$). Four equations represent the matching conditions at $R = \bar{R}$:

$$U_< = U_> , \; g_< = g_> , \; U'_< = U'_> , \; g'_< = g'_> . \tag{18}$$

These determine the four constants A, B, C, D through a set of four linear algebraic equations. The function U(R) thus obtained is plotted on Fig. 1. This is the principal result of the present work: The node representing the spurious state occurs at larger R than for the non-variational case, and this decrease in effective attraction is sufficient to destroy the second node.[13] The variational treatment thus does not give any indication of a resonance below the Ps threshold. The radically different behavior produced by the inclusion of the non-adiabatic terms leads us to conclude that the resonance found in Ref. (1) is probably spurious.

V. DISCUSSION AND CONCLUSIONS

To explain the relation between the present work and that of Ref. 1, let us recall that the latter considered the scattering of positrons on hydrogen above the threshold for positronium formation, using a polarized orbital type of wave function in both e^+-H and Ps-P channels. In our notation

$$\begin{aligned}\psi &= \chi_1(\mathbf{x})\,[1 + G_H(\mathbf{x},\mathbf{r})]\,\phi_H(r)\\ &\quad + \chi_2(\mathbf{R})\,[1 + G_{Ps}(\mathbf{R},\boldsymbol{\zeta})]\,\phi_{Ps}(\zeta).\end{aligned} \tag{19}$$

If the Schrödinger equation $[H-E]\psi = 0$ is projected onto $\phi_H(r)$ and $\phi_{Ps}(\zeta)$ in turn, the coupled equations used in Ref. 1 are obtained [their Eq. (16)]. These are as follows:

$$\begin{aligned}&[\nabla_x^2 + k_1^2 - V_1(x) - V_{2H}(x)]\,x_1(\mathbf{x}) = \int d^3r\,\phi_H(r)\\ &\qquad [-\nabla_x^2 - k_1^2 + V(\mathbf{r},\mathbf{x})]\,[1 + G_{Ps}(\mathbf{R},\boldsymbol{\zeta})]\,\phi_H(r)\,\chi_1(\mathbf{x}) = 0\\ &[\nabla_R^2 + k_2^2 - 2V_{2Ps}(R)]\,\chi_2(\mathbf{R}) = \int d^3\boldsymbol{\zeta}\,\phi_{Ps}(\zeta)\\ &\qquad [-\nabla_R^2 - k_2^2 + 2V(\mathbf{R},\boldsymbol{\zeta})]\,[1 + G_H(\mathbf{x},\mathbf{r})]\,\phi_{Ps}(\zeta)\,\chi_2(\mathbf{R}) = 0\end{aligned} \tag{20}$$

where the second-order potentials are the adiabatic polarization potentials of hydrogen [including several multipoles] and positronium [dipole distortion only], and where

$$V(\mathbf{r},\mathbf{x}) = 2\left[\frac{1}{x} - \frac{1}{|\mathbf{x}-\mathbf{r}|}\right], \tag{21}$$

and $V(\mathbf{R},\boldsymbol{\zeta})$ is given in Eq. (3). [A further neglect of all terms in G_H, G_{Ps} on the right side of Eq. (20) does not concern us here]. If Eq. (20) is now solved, the eigenphases or reaction matrix satisfy a minimum principle, but only if certain non-adiabatic terms are added. These are complicated and involve cross-channel couplings, but for the diagonal Ps term the form is

$$\int d^3R\, \chi_2(\mathbf{R}) \left[-\frac{1}{2} N \,(\nabla_R^2 + k_2^2) + W + V_N \frac{d}{dx}\right] \chi_2(\mathbf{R}), \tag{22}$$

where N, W, V_N were defined in Eq. (11), and a similar correction term appears in the diagonal H term. The authors of Ref. 1 emphasize that, since they have omitted the non-adiabatic correction terms their results cannot be considered quantitative. We have here attempted, by including terms of this type in an optimal variational calculation, to indicate that the most likely result of the quantitative extension of the work of Ref. 1 would be the disappearance of the resonance.

Recently, another above-threshold calculation has been reported,[14] which does not obtain the resonance discussed in Ref. (1). The method is very similar to that of Ref. (1), including both ground-state hydrogen and Ps as well as adiabatic polarization potentials. A unique coordinate system, introduced into the Ps-P channel to simplify the form of the coupled equations, also provides a spurious centrifugal potential. It seems that this extra potential serves inadvertently to simulate the effect of the non-adiabatic terms we have discussed above, and hence to eliminate the resonance.

An interesting question may be raised now concerning the Ps - He^+ channel in e^+-He scattering. This system is the same as Ps - P at large distances, but its additional Van der Waals attraction might be just enough to produce the resonance. The cross-section near threshold for e^+-He scattering has been measured,[15] although the analysis of the experiment is not straightforward. It is possible that a resonance near threshold is needed to bring about agreement between experiment[15] and theory.[16]

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TABLE I

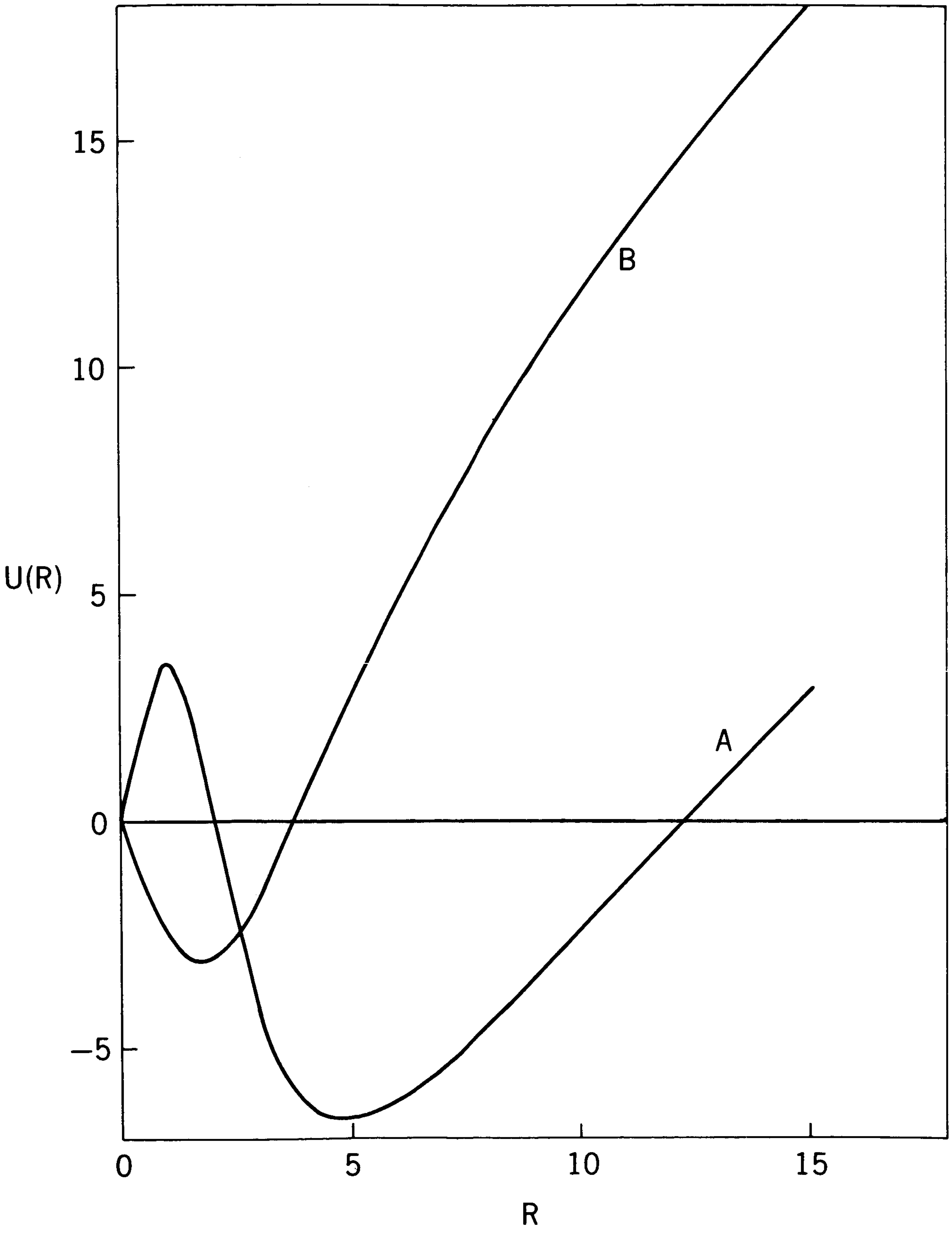
Potentials Needed for the Numerical Solution of the Scattering Problem

R	$-V_2$	N	V_N	W
0	0	0	0	0
0.2	0.282	0.198	-0.920	0.801
0.4	0.745	0.661	-1.300	1.944
0.6	1.108	1.173	-1.197	2.613
0.8	1.306	1.586	-0.845	2.752
1.0	1.358	1.842	-0.436	2.536
1.5	1.135	1.873	+0.276	1.521
2.0	0.785	1.469	0.464	0.729
2.5	0.504	1.026	0.403	0.314
3.0	0.316	0.680	0.288	0.128
4.0	0.127	0.291	0.121	1.97 (-2)
5.0	5.60 (-2)	0.132	4.92 (-2)	2.90 (-3)
7.5	1.14 (-2)	2.71 (-2)	7.21 (-3)	2.32 (-5)
10.0	3.60 (-3)	8.60 (-3)	1.72 (-3)	1.76 (-7)
$R \to \infty$	$\sim 36\ R^{-4}$	$\sim 86\ R^{-4}$	$\sim 172\ R^{-5}$	Exponential

FIGURE CAPTIONS

Fig. 1. Radial wave Functions $U = R\chi$, for $\epsilon = 0$. Curve A is non-variational and shows two nodes, while curve B is variational and has only one. The functions are normalized to unit slope asymptotically, with R measured in Bohr radii.

Fig. 2. Energy level diagram for the e^+-e^--P system. The two bound states found in the non-variational method are shown: A is the spurious level, and B respresents the resonance found below the Ps threshold. The diagonal hatching indicates the scattering continua. The terminology "open" or "closed" channel is meaningful only below $E = -1/2$.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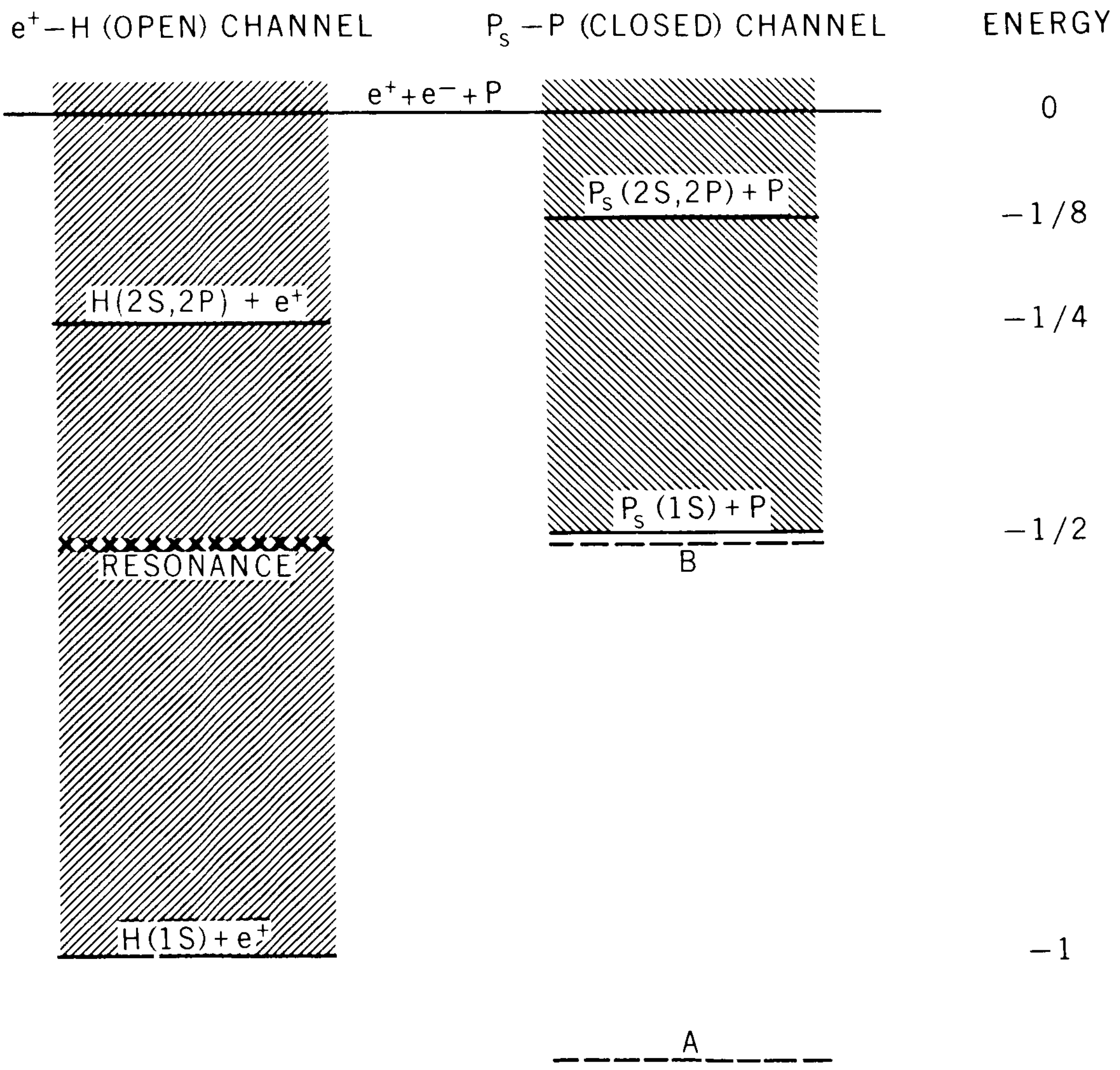
B


e^+–H (OPEN) CHANNEL
P_s –P (CLOSED) CHANNEL
ENERGY
$e^+ + e^- + P$
0
P_s (2S,2P) + P
−1/8
H(2S,2P) + e^+
−1/4
P_s (1S) + P
−1/2
RESONANCE
B
H(1S) + e^+
−1
A