Boundary condition model for the linewidths of protonium

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We have calculated the annihilation widths of s- and p-state protonium using a coupled channel model which incorporates an absorptive boundary condition derived from the WKB approximation. The boundary condition yields results nearly independent of the point at which the condition is applied. The results are compared with the black sphere model.

[NUCLEAR REACTIONS protonium $\bar{p}p$, calculated level shifts and widths, boundary condition model.]

I. INTRODUCTION

Protonium, the bound state of a proton and an antiproton, is a very large system on the nuclear scale. Its mean radius in the 1s state is 86.5 fm, an order of magnitude greater than the range of the strong interactions. Thus, to a good approximation, the system is described by hydrogenlike wave functions. Nonetheless, the hadronic forces play an important role in the dynamics of the system since they lead to its destruction through annihilation into mesons. It is the effect of these strong interactions on the atomic dynamics which is the subject of this paper.

The dynamics of the atomic bound state of a proton and an antiproton, protonium, is most easily visualized by reference to the effective potential shown schematically in Fig. 1. The system exists for most of its lifetime in the broad potential well lying between r_1 and r_2 formed by the attractive Coulomb potential and (for $l \neq 0$) the centrifugal potential. We will refer to this shallow well as the "atomic well"; for 2p levels the corresponding radii are $r_1 \approx 30$ fm and $r_2 \approx 200$ fm. In the region with r less than a few fm, the potential is dominated by strong short range hadronic forces, the outer parts of which are given by meson exchanges. The problem is complicated by the fact that pion or other isovector meson exchanges mix $n\bar{n}$ components into the dominantly $p\bar{p}$ wave function. In a previous[1] article it was shown that the potential including the coupling to the $n\bar{n}$ channel is sufficiently attractive in each of the 2p states to give additional "inner" classically allowed regions at separations $R \leq 1$–3 fm. For s states there is no barrier and the entire region from r_a to r_2 is classically allowed. The potential has not been sketched in the neighborhood of the origin ($r < r_a$) because it is both poorly known and complex (absorptive) in this region. Particles bound in the atomic well will, in time, leak through the barrier to be pulled together by the strong attractive forces to be later annihilated within the central region. For s states the lack of a barrier makes the annihilation rate much higher than for p states. The combination of attraction and absorption makes the central region appear nearly "black"; almost all the particles which enter the region of hadronic forces are eventually absorbed. This absorption rate is the principal quantity to be calculated in this article.[2]

In Ref. 1 we calculated the annihilation widths using the WKB result: $\Gamma = \nu e^{-2I}$ where $\nu = n^{-3} m \alpha^2 \times (2\pi)^{-1}$ is the radial oscillation frequency in the atomic well. I is the usual integral over the barrier $I = \int_{r_1}^{R} \kappa \, dr$, $\kappa = ik$, where $k = [2m(E - V_{eff})]^{1/2}$, and r_1 and R are the turning points shown in Fig. 1. The calculation is based on a global form of the WKB approximation which requires the validity of WKB wave functions in each region except in the annihilation region and which assumes the ability of the WKB connection formulas to relate these wave functions. To include absorption, the WKB wave function in the inner region is assumed

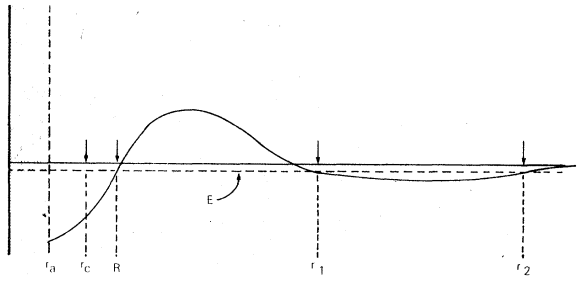

FIG. 1. Schematic drawing of the effective potential for protonium. The cross-hatched "absorptive" region is described by a boundary condition at r_c which lies in the inner classically allowed region between r_c and R. The region between r_1 and r_2 is the atomic well, and the region between R and r_1, the barrier region. The depth of the atomic well is greatly exaggerated. Typical values are $r_a \sim 0.5$ fm, $R \sim 1$–2 fm, $r_1 \sim 30$ fm, and $r_2 \sim 200$ fm for p states.

to consist of purely inward moving waves.[3] The model gives absolute predictions for linewidths of the $2p$ states of protonium once a form for the meson exchange potential is assumed. The potential is used only in regions in which it is well known: in the atomic well to calculate ν and in the barrier to calculate I.

In order to do better we can numerically solve the Schrödinger equation for the coupled $p\bar{p}$-$n\bar{n}$ system. The principal problem is to properly include the central absorptive region. The traditional methods of treating absorption are to employ either an absorptive boundary condition[4,5] or to use a complex potential[6] to describe the coupling to annihilation channels. More complete references can be found in a recent review of nucleon-antinucleon systems.[7] In this article we formulate a boundary condition model which has the following features: (a) the absorption is maximal in a WKB sense, (b) both $p\bar{p}$ and $n\bar{n}$ channels are included explicitly, and (c) the absorption is only weakly dependent on the radius at which the boundary condition is applied. Because of (c) the present formulation is nearly parameter-free in the spirit of the black sphere model,[1] provided the hadronic potential is known in outer regions ($r > r_a$).

In the next section we review the form of the Schrödinger equation for protonium and formulate the absorptive boundary condition. Results and a brief discussion are given in the final section.

II. THE MODEL

For completeness we review the equations describing protonium which were previously given in Ref. 1.

Protonium is described by the coupled channel Schrödinger equation

$$H\Psi = E\Psi\,,$$

$$\Psi = \begin{pmatrix} \psi_p \\ \psi_n \end{pmatrix} \equiv \begin{pmatrix} \psi(\bar{p}p) \\ \psi(\bar{n}n) \end{pmatrix}, \tag{1}$$

$$H = K + V = \begin{pmatrix} p^2/2m & 0 \\ 0 & p^2/2m \end{pmatrix} + \begin{pmatrix} V_c + V_0 & V_{pn} \\ V_{pn} & 2\delta m + V_0 \end{pmatrix},$$

where $m = m_p/2$, $\delta m = m_n - m_p$, $V_C = -\alpha/r$; V_0 and V_{pn} are the diagonal and the off-diagonal parts of the hadronic potential. The contribution of pion exchange to V_0 is given by the conventional form

$$V_\pi = -\tfrac{1}{3} f^2 [\vec{\sigma}_1 \cdot \vec{\sigma}_2 + Y(x) S_{12}] e^{-x}/r\,, \tag{2}$$
$$Y(x) = 1 + 3/x + 3/x^2, \quad x = m_\pi r, \quad f^2 = 0.079\,,$$

where S_{12} is the tensor operator. The off-diagonal contribution of π exchange to the potential is $V_{pn} = -2V_\pi$. In addition to π exchange we have included the isoscalar ω and σ_0 exchanges with a common mass m_ω; thus

$$V_0 \approx V_\pi - (4\pi r)^{-1} G_0^2 e^{-m_\omega r}/r, \quad G_0^2 = G_\sigma^2 + G_\omega^2\,. \tag{3}$$

This simple form for ω, σ_0 exchange is the same as was used in Ref. 1 and is justified on the basis of the insensitivity of the results to G_0^2 within reasonable limits ($G_0^2/4\pi \approx 20$–40). The vector meson exchanges are relatively unimportant for the atomic (vs quasinuclear) states calculated here.

Since the $\bar{p}p$ and $\bar{n}n$ channels are coupled only through short range strong interactions, we can write immediately the reduced wave functions (i.e., the wave function times r) for large r:

$$\psi_p(r) \approx A_p W_{\kappa\mu}(\lambda r)\,, \quad \kappa = 2m\alpha/\lambda\,, \quad \mu = l + \tfrac{1}{2}\,, \quad \lambda = (-8mE)^{1/2}\,, \tag{4}$$

where $W_{\kappa\mu}$ is Whittaker's function[8] and

$$\psi_n(r) \approx A_n r h_l^{(1)}(i\beta r)\,, \quad \beta = [2m(2\delta - E)]^{1/2}\,, \tag{5}$$

where $h_l^{(1)}$ is the spherical Hankel function.[8]

Given a trial value of the energy $E = (E_R + iE_I)$ and the relative normalization $A = A_n/A_p$ we now use Eqs. (4) and (5) to start the numerical integration of the coupled Schrödinger equation (1). We have used 14 fm as a starting point; this is substantially outside the range of the strong interactions.[9] The integration carries our solution into the inner classically allowed region in which the hadronic attraction overcomes the centrifugal barrier (See Fig. 1). As we have shown in Ref. 1 this inner region begins at a value of R between 1–3 fm for $2p$ states; this is outside the absorptive region.

The existence of this inner classically allowed interval $C \equiv [r_a, R]$ in which V is nearly real allows us to formulate incoming wave boundary conditions within the framework of the WKB approximation. At some point r_c within C we now impose a boundary condition which approximates pure absorption. The most common WKB prescription, the "continuum model,"[10] assumes that $\psi \sim \exp \times(-iKr)$ (or in terms of the logarithmic derivative $\psi'/\psi = -iK$) in the neighborhood of r_c. The constant may be taken as a parameter adjusted to maximize absorption[4] or as a local momentum.[5] Reference 5 also uses a form of the WKB approximation which incorporates the centrifugal barrier. We use a variant of this condition which also follows from the WKB approximation, but which includes the channel coupling and hadronic forces.

As a preliminary, we study the eigenvectors and eigenvalues of the potential matrix V,[1,11] with com-

ponents

$$\begin{pmatrix} V_p & V_{pn} \\ V_{pn} & V_n \end{pmatrix}, \quad V_p \equiv V_c + V_0, \quad V_n \equiv 2\delta m + V_0. \tag{6}$$

The eigenvalues of the potential matrix are

$$v_\pm = \tfrac{1}{2}(V_n + V_p) \pm \left[\left(\frac{V_n + V_p}{2}\right)^2 - V_p V_n + V_{pn}^2\right]^{1/2}. \tag{7}$$

The corresponding eigenvectors $\phi^\pm = (\phi_p^\pm, \phi_n^\pm)$ satisfy

$$\phi_n^\pm = [(v^\pm - V_p)/V_{pn}]\,\phi_p^\pm \equiv R_\pm \phi_p^\pm. \tag{8}$$

Since the eigenvectors are orthogonal and may be normalized, we can define

$$\begin{aligned} \phi_p^\pm &= (1 + R_\pm^2)^{-1/2}, \\ \phi_n^\pm &= R_\pm (1 + R_\pm^2)^{-1/2}. \end{aligned} \tag{9}$$

An overall phase function of r which is common to ϕ_p and ϕ_n can be absorbed into the expansion coefficients. Equations (9) establish the relative amounts of $\bar{p}p$ and $\bar{n}n$ in the composite wave function as a function of r. At large separations v_{pn} is negligible and we see that v_+ corresponds to the $\bar{n}n$ potential while v_- corresponds to the $\bar{p}p$ potential.[1] In the region of strong interactions $V_p \approx V_n$ holds because the Coulomb force and the n-p mass difference are relatively small compared to the hadronic potentials. This near equality, when combined with Eqs. (7) and (8), leads to the result that R_+ and R_- are nearly constant and equal to ± 1 in this region. This is merely a statement of the fact that in the absence of isospin breaking forces, the Schrödinger equation can be diagonalized in an isospin basis. Summarizing, at large separations the eigenvectors of the potential matrix correspond to a charge basis set, while at small separations they correspond to an isospin basis set.

The matrix U, whose rows are ϕ^+ and ϕ^-, is a unitary matrix which diagonalizes V. Now let us assume that in the neighborhood of the boundary radius r_c the function $U(r)$ is smooth enough that the commutator of $U(r)$ with the kinetic energy nearly vanishes:

$$[U(r), p^2/2m] \approx 0. \tag{10}$$

The validity of this assumption follows from the near constancy of $U(r)$ in the region of strong interactions, $U(r)$ being a function solely of $R_\pm$, which we have seen is nearly constant in this region. Even at larger separation we expect the approximation to be reasonable since the potentials are smoothly varying.

With this assumption, U is used to diagonalize Eq. (1) yielding the separated equations

$$\left(\frac{p^2}{2m} + v_\pm - E\right)\psi_\pm = 0, \tag{11}$$

where

$$\psi_\pm = \phi_p^\pm \psi_p + \phi_n^\pm \psi_n. \tag{12}$$

The eigenpotential V_- becomes the $p\bar{p}$ potential at large separation and is always more attractive than V_+ (note that $V_n > V_p$ for large r). This suggests that we impose boundary conditions at r_c:

(a) ψ_+ vanishes at r_c,

(b) ψ_- corresponds to incoming waves at r_c.

Condition (a) may be written as

$$\phi_p^+ \psi_p + \phi_n^+ \psi_n = 0 \quad (\text{at } r_c),$$

or, using the orthogonality of ϕ^+ and ϕ^-, as

$$\text{(a')}: \quad \psi_n/\psi_p = \phi_n^-/\phi_p^- \equiv R_-.$$

Within the framework of the WKB approximation, conditon (b) can be expressed as

$$\begin{aligned} \psi_- &\propto k_-^{-1/2} \exp\left(-i\int^r k_- dr\right), \\ k_- &= [2m(E - v_-)]^{1/2}. \end{aligned} \tag{13}$$

Differentiating, we get

$$\text{(b')}: \quad \psi_-'/\psi = -ik_- + (m/2k_-^2)\frac{dv_-}{dr}.$$

This condition may be expressed in terms of ψ_p, ψ_n by use of Eqs. (9) and (12): $\psi_- = (\psi_p + R_-\psi_n) \times (1 + R_-^2)^{-1/2}$ in the neighborhood of r_c. Equations (a') and (b') are the absorptive boundary conditions. They are valid provided the potential is sufficiently smooth in the neighborhood of the point of application. The right-hand side of (b') involves an imaginary term which is the form used in the continuum model with the parameter k_- given by the local momentum corresponding to the eigenpotential v_-. The second term, which is essential, provides a real part which depends on both centrifugal and hadronic potentials.

With the exception of the $^3P_0$ state, the turning points for p states are relatively close to the annihilation radii. Because of this, the standard WKB formula, Eq. (13), and the corresponding boundary condition (b') will be inaccurate for these states. To improve the situation we have used a generalized form of the WKB wave function which is also accurate near the turning point. As is shown in standard texts,[12] an approximate solution to the Schrödinger equation which is accurate in the classically allowed region up to a linear turning point is

$$\psi(r) \approx A\xi^{1/2} k^{-1/2} Z(\xi), \tag{14}$$

where

$$\xi = \int_R^r k\,dr\,,$$

and where R is the turning point. The function Z is a linear combination of Bessel functions of order $\frac{1}{3}$:

$$CJ_{1/3}(\xi) + DY_{1/3}(\xi)\,.$$

Far from the turning point in the classically allowed region Eq. (14) reduces to the standard WKB result (13) for suitable C and D. The correct choice of constants to give ingoing waves yields

$$Z(\xi) = J_{1/3}(\xi) - iY_{1/3}(\xi) \equiv H^{(2)}_{1/3}(\xi)\,. \qquad (15)$$

Combining (14) and (15) gives the improved form for the ingoing wave boundary condition:

$$\text{(b)}'': \quad \psi_-'/\psi_- = k[H^{(2)\prime}_{1/3}(\xi)/H^{(2)}_{1/3}(\xi)] - \tfrac{1}{2}[(k'/k) - (k/\xi)]\,.$$

This boundary condition is found to give a significantly improved stability for the eigenvalues as will be shown in the next section.

The coupled Schrödinger equation (1) was integrated inward repeatedly with (4) and (5) providing the starting values. The complex parameters A and E were varied (using a form of Newton's method) until the boundary conditions were satisfied. Finally, the point of application of the boundary condition, r_c, was varied to determine the sensitivity of E and A to this parameter.

It should be emphasized that the smoothness assumptions were applied only in the neighborhood of r_c in order to infer the boundary conditions. The full coupled equations were solved numerically from the starting radius to r_c. This frees the calculation from the use of WKB connection formulas implicit in Ref. 1.

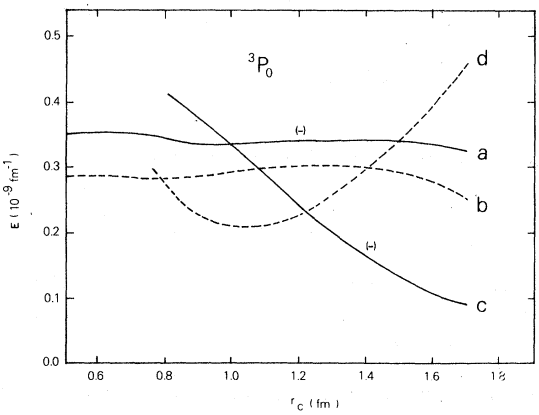

FIG. 2. Annihilation width and energy shift vs boundary condition radius r_c for the $^3P_0$ state. The classical turning point is at approximately 2.5 fm. The importance of the dv_-/dr term in Eq. (6) is illustrated. Curves (a) and (b) use the full boundary conditions and curves (c) and (d) omit the derivative term. The dashed lines give the negative of the imaginary part of E, while the solid lines give the negative of the level shift.

III. RESULTS AND DISCUSSION

Figure 2 shows the calculated energy eigenvalue for the $^3P_0$ state of protonium as a function of the

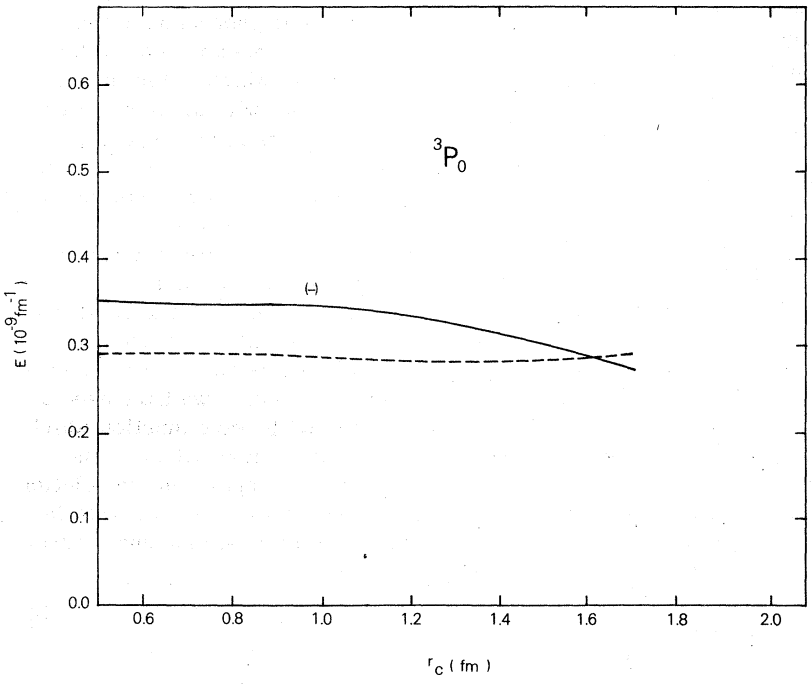

FIG. 3. Annihilation width and energy shift vs boundary condition radius r_c for the $^3P_0$ state. The boundary condition b'' is used in this and all subsequent figures. The dashed curves give the negative of the imaginary part of E. The solid lines give the real parts, with the appropriate sign indicated by the curve.

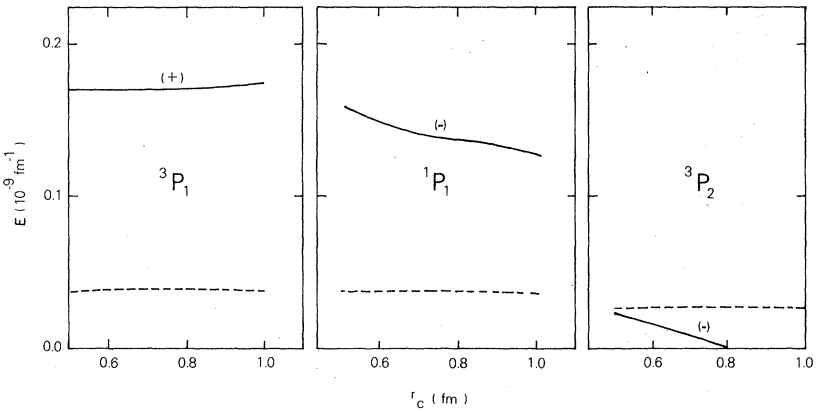

FIG. 4. Same as Fig. 3 for $^3P_2$, $^3P_1$, and $^1P_1$ states.

boundary radius r_c. The corresponding turning point is at approximately 2.5 fm. Note the constancy of both real and imaginary parts of E except as r_c approaches the turning point, where the WKB wave function used in the formulation of the boundary condition becomes invalid. In this state there is enough distance between the turning point and the annihilation radius ($r_a \sim 0.5$ fm) for $E(r_c)$ to stabilize.

We should note here that the term proportional to dv_-/dr in the boundary condition is essential for this independence. The term provides a real part which is not negligible compared to $-ik_-$. A calculation without the derivative term is also included in Fig. 2 for comparison.

Were the WKB wave functions exact, the energy and normalization constants would be rigorously independent of r_c. The observed near constancy of these quantities in an *ex post facto* verification of the adequacy of the approximation in this region. The result for the $^3P_0$ state using the improved boundary condition is shown in Fig. 3, while results for the other p states are shown in Fig. 4. Note that the imaginary parts of E are constant to a high degree of accuracy and hence the corresponding level widths $\Gamma(=-2E_I)$ are well determined. The level shifts ϵ $(=\mathrm{Re}(E) - E_{\mathrm{Bohr}})$ are not quite so well determined, although except for the $^3P_2$ state they too are at least approximately constant. In Fig. 5 the superiority of the improved boundary condition is made evident.

The linewidths and energy shifts are collected in Table I along with the widths predicted by the black sphere model of Ref. 1. The latter model is seen to give results in qualitative agreement with the present values, overestimating them somewhat. We note here that the f wave component of the $^3P_2$ state was not included in the present calculation.

Figure 6 presents the annihilation of the $^1S_0$ state using the same technique. We have chosen the $^1S_0$ rather than the coupled triplet ($^3S_1 - {}^3D_1$)

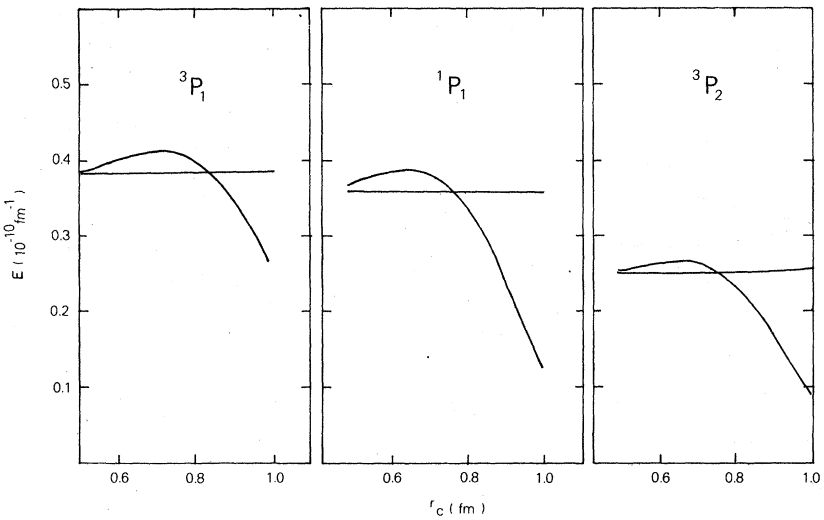

FIG. 5. Comparison of E_I for the $^3P_2$, $^3P_1$, and $^1P_1$ state using boundary condition b′ (curved lines) and b″. The latter boundary condition is valid up to the turning point and hence gives very stable results.

TABLE I. Comparison of black sphere model (Ref. 1) and the present calculation. The parameters used are $f^2 = 0.079$, $G_0^2 = 30$, $M_\omega = 783$ MeV, $m = 938/2$ MeV, $\delta m = 1.294$ MeV, $m_\pi = 137$ MeV. $R^{(1)}$ and $\Gamma^{(1)}$ are taken from Ref. 1 and $\Gamma^{(2)}$ and $\epsilon^{(2)}$ from the present model. $\epsilon^{(1)}$ vanishes in the black sphere model. The results of the $^3P_2$ calculations cannot be directly compared since the present calculation does not include the coupling to f waves.

State	$R^{(1)}$ fm	$\Gamma^{(1)}_{ann}$ (eV)	$\Gamma^{(2)}_{ann}$ (eV)	$\epsilon^{(2)}$ (eV)
$^3P_0$	2.39	0.194	0.118	−0.069
$^3P_1$	1.30	0.030	0.016	+0.035
($^3P_2$)	1.50	0.043	(0.010)	(small)
$^1P_1$	1.20	0.026	0.014	−0.028

because of its simplicity, but expect similar results for the two states. In the absence of the off-diagonal parts of the tensor force, the two states give identical results with the potential used. Unfortunately the independence of ϵ and Γ on r fails drastically at small separations ($r_c \lesssim 0.6$ fm). This failure may be a numerical artifact or may simply indicate a breakdown of the WKB approximation at small separations. In any case the meson exchange potential used is not to be trusted at separations smaller than 0.6 fm. The imaginary part of the energy eigenvalue is sufficiently stable that we can estimate E_I to be 0.25×10^{-5} fm^{-1} to about 10%. The level shift, while varying considerably over the same interval, is approximately of the same magnitude. When converted into energy and time units the results are $\Gamma(^1S_0) \approx 0.9$ keV $\approx 1.5 \times 10^{18}$ s^{-1} and $\epsilon(^1S_0) \approx 0.45$ keV. The positive sign of the shift indicates that the state is less strongly bound than in the absence of the strong interactions. The result is in reasonable accord with previous estimates.[3,13]

In conclusion, we have formulated a boundary condition model for protonium. The coupling of the $\bar{n}n$ to the $\bar{p}p$ channel is incorporated as is the strong absorption. A novel feature of the model is the approximate independence of the annihilation widths, energy shifts, and relative normalization parameter on the point at which the boundary condition is applied. The method might prove useful in other problems which involve strong absorption.

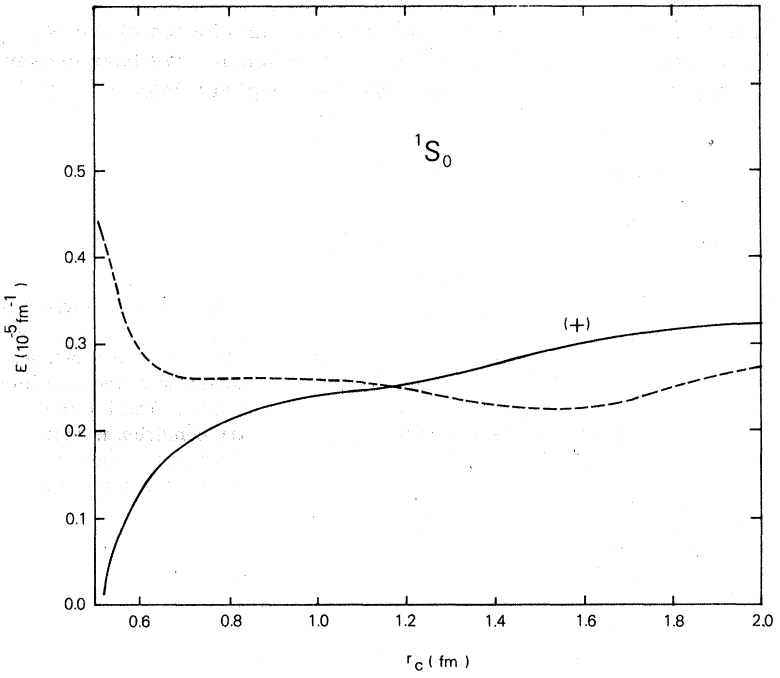

FIG. 6. Same as Fig. 3 for the $^1S_0$ state.

Work is in progress applying this model to the $\bar{p}p$ scattering problem. This, the effects of the inclusion of the off-diagonal portion of the tensor force, and alternatives to boundary condition (a) will be discussed in a subsequent article.

It is a pleasure to thank Professor H. Pilkuhn for correspondence and Dr. W. Gibbs, Dr. B. F. Gibson, and Dr. G. J. Stevenson for their hospitality at the Los Alamos Scientific Laboratory, where part of the work was done.

[1]W. B. Kaufmann and H. Pilkuhn, Phys. Rev. C 17, 315 (1978).

[2]We should also mention that in the absence of Stark mixing the competing radiative ($2p \rightarrow 1s$) transitions are approximately a factor of 100 times smaller. Thus for the p-state calculations our result is appropriate for p capture in gaseous hydrogen for which Stark mixing is small.

[3]WKB models were first proposed for $\bar{p}p$ scattering by J. S. Ball and G. Chew, Phys. Rev. 109, 1385 (1958), and for protonium by B. R. Desai, *ibid.* 119, 1385 (1960); 119, 1390 (1960).

[4]M. S. Spergel, Nuovo Cimento 47A, 538 (1967).

[5]O. D. Dalkarov and F. Myhrer, Nuovo Cimento 40A, 152 (1977).

[6]F. Myhrer and A. Gersten, Nuovo Cimento 37A, 21 (1977).

[7]I. S. Shapiro, Phys. Rep. 35C,129 (1978).

[8]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun, National Bureau of Standards Applied Mathematics Series No. 55 (U. S. G. P. O., Washington, D. C., 1964), Chaps. 9 and 13.

[9]We have also increased the initial point to 20 fm with no significant change in the energy eigenvalue.

[10]See, for example, J. Blatt and V. Weisskopf, *Theoretical Nuclear Physics* (Wiley, New York, 1952), p. 351.

[11]This method was used by R. Christian and E. Hart, Phys. Rev. 77, 441 (1950), to include coupled spin channels in nucleon-nucleon scattering.

[12]L. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), 3rd edition, p. 272. See Also Ref. 11.

[13]O. D. Dalkarov and V. M. Samoilov, Zh. Eksp. Teor. Fiz. Pis'ma Red. 16, 353 (1972) [JETP Lett. 16, 249 (1972)]. See also Ref. 7.