Faddeev calculation of e^--Ps scattering lengths

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The modified Faddeev equations in configuration space are applied to solve numerically the problem of the zero-energy elastic scattering of an electron by positronium at zero angular momentum. The singlet and triplet scattering lengths are calculated and zero-energy limits of elastic and ortho-para conversion cross sections are established. The results confirm and improve previous variational estimations of these parameters.

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I. INTRODUCTION

Since the experimental discovery of the negative ion positronium [1], the $e^-e^-e^+$ system has become a subject of intensive theoretical study. In particular, high-accuracy variational calculations of its bound state Ps^- have been performed [2]. Another problem of considerable interest is the elastic e^--Ps scattering at low energies. Theoretical calculations of the cross sections for the electron impact on Ps could provide a guide for possible experiments of fundamental interest [3,4] including tests of charge conjugation in the leptonic systems $e^-e^-e^+$ and $e^-e^-e^+$.

Previously, the low-energy e^--Ps scattering has been treated via the Kohn variational principle [3,4] and adiabatic method [5,6]. We find it worthwhile to solve the problem in a completely different way by solving the Faddeev equation in configuration space. In this paper, we apply the Faddeev approach to calculate the s-wave e^--Ps scattering lengths.

General motivation of our interest in the problem is that this is an application of the configuration space Faddeev method to scattering states of a purely Coulomb three-body system. As is known, in this case one cannot exploit directly the standard version of the Faddeev equations, for they are noncompact and should be modified via a cutoff procedure due to Merkuriev [7]. The modified Faddeev equations were established long ago but have never been solved numerically; here we will attempt to do so. We believe it will stimulate further development of the Faddeev approach in order to study more complicated processes of atomic and mesoatomic physics.

II. MODIFIED FADDEEV EQUATIONS

Throughout the paper we use the atomic units (a.u.) $\hbar=e^2=m_e=1$, so that the length unit is the Bohr radius a_0.

The particles are numbered by the label $\alpha=1,2,3$: $(e^-,e^-,e^+)=(1,2,3)$. Configuration space is parametrized by the scaled Jacobi vectors $\{\mathbf{x}_\alpha,\mathbf{y}_\alpha\}$. In our case of equal particle masses, they are related to the position vectors of the particles $\mathbf{r}_\alpha$ as follows (for $\alpha=1$):

$$\mathbf{x}_1=(\mathbf{r}_2-\mathbf{r}_3)\ , \qquad \mathbf{y}_1=\frac{2}{\sqrt{3}}\left[\mathbf{r}_1-\frac{\mathbf{r}_2+\mathbf{r}_3}{2}\right]\ . \tag{1}$$

Cyclic permutations of indices in (1) yield the Jacobi vectors with other α's. Relation between them is given by the orthogonal transform

$$\mathbf{x}_\beta=-\tfrac{1}{2}\mathbf{x}_\alpha+\epsilon_{\beta\alpha}\frac{\sqrt{3}}{2}\mathbf{y}_\alpha\ , \qquad \mathbf{y}_\beta=-\epsilon_{\beta\alpha}\frac{\sqrt{3}}{2}\mathbf{x}_\alpha-\tfrac{1}{2}\mathbf{y}_\alpha\ , \tag{2}$$

with $\epsilon_{\beta\alpha}=(-1)^{\beta-\alpha}\mathrm{sgn}(\alpha-\beta)$.

When the total angular momentum L of the system is fixed, the three-body dynamics is constrained onto three-dimensional internal space [8] which can be parametrized, for instance, by the coordinates

$$x_\alpha=|\mathbf{x}_\alpha|\ , \quad y_\alpha=|\mathbf{y}_\alpha|\ , \quad \theta_\alpha=\arccos(\hat{\mathbf{x}}_\alpha,\hat{\mathbf{y}}_\alpha)\ . \tag{3}$$

The s-wave ($L=0$) state is governed by the Hamiltonian [8]

$$H=H_0+\sum_{\alpha=1}^{3}V_\alpha(x_\alpha)\ , \tag{4}$$

where V_α stand for the potentials of the Coulomb interactions between the particles:

$$V_1(x)=V_2(x)=-\frac{1}{x}\ , \quad V_3(x)=\frac{1}{x}\ ,$$

and H_0 is the s-wave kinetic energy operator:

$$H_0=-x_\alpha^{-2}\partial_{x_\alpha}x_\alpha^2\partial_{x_\alpha}-y_\alpha^{-2}\partial_{y_\alpha}y_\alpha^2\partial_{y\alpha}-\left[\frac{1}{x_\alpha^2}+\frac{1}{y_\alpha^2}\right]\csc\theta_\alpha\partial_{\theta_\alpha}\sin\theta_\alpha\partial_{\theta_\alpha}\ . \tag{5}$$

As mentioned in the Introduction, one cannot exploit the usual form of the Faddeev equations related to the Hamiltonian (4):

$$(H_0+V_\alpha-E)\Psi_\alpha=-V_\alpha\sum_{\beta(\neq\alpha)}\Psi_\beta\ , \tag{6}$$

where Ψ_α are the Faddeev components of the total wave function. The reason for failure of Eqs. (6) is that the Coulomb potentials in the right-hand side of (6) yield a long-range coupling of the Faddeev components in the so-called three-body region where all three particles are well separated asymptotically. This results in noncompactness of Eqs. (6) in the continuum spectrum. A method to get rid of this problem is due to Merkuriev [7] and is as follows.

Each Coulomb potential is decomposed into the two parts

$$\begin{aligned} V_\alpha^{(s)}(x_\alpha,y_\alpha)&=V_\alpha(x_\alpha(x_\alpha)\zeta(x_\alpha,y_\alpha)\ ,\\ V_\alpha^{(l)}(x_\alpha,y_\alpha)&=V_\alpha(x_\alpha)[1-\zeta(x_\alpha,y_\alpha)]\ , \end{aligned} \tag{7}$$

where ζ_α is a cutoff function. Its form can be rather arbitrary within some general requirements. Namely, let Ω_α be domain of the (x_α,y_α) plane where $y_\alpha\geq x_\alpha^\nu$ with $\nu>2$. Then asymptotically, as $y_\alpha\to\infty$, the cutoff function is to achieve fast enough the limits

$$\zeta_\alpha(x_\alpha,y_\alpha)\to\begin{cases}1 & \text{if } (x_\alpha,y_\alpha)\in\Omega_\alpha\\ 0 & \text{otherwise.}\end{cases}$$

Thus $V_\alpha^{(s)}$ may be regarded as a short-range potential that vanishes asymptotically in the three-body region (where $x_\alpha\sim y_\alpha\to\infty$) whereas the long-range potential $V_\alpha^{(l)}$ goes to zero in the two-body sector Ω_α.

In terms of the potentials (7) the Hamiltonian (4) can be written as

$$H=H_{\rm as}+\sum_\alpha V_\alpha^{(s)}\ ,\quad H_{\rm as}=H_0+\sum_\alpha V_\alpha^{(l)}\ . \tag{8}$$

The operator $H_{\rm as}$ incorporates the long-range tail of the total Coulomb potential.

Using the representation (8), one now can construct the Faddeev equations in the standard way, treating $H_{\rm as}$ as an unperturbed Hamiltonian. This leads to the modified Faddeev equations

$$(H_{\rm as}+V_\alpha^{(s)}-E)\Psi_\alpha(x_\alpha,y_\alpha,\theta_\alpha)=-V_\alpha^{(s)}\sum_{\beta\neq\alpha}\Psi_\beta(x_\beta,y_\beta,\theta_\beta)\ . \tag{9}$$

The sum of the Faddeev components gives the total wave function

$$\Psi=\sum_\alpha\Psi_\alpha\ . \tag{10}$$

Note that the number of the modified Faddeev equations can be reduced from three to two when two particles are identical. For the $e^-e^-e^+$ system, these are the particles 1,2. The coordinate part of the wave function possesses additional quantum number $p=\pm1$, being parity with respect to electron exchange: $P_{21}\Psi=p\Psi$. Thus $p=+1(-1)$ for the singlet (triplet) spin state of electrons.

For fixed parity state, the Faddeev components obey the (anti) symmetry relations $P_{21}\Psi_1=p\Psi_2, P_{21}\Psi_3=p\Psi_3$ (the cutoff functions ζ_1 and ζ_2 are to be equal). In terms of the coordinates (3) they become

$$\begin{aligned}\Psi_1(x,y,\theta)&=p\Psi_2(x,y,\pi-\theta)\ ,\\ \Psi_3(x,y,\theta)&=p\Psi_3(x,y,\pi-\theta)\ .\end{aligned}$$

Therefore Eqs. (9) are reduced to the set of two equations for the components Ψ_1 and Ψ_3:

$$[H_0+V_1(x)+V_2^{(l)}(x_{21},y_{21})+V_3^{(l)}(x_{31},y_{31})-E]\Psi_1(x,y,\theta)=-V_1^{(s)}(x,y)[p\Psi_1(x_{21},y_{21},\pi-\theta_{21})+\Psi_3(x_{31},y_{31},\theta_{31})]\ , \tag{11}$$

$$[H_0+V_3(x)+V_1^{(l)}(x_{13},y_{13})+V_2^{(l)}(x_{23},y_{23})-E]\Psi_3(x,y,\theta)=-V_3^{(s)}(x,y)[\Psi_1(x_{13},y_{13},\theta_{13})+p\Psi_1(x_{23},y_{23},\pi-\theta_{23})]\ ,$$

where $x_{\beta\alpha}$, $y_{\beta\alpha}$, and $\theta_{\beta\alpha}$ stand for the coordinates x_β, y_β, and θ_β expressed through $x_\alpha=x$, $y_\alpha=y$, and $\theta_\alpha=\theta$ according to (2).

III. BIPOLAR EXPANSION

For computational purposes, once can reduce the dimension of Eqs. (9) by expanding the Faddeev components into an auxiliary basis, at the expense of dealing with an infinite number of partial equations. To this end, we make use of the bipolar expansion which has been exploited extensively in the trinucleon problem [9–11] and more recently, in the Coulomb three-body bound-state problems [12]. In our case of zero total angular momentum, this is the expansion of the Faddeev components into Legendre polynomials, the eigenfunctions of the angular part of the operator (5) being

$$\Psi_\alpha(x,y,\theta)=\sum_{\ell_\alpha}\frac{F_{\ell_\alpha}^{(\alpha)}(x,y)}{xy}\tilde P_{\ell_\alpha}(\cos\theta)\ , \tag{12}$$

where $\tilde P_\ell$ are the normalized Legendre polynomials: $\tilde P_\ell(u)=\sqrt{\ell+1/2}P_\ell(u)$.

Substituting Eq. (12) into Eqs. (11) leads one to an infinite set of two-dimensional integrodifferential equations for the partial components of Ψ_1, Ψ_3:

$$\begin{aligned}(-\Delta_{\ell_1}+V_1-E)F_{\ell_1}^{(1)}+\sum_{\ell_1'}[W_{\ell_1\ell_1'}^{(2)}+W_{\ell_1\ell_1'}^{(3)}]F_{\ell_1'}^{(1)}&=-pV_1^{(s)}\left\{\sum_{\ell_1'}(-)^{\ell_1'}\hat h_{\ell_1\ell_1'}F_{\ell_1'}^{(1)}+\sum_{\ell_3}(-)^{\ell_1}\hat h_{\ell_1\ell_3}F_{\ell_3}^{(3)}\right\}\ ,\\ (-\Delta_{\ell_3}+V_3-E)F_{\ell_3}^{(3)}+\sum_{\ell_3'}[W_{\ell_3\ell_3'}^{(1)}+W_{\ell_3\ell_3'}^{(2)}]F_{\ell_3'}^{(3)}&=-2V_3^{(s)}\sum_{\ell_1}\hat h_{\ell_3\ell_1}F_{\ell_1}^{(1)}\ ,\end{aligned} \tag{13}$$

where $-\Delta_\ell$ are the partial components of the kinetic energy operator (5):

$$-\Delta_\ell = -\partial_x^2 - \partial_y^2 + \ell(\ell+1)\left[\frac{1}{x^2}+\frac{1}{y^2}\right] .$$

The coupling due to the functions $W_{nm}^{(\alpha)}$ comes from the long-range potentials $V_\beta^{(l)}$ of Eqs. (11), for instance,

$$W_{nm}^{(2)}(x,y) = \int_{-1}^{1} du\, \tilde{P}_n(u)\tilde{P}_m(u) V_2^{(l)}(x',y') ,$$

where $u=\cos\theta$,

$$x'(x,y,u) = x_{21} = \left[\frac{1}{4}x^2 - \frac{\sqrt{3}}{2}xyu + \frac{3}{4}y^2\right]^{1/2} ,$$

$$y'(x,y,u) = y_{21} = \left[\frac{3}{4}x^2 + \frac{\sqrt{3}}{2}xyu + \frac{1}{4}y^2\right]^{1/2} . \tag{14}$$

The operators $\hat{\mathbf{h}}_{\ell\ell'}$ yield the standard integral coupling of the partial Faddeev components:

$$(\hat{\mathbf{h}}_{\ell\ell'}F)(x,y) = \int_{-1}^{1} du \frac{xy}{x'y'} \tilde{P}_\ell(u)\tilde{P}_{\ell'}(u')F(x',y') ,$$

where x',y' are defined by (14) and

$$u'(x,y,u) = \cos\theta_{21} = (2x'y')^{-1}\left[-xyu + \frac{\sqrt{3}}{2}(x^2-y^2)\right] . \tag{15}$$

In the derivation of Eqs. (13) use has been made of the symmetry relations

$$x_{31}(-u) = x_{13}(u) = x_{23}(-u) = x_{12}(-u) = x_{21}(u) = x'(u) ,$$

$$y_{31}(-u) = y_{13}(u) = y_{23}(-u) = y_{12}(-u) = y_{21}(u) = y'(u) ,$$

$$-\cos\theta_{31}(-u) = \cos\theta_{13}(u) = -\cos\theta_{23}(-u) = \cos\theta_{32}(u) = -\cos\theta_{12}(-u) = \cos\theta_{21}(u) = u' ,$$

where the functions x', y', and u' are defined in (14) and (15). These relations from (2) are responsible for sign factors by the integral terms of Eqs. (13).

In the expansion (12) for the component Ψ_1 the partial indices ℓ_1 run over all nonnegative integers ($\ell_1=0,1,2,\ldots$) whereas for the component Ψ_3 only even/odd indices are involved, depending on parity: $\ell_3=0,2,4,\ldots$ if $p=+1$ and $\ell_3=1,3,5,\ldots$ if $p=-1$.

Equations (13) are subject to the boundary conditions

$$F_{\ell\alpha}^{(\alpha)}(x=0,y) = F_{\ell\alpha}^{(\alpha)}(x,y=0) = 0 . \tag{16}$$

For the scattering problem, one also has to impose an asymptotic condition. We shall consider the problem of the zero-energy e^--Ps elastic scattering where $E=-\frac{1}{4}$ a.u. is the binding energy of the Ps ground state. In this case, all partial components vanish asymptotically except for the component $F_0^{(1)}$ which contains zero-energy asymptotic state:

$$F_{\ell\alpha}^{(\alpha)}(x,y\to\infty) \sim \begin{cases} \varphi_0(x)\left(\frac{\sqrt{3}}{2}y - A\right) & \text{if } \alpha=1, \ell_\alpha=0 \\ 0 & \text{otherwise} , \end{cases} \tag{17}$$

where φ_0 stands for the radial wave function of positronium and $\sqrt{3}y/2$ is the distance between the incoming electron and the positronium center of masses [see Eqs. (1)]. The constant A is scattering length to be calculated.

IV. RESULTS AND DISCUSSION

First, we have to fix the cutoff functions ζ_α which are input parameters of the method. Of course, the total wave function (and, therefore, scattering length) must be independent of the particular choice of the cutoff. However, one should expect that only in the limit when all partial channels of Eqs. (13) are taken into account. For a truncated set of Eqs. (13), results obtained with different cutoffs will differ, but the difference must vanish with increase of the number of partial waves included. This provides a rather strong test of the selfconsistency of the method and convergence of the bipolar expansion.

In our calculations, we take all cutoff functions to be of the same form,

$$\zeta_\alpha(x,y) = 2\left[1+\exp\left[\frac{(x/x_0)^\nu}{y/y_0+1}\right]\right]^{-1} .$$

We make the following remarks on choosing the cutoff parameters. According to the compactness requirements [7], ν must be greater than 2. There are no principal restrictions on x_0, and y_0. However, the parameter x_0 is rather important, for it determines the effective range of the short-range potentials $V_\alpha^{(s)}$. The larger x_0, the more $V_\alpha^{(s)}(x,y)$ is spread over the x axis. Thus, in order to diminish the integral coupling of the Faddeev components, x_0 should be taken small enough. But with decrease of x_0 the coupling due to the matrix elements $W_{\ell\ell'}^{(\alpha)}$ increases, so that x_0 should not be too small. Interplay of these factors determines the optimal region where x_0 is to be chosen from. We found that x_0 being around the size of the positronium atom is the optimal choice. In our calculations, we use two sets of the cutoff parameters:

$$\nu=2.3 , \quad x_0=2 , \quad y_0=10 , \tag{18}$$

$$\nu=2.6 , \quad x_0=1.8 , \quad y_0=5 . \tag{19}$$

To solve the problem (13), (16), and (17) numerically, we adopt a method proposed previously for the neutron-deuteron scattering problem [13]. It consists of the finite-difference approximation of Eqs. (13) in the Cartesian coordinates on a rectangle $Q=\{x,y\}$

$\in[0,x_{max}]\otimes[0,y_{max}]$ which is meshed by a nonuniform rectangular grid. The integral terms of Eqs. (13) are calculated by the eight-point Gauss quadruture formula with a linear interpolation of integrands in between the grid points.

At the boundaries of Q we set all partial components to be zero except for the component F_0^1 at $y=y_{max}$ where the condition $F_0^1(x,y_{max})=\varphi_0(x)$ is imposed. Thereby the asymptotic behavior (17) is ensured (up to a normalization factor) and the scattering length is derived from the y dependence of the solution in the asymptotic region. The x independence of A obtained in this way provides a stability test of the method.

Both grids in x and y are taken to be piecewise uniform with successive doubling of step at several points. To fix an adequate grid, we solve the problem with three partial channels of Eqs. (13) and vary all grid parameters until stability of result within 0.5% is achieved. A typical grid providing such an accuracy consists of $N_x\times N_y=34\times45$ points

$$x=0(0.3)4.5(0.6)12.6(1.2)21\ ,$$

$$y=0(0.4)4.4(0.8)12.4(1.6)25.2(3.2)50.8(6.4)108.4\ ,$$

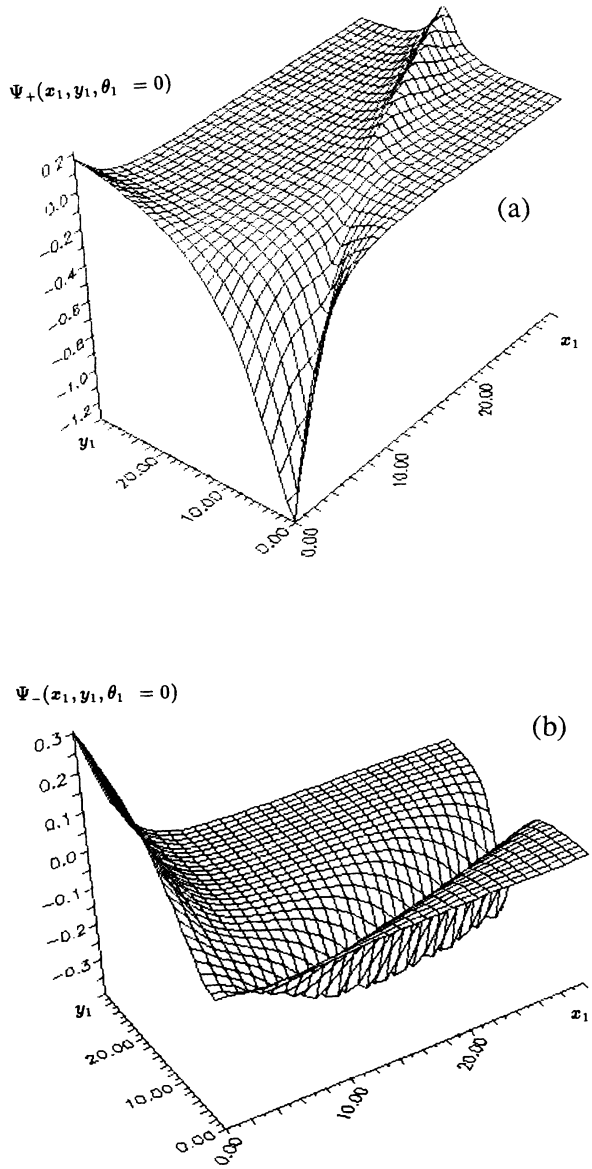

FIG. 1. The singlet (a) and triplet (b) wave functions (21) of the zero-energy e^--Ps scattering as functions of x_1,y_1 at fixed angle $\theta_1=0$.

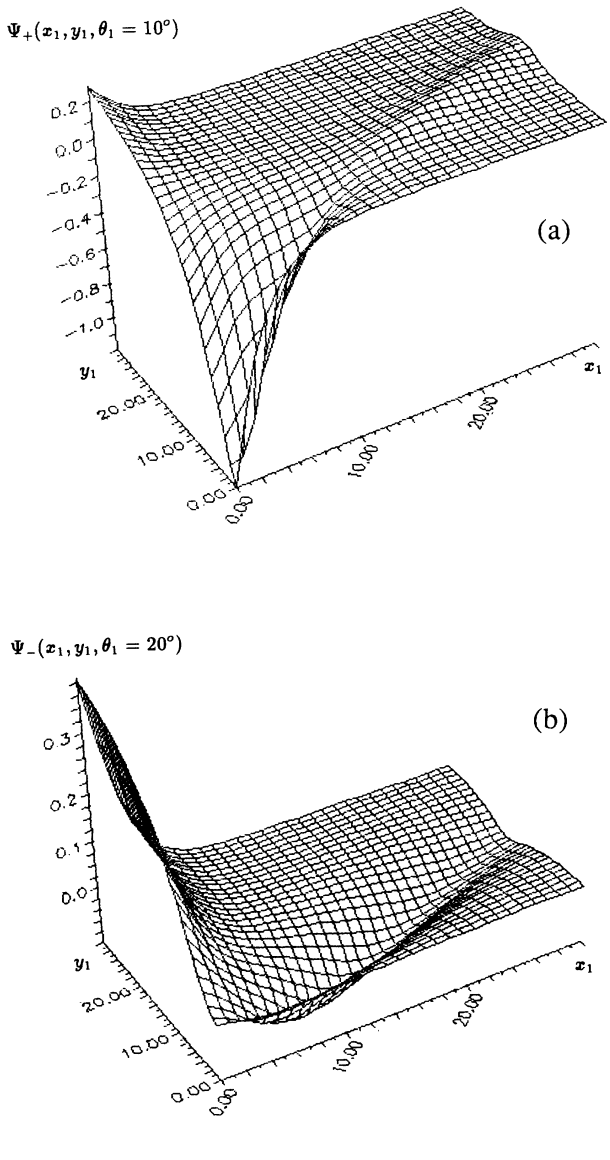

FIG. 2. (a) Singlet wave function at $\theta_1=10°$. (b) Triplet wave function at $\theta_1=20°$.

TABLE I. The singlet ($p=+1$) scattering length for two different uses of the cutoff parameters (18) (A_+) and (19) (A'_+); N is the number of partial channels of Eqs. (13) taken into account; $\{\ell_1\}$ and $\{\ell_3\}$ are corresponding sets of partial angular momenta for the components Ψ_1 and Ψ_3.

N	2	3	4	5	6	8
$\{\ell_1\}$	0	01	012	012	0123	01234
$\{\ell_3\}$	0	0	0	02	02	024
A_+ (a.u.)	16.5337	12.0560	11.9467	11.8116	11.9826	11.9846
A'_+ (a.u.)	15.9591	12.0475	11.9481	11.7851	11.9820	11.9853

where $a(h)b$ means that within the interval $[a,b]$ the grid step is h.

Tables I and II present the convergence of the scattering lengths with increase of the number of bipolar harmonics taken into account. In both the singlet and triplet cases the convergence is achieved for $N=8$ and the limiting values are fairly independent of cutoff. Thus, our final values for the scattering lengths are

$$A_+ = 11.98a_0 \ , \quad A_- = 4.78a_0 \tag{20}$$

which yield the following zero-energy limits for the total elastic and ortho-para conversion cross sections:

$$\sigma_{el}(0) = (\tfrac{1}{4}A_+^2 + \tfrac{3}{4}A_-^2)4\pi a_0^2 = 212.07\pi a_0^2 \ ,$$

$$\sigma_c(0) = \tfrac{1}{4}(A_+ - A_-)^2 \pi a_0^2 = 12.96\pi a_0^2 \ .$$

These results are in agreement with the variational estimations of Ref. [4]: $A_+ = (12.0\pm0.3)a_0$, $A_- = (4.6\pm0.4)a_0$, and $\sigma_{el}(0) = 208\pi a_0^2$.

The adiabatic calculation of Ref. [5] gives $A_+ = 13.16a_0$, $A_- = 4.90a_0$ (these numbers are derived from Table I of Ref. [5] where a different representation of the S matrix has been used). Some 10% disagreement with our result (20) in the singlet case can be accounted for by the fact that the convergence in the number of adiabatic channels is not quite achieved as is seen from Table I of Ref. [5].

Note that in Ref. [14] an estimation of the singlet scattering length was made by making use of variational wave function of the Ps^- state. Somewhat surprisingly, the result of this work $A_+ = (12.233\pm0.006)a_0$ is rather good though the accuracy seems to be overestimated.

For a better understanding of the scattering dynamics, let us now consider structure of the total wave function which is composed of the partial Faddeev components according to (10) and (12):

$$\Psi = \sum_\alpha \sum_{l_\alpha} \frac{F_{l_\alpha}^{(\alpha)}(x_\alpha, y_\alpha)}{x_\alpha y_\alpha} \tilde{P}_{l_\alpha}(\cos\theta_\alpha) \ . \tag{21}$$

TABLE II. The triplet ($p=-1$) scattering length. The same notation as in Table I.

N	2	3	4	6	8
$\{\ell_1\}$	0	01	012	0123	01234
$\{\ell_3\}$	1	1	1	13	135
A_- (a.u.)	4.8971	4.6589	4.8491	4.8091	4.7839
A'_- (a.u.)	4.9011	4.6902	4.8775	4.8209	4.7890

Figure 1 shows the singlet and triplet wave functions at fixed angle $\theta_1=0$. One can clearly see two asymptotic states propagating along the directions $x=0$ and $x=\sqrt{3}y$ on the $\{x,y\}$ plane:

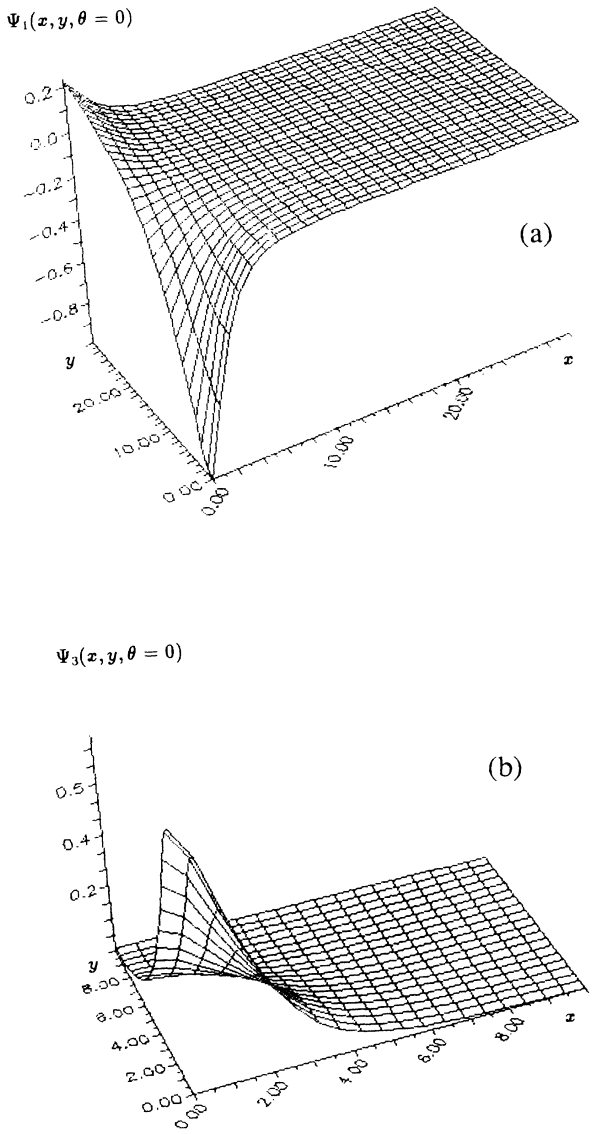

FIG. 3. The singlet Faddeev components $\Psi_1(x,y,\theta)$ (a) and $\Psi_3(x,y,\theta)$ (b) at $\theta=0$.

$$\Psi=\tilde{\varphi}_0(x)\left[1-\frac{2A_p}{\sqrt{3}y}\right]+p\tilde{\varphi}_0(x')\left[1-\frac{2A_p}{\sqrt{3}y'}\right], \quad (22)$$

where x' and y' are defined in (14) and $\tilde{\varphi}_0(x)=\varphi_0(x)/x$ is the (renormalized) positronium ground state. The direction $x=\sqrt{3}y$ corresponds to the maximum of the second two-body bound state of Eq. (21) at $x'=0$. Out of these two directions, the wave function vanishes asymptotically. Apparently, there are two different regions of configuration space: the inner domain where dynamics is essentially three body, and the asymptotic domain where one of the electrons catches the positron to form a positronium atom. The singlet wave function changes its sign when passing from one region to another. This is due to orthogonality of the scattering state to the bound state of Ps^-. Note that the inner domain is much more spread over in the case of the singlet compared to that of the triplet.

The second asymptotic state of Eq. (22) exists only at $\theta_1=0$. When $\theta_1\neq 0$, the argument x' of the positronium wave function is bounded away from zero everywhere, so that this term vanishes asymptotically. For small θ_1 it leaves a fading trace at finite distances, as is seen from Fig. 2. With further increase of θ_1 it disappears completely.

It is worthwhile to compare the complicated structure of the wave function with that of the Faddeev components (12) shown in Fig. 3 for the singlet state. The Faddeev components are rather smooth and well localized in the x axis. It illustrates the usual practical advantage of the Faddeev method compared to methods dealing with the total wave function.

There is one additional point we would like to outline. The efficiency of the bipolar expansion method depends drastically on convergence in the number of partial channels taken into account. In our case of equal particle masses the convergence turned out to be quite satisfactory. However, one might expect it to be getting worse with increase of mass differences. Recently [15], a method was proposed to overcome this shortcoming of the bipolar expansion. It consists of directly solving the three-dimensional Faddeev equations (11) via a supine expansion in all three variables. The results of Ref. [15] for the bound states of Ps^- and $pp\mu^-$ systems are rather encouraging and the approach seems to be worthwhile to apply to scattering reactions in systems like $d+(t\mu^-)$ and e^-+H.

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