Conf-950706--1

LA-UR- 95 - 790

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

TITLE: FADDEEV CALCULATION OF $p\mu + p$ COLLISIONS; EFFECT OF
HYPERFINE SPLITTING ON THE CROSS SECTIONS

AUTHOR(S): CHI-YU HU
ANDREI A. KVITSINSKY
JAMES S. COHEN

RECEIVED
MAR 10 1995
OSTI

SUBMITTED TO: JOURNAL OF PHYSICS B

MASTER

By acceptance of this article, the publisher recognizes that the U.S. Government retains a non-exclusive, royalty-free license to publish or reproduce the published form this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article's work performed under the auspices of the U.S. Department of Energy.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

12

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Faddeev calculations of $p\mu + p$ collisions: Effect of hyperfine splitting on the cross sections

Chi-Yu Hu[†], Andrei A Kvitsinsky^{†‡} and James S Cohen[§]

[†]*Department of Physics, California State University, Long Beach, California 90840, USA*

[§]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

(February 27, 1995)

Abstract

The Faddeev equations, modified to remove long-range coupling between different channels, are solved in the total-angular-momentum representation for $p\mu + p$ collisions. S-wave elastic and hyperfine-transition cross sections are calculated with and without explicit inclusion of the hyperfine splitting ΔE . For hyperfine quenching the simpler approach without hyperfine splitting is found adequate at collision energies above about ΔE , but for elastic scattering it becomes adequate at somewhat higher energies. The present cross sections tend to fall in between earlier calculations done using a large standard adiabatic expansion and those done using a two-state improved adiabatic expansion, but are closer to the former.

[‡]Permanent address: Department of Mathematical and Computational Physics, Institute for Physics, St. Petersburg State University, 198904 St. Petersburg, Russia.

PACS numbers: 36.10.Dr, 11.80.Jy, 34.40.+n, 34.50.-s

Typeset using REVTeX

I. INTRODUCTION

For three decades the Faddeev equations [1] have provided a rigorous approach to three-body scattering problems. However, the method was generally considered impractical for systems involving long-range forces, with the pure Coulomb system being most intractable. Hence the method was popular in nuclear physics but rather rare in atomic physics. Merkuriev [2] has solved this long-standing problem. In his modified Faddeev equations (MFE), the configuration space of a three-body Coulomb system is divided into a three-body sector, where all three particles are far apart, and the region of two-body clusters, where the various two-particle interactions dominate. In order to lower the dimensionality of the equations, the total-angular-momentum representation has been developed [3], which reduces the Faddeev equations to a small number of three-dimensional differential equations. For numerical solution one can then apply the bipolar expansion method [4] or a direct solution via a global spline expansion in all variables [5]. The latter approach has recently been implemented using quintic splines and applied successfully to the processes $e^- + \text{Ps}$ [5,6], $e^\pm + \text{H}$ [7], and to scattering length calculations for the symmetric mesic atomic systems [5]. In the present work, the method is applied to $p\mu + p$ scattering.

The mesic atomic collisions have usually been treated by expanding the scattering wave function in adiabatic molecular states — the method of perturbed stationary states (PSS) [8,9]. Convergence of the cross sections by that expansion is slow, typically requiring as many as 1000 states. Most of these states lie in the continuum and are necessitated by the finite mass of the muon (e.g., $m_\mu/m_p \sim 0.1$), which is neglected at zeroth order in the adiabatic representation.¹ The convergence of the adiabatic representation can be greatly accelerated by modification of the reduced mass. In the *two-state* calculation of systems like $p\mu + p$, the *effective* mass is just the reduced mass of the atom($p\mu$) + nucleus(p) instead of the reduced mass of the nuclei($p + p$) appropriate in the usual PSS method. For calculations with an

---

¹The precise masses used in the present work are $m_\mu = 206.769m_e$ and $m_p = 1836.1515m_e$.

intermediate number of states, it is not so simple, but Bracci *et al* [10] have suggested a procedure for optimizing the mass for PSS calculations involving an arbitrary finite number of basis states.

In the present work we take a different approach to improving the efficiency of treating muonic atom collisions. We use the Faddeev approach — modified for the long-range force — which naturally uses the mass physically appropriate in each scattering channel. Thus muon-exchange and hyperfine-quenching cross sections can be obtained accurately in calculations including only the two channels of experimental interest. In this respect the method is akin to the method of nonadiabatic coupled rearrangement channels, which has been successfully applied to the asymmetric collision $d\mu + t$ [11]. The formulation for the hyperfine-transition cross sections is exact with two Faddeev equations, just as the underlying Schrödinger equation is. The price that is paid for the small number of equations is their high dimensionality — they are three-dimensional differential equations. If we were to decompose these equations on a basis, we would again get an infinite set of coupled equations. Instead, our approach is not to use any intermediate decomposition but to solve the exact equations directly via a spline expansion in each coordinate. The approximation is made in using a finite number of splines.

Our main thrust in the present work is to re-examine the elastic and hyperfine-transition cross sections for $p\mu + p$ and to answer the question as to how high an energy is required before the cross sections can be simply obtained from calculations of muon exchange that ignore the splittings. The hyperfine splitting of the muonic atom ground state is

$$\Delta E(p\mu) = 0.1820 \text{ eV } (F = 0 \text{ and } 1) , \quad (1)$$

where F is the total spin of the muonic atom. The $p\mu + p$ system is of particular interest in that it is the only case where the presumably converged adiabatic representation cross sections differ significantly from the two-state adiabatic [12] and improved adiabatic [13] calculations utilizing the effective mass mentioned above.

Electron screening and molecular binding effects are not taken into account in the present

work; they are negligible at energies above about 1 eV. Also, only S waves ($J = 0$) are treated so the calculations are restricted to energies below 10 eV.

II. MODIFIED FADDEEV EQUATIONS FOR SYMMETRIC SYSTEMS

The usual Faddeev equations are rearranged in the MFE so that the right-hand sides, which couple the Faddeev amplitudes in different channels, involve only short-range interactions. Thus complete decoupling of the scattering amplitudes in different channels is accomplished in the asymptotic region. The total wave function is given by

$$\Psi = \psi_1 + \psi_2 + \psi_3, \quad (2)$$

where ψ_α is the Faddeev amplitude in channel α . The MFE for the components are

$$(H_{as} + V_\alpha^{(s)} - E)\psi_\alpha = -V_\alpha^{(s)} \sum_{\beta \neq \alpha} \psi_\beta \quad (3)$$

where the asymptotic Hamiltonian

$$H_{as} = H_0 + \sum_\alpha V_\alpha^{(l)} \quad (4)$$

includes the kinetic energy operator H_0 and the long-range potentials. A cutoff function ζ is employed to separate the short- and long-range potentials,

$$V_\alpha^{(s)}(x_\alpha, y_\alpha) = V_\alpha(x_\alpha)\zeta_\alpha(x_\alpha, y_\alpha) \quad (5a)$$

and

$$V_\alpha^{(l)}(x_\alpha, y_\alpha) = V_\alpha(x_\alpha)[1 - \zeta_\alpha(x_\alpha, y_\alpha)], \quad (5b)$$

respectively. The cutoff function used in the present work is

$$\zeta_\alpha(x_\alpha, y_\alpha) = 2 \left[1 + \exp \left(\frac{(x_\alpha/x_0)^\nu}{y_\alpha/y_0 + 1} \right) \right]^{-1}. \quad (6)$$

The parameters ν , x_0 , and y_0 are chosen such that ζ tends to unity in the limit $x_\alpha \ll y_\alpha \rightarrow \infty$ and vanishes when $x_\alpha \sim y_\alpha \rightarrow \infty$, thus providing asymptotic decoupling of the scattering

channels [2]. Here x_α and y_α are the lengths of the mass-scaled Jacobi vectors. For the present work we chose $\nu = 2.3$, $x_0 = 2.0$, and $y_0 = 5.0$. In terms of the masses m_α , position vectors $\vec{r}_\alpha$, and charges z_α of the three particles and the total mass $M = m_1 + m_2 + m_3$ $[(\alpha, \beta, \gamma) = \text{cyclic } (1, 2, 3) \text{ in the following definitions}]$,

$$\vec{x}_\alpha = \tau_\alpha(\vec{r}_\beta - \vec{r}_\gamma), \quad (7a)$$

and

$$\vec{y}_\alpha = \mu_\alpha \left(\vec{r}_\alpha - \frac{m_\beta \vec{r}_\beta + m_\gamma \vec{r}_\gamma}{m_\beta + m_\gamma} \right) \quad (7b)$$

where

$$\tau_\alpha = \sqrt{\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma}} \quad (8)$$

and

$$\mu_\alpha = \sqrt{2m_\alpha \left(1 - \frac{m_\alpha}{M} \right)}. \quad (9)$$

We also define the scaled charges

$$q_\alpha = z_\beta z_\gamma \tau_\alpha \quad (10)$$

such that the Coulomb potentials are given by

$$V_\alpha(x_\alpha) = q_\alpha / x_\alpha. \quad (11)$$

The Jacobi vectors for different channels are related by an orthogonal transformation so that

$$\vec{x}_\beta = c_{\beta\alpha} \vec{x}_\alpha + s_{\beta\alpha} \vec{y}_\alpha \quad (12a)$$

$$\vec{y}_\beta = -s_{\beta\alpha} \vec{x}_\alpha + c_{\beta\alpha} \vec{y}_\alpha \quad (12b)$$

where

$$c_{\beta\alpha} = - \left(\frac{m_\beta m_\alpha}{(M - m_\beta)(M - m_\alpha)} \right)^{\frac{1}{2}} \quad (13a)$$

and

$$s_{\beta\alpha} = (-1)^{\beta-\alpha} \text{sgn}(\alpha - \beta) (1 - c_{\beta\alpha}^2)^{\frac{1}{2}} . \quad (13b)$$

In the case of S waves, the kinetic-energy operator reduces to

$$H_0 = -x_\alpha^{-2} \partial_{x_\alpha} x_\alpha^2 \partial_{x_\alpha} - y_\alpha^{-2} \partial_{y_\alpha} y_\alpha^2 \partial_{y_\alpha} - (x_\alpha^{-2} + y_\alpha^{-2}) \csc \theta_\alpha \partial_{\theta_\alpha} \sin \theta_\alpha \partial_{\theta_\alpha} \quad (14)$$

where

$$\theta_\alpha = \arccos \left(\frac{\vec{x}_\alpha \cdot \vec{y}_\alpha}{x_\alpha y_\alpha} \right) . \quad (15)$$

For the $p + p\mu$ system in which particles 1 and 2 (the nuclei) are identical, we have

$$\psi_1(x, y, \theta) = \wp \psi_2(x, y, \pi - \theta) \quad (16)$$

where $\wp = \pm 1$ for antisymmetric and symmetric spin states of the identical nuclei, as required to give the correct overall symmetry of the total wave function. Owing to the repulsion between the nuclei, two-body bound states are not formed in channel 3 and explicit use of channel 3 is obviated. Thus further simplification can be achieved by choosing the cutoff functions such that

$$\zeta_1 = \zeta_2 \equiv \zeta \quad (17a)$$

and

$$\zeta_3 \equiv 0 . \quad (17b)$$

The MFE then reduce to just one equation,

$$\left[H_0 + V_1(x_1) + V_3(x_{31}) + V_2^{(i)}(x_{21}, y_{21}) - E \right] \psi_1(x_1, y_1, \theta_1) = -\wp V_1^{(s)}(x_1, y_1) \psi_1(x_{21}, y_{21}, \pi - \theta_{21}) , \quad (18)$$

where $x_{\beta\alpha}$, $y_{\beta\alpha}$, and $\theta_{\beta\alpha}$ are the coordinates in channel β expressed through those of channel α by (12). The total wave function is

$$\Psi = \psi_1 + \psi_2 = (1 + P_{12})\psi_1 \quad (19)$$

where P_{12} is the operator interchanging particles 1 and 2 (protons). Below excitation channels, the asymptotic conditions are

$$\psi_1(x_1, y_1, \theta_1)_{y_1 \rightarrow \infty} \sim \frac{1}{k_1 y_1} \varphi_0(x_1) [\sin(k_1 y_1) + \tan \delta \cos(k_1 y_1)] \quad (20a)$$

and

$$\psi_1(x_1, y_1, \theta_1)_{x_1 \rightarrow \infty} \sim 0 \quad (20b)$$

where $\varphi_0(x_1)$ is the ground-state wave function of muonic atom, δ is the phase shift, and k_1 is the momentum conjugate to y_1 .

In order to facilitate numerical procedures, a scaled wave function is defined such that

$$\phi(x, y, \theta) = xy\psi_1(x, y, \theta) = \varphi(x) \frac{\sin ky}{k} - F(x, y, \theta) . \quad (21)$$

Here we have introduced $\varphi(x) = x\varphi_0(x)$ as the scaled two-body ground-state wave function.

In terms of the scattering amplitude $F(x, y, \theta)$, Eq. (18) becomes

$$[\widetilde{H}_0 + V_1(x) + W(x, y, \theta) - E] F(x, y, \theta) + \wp \frac{xy}{x_{21}y_{21}} V_1^{(s)}(x, y) F(x_{21}, y_{21}, \pi - \theta_{21}) = g \quad (22)$$

where

$$W(x, y, \theta) = V_3(x_{31}) + V_2(x_{21})[1 - \zeta(x_{21}, y_{21})] , \quad (23)$$

$$\widetilde{H}_0 = -\partial_x^2 - \partial_y^2 - \left(\frac{1}{x^2} + \frac{1}{y^2} \right) \csc \theta \partial_\theta \sin \theta \partial_\theta , \quad (24)$$

and

$$g = \varphi(x) \frac{\sin ky}{k} W(x, y, \theta) + \wp \frac{xy}{x_{21}y_{21}} \varphi(x_{21}) \frac{\sin(ky_{21})}{k} V_1^{(s)}(x, y) . \quad (25)$$

In the numerical procedure, we introduce new variables t and r related to x and y by the nonlinear mapping

$$x(t) = \frac{1}{\lambda} \ln \left(\frac{1}{1-t} \right) \quad (26a)$$

and

$$y(r) = h \left[\left(1 + \frac{y_{\max}}{h} \right)^r - 1 \right] . \quad (26b)$$

Thus the variable domains are changed from $\{x, y\} \in [0, \infty] \times [0, y_{\max}]$ to $\{t, r\} \in [0, 1] \times [0, 1]$, and the grid distribution can be changed easily by adjusting the mapping parameters λ and h . The logarithmic mapping $t \rightarrow x$ is suitable for bound states, and the parameter λ is chosen to give the exact two-body binding energy E_0 . The exponential mapping $r \rightarrow y$ gives the y -grid a geometrical progression, which is suitable for the scattering dynamics along y .

The asymptotic conditions (20) are imposed at finite $y = y_{\max}$ with a large enough $y_{\max}$ to yield a stable solution. In terms of the new variables, the boundary conditions on $F(t, r, \theta)$ are

$$F|_{t=0} = F|_{r=0} = 0 , \quad (27a)$$

$$\partial_t^n F|_{t=1} = 0 \quad (\text{for } n = 0, 1) , \quad (27b)$$

$$\partial_\theta F|_{\theta=0, \pi} = 0 , \quad (27c)$$

$$F|_{r=1} = -\frac{\tan \delta}{k} \cos(ky_{\max}) , \quad (27d)$$

$$\partial_r F|_{r=1} = -\frac{\tan \delta}{k} \partial_r \cos(ky)|_{y=y_{\max}} , \quad (27e)$$

and

$$\partial_r^2 F|_{r=1} = -\frac{\tan \delta}{k} \partial_r^2 \cos(ky)|_{y=y_{\max}} . \quad (27f)$$

III. FADDEEV EQUATIONS INCLUDING THE HYPERFINE INTERACTION

The representation of the wave function described in Sec. II ignores the hyperfine effect but is expected to be suitable for energies large compared with the hyperfine splitting. Otherwise the Faddeev component ψ_1 involves the spin degree of freedom explicitly and becomes the vector

$$\psi_1 = \chi_1 \phi_1 + \chi_2 \phi_2 \quad (28)$$

where χ_1 and χ_2 are the spin-coupled functions of the nucleus and the muon and ϕ_1 and ϕ_2 are the spatial parts of the Faddeev component.

With the hyperfine interaction included, the three-body functions χ_i correspond to fixed spins of the particles 2 and 3 (nucleus and muon). For $pp\mu$ they are given by

$$\chi_1 = \frac{1}{\sqrt{6}}[(++-) + (+-+) - 2(-++)] \quad (\text{for } S_{23} = 0) \quad (29a)$$

and

$$\chi_2 = \frac{1}{\sqrt{2}}[(++-) - (+-+)] \quad (\text{for } S_{23} = 1) \quad (29b)$$

where, for instance, $(++-) \equiv |\uparrow\rangle_1 |\uparrow\rangle_2 |\downarrow\rangle_3$. The Faddeev equation becomes

$$(H_0 + V_1 + V^{(\text{hf})} + W_1 - E)\psi_1 = -(V_1^{(s)} + V^{(\text{hf})})P_{12}\psi_1 \quad (30)$$

which differs from Eq. (18) by the presence of the potential of hyperfine interaction $V^{(\text{hf})}$ between particles 2 and 3.

Calculating matrix elements of the operator P_{12} in the spin basis yields

$$\langle \chi_1 | P_{12} | \chi_1 \rangle = -\langle \chi_2 | P_{12} | \chi_2 \rangle = -\frac{1}{2} \quad (31a)$$

and

$$\langle \chi_1 | P_{12} | \chi_2 \rangle = \langle \chi_2 | P_{12} | \chi_1 \rangle = \frac{\sqrt{3}}{2}. \quad (31b)$$

Therefore, upon projecting on χ_i , Eq. (30) goes over into a set of two coupled equations for spatial components of (28)

$$(H_0 + V_1 + W_1 + \Delta_1 - E)\phi_1 = -(V_1^{(s)} + \Delta_1)P_{12} \left(-\frac{1}{2}\phi_1 + \frac{\sqrt{3}}{2}\phi_2 \right) \quad (32a)$$

$$(H_0 + V_1 + W_1 + \Delta_2 - E)\phi_2 = -(V_1^{(s)} + \Delta_2)P_{12} \left(\frac{\sqrt{3}}{2}\phi_1 + \frac{1}{2}\phi_2 \right). \quad (32b)$$

The Δ_i are matrix elements of the potential $V^{(\text{hf})}$ which is diagonal in the spin basis χ_i ; i.e.,

$$\langle \chi_i | V^{(\text{hf})} | \chi_j \rangle = \delta_{ij} \Delta_i. \quad (33)$$

Rigorously speaking, the Δ_i depend on the internuclear distance, but the effect of the variation has been demonstrated to be negligibly small [16]. We now make use of the standard approximation that reduces hyperfine effects in the three-body problem to the energy splitting of the two states. Namely, we neglect the terms Δ_i in the r.h.s. of Eqs. (32) whereas in the l.h.s., we replace them by constants $\Delta_1 = 0$ and $\Delta_2 = \Delta E$, where $\Delta E > 0$ is the splitting between singlet ($F = 0$) and triplet ($F = 1$) hyperfine states of the muonic atom given in Eq. (1).

This leads to the coupled equations

$$(H_0 + V_1 + W_1 - E)\phi_1 = -V_1^{(s)}P_{12} \left(-\frac{1}{2}\phi_1 + \frac{\sqrt{3}}{2}\phi_2 \right) \quad (34a)$$

$$(H_0 + V_1 + W_1 + \Delta E - E)\phi_2 = -V_1^{(s)}P_{12} \left(\frac{\sqrt{3}}{2}\phi_1 + \frac{1}{2}\phi_2 \right). \quad (34b)$$

The scattering problem for these equations is solved numerically in the framework of the K -matrix approach.

IV. RELATION BETWEEN RESULTS OBTAINED WITH AND WITHOUT HYPERFINE SPLITTING

If the hyperfine splitting is neglected, the K -matrix associated with Eqs. (34) is related (approximately) to that of Eq. (18) by a unitary transformation

$$\mathbf{K} \equiv \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} = \mathbf{U} \begin{bmatrix} K_+ & 0 \\ 0 & K_- \end{bmatrix} \mathbf{U}^\dagger \quad (35)$$

where

$$K_\pm = \tan \delta_\pm . \quad (36)$$

For $p\mu + p$ ($s_{nuc} = \frac{1}{2}$)

$$\mathbf{U} = \frac{1}{2} \begin{bmatrix} 1 & -\sqrt{3} \\ \sqrt{3} & 1 \end{bmatrix} \text{ for } S = \frac{1}{2} \quad (37a)$$

and

$$\mathbf{U} = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} \text{ for } S = \frac{3}{2} . \quad (37b)$$

The $\mathbf{U}$ matrices apply to even J (including S waves calculated in the present work); the $\mathbf{U}$ matrices for odd J are the same *except* with the matrix columns interchanged.

Note that the operator $\mathbf{U}$ diagonalizes the r.h.s. of Eqs. (34),

$$\mathbf{U}^\dagger \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix} \mathbf{U} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} . \quad (38)$$

Upon the unitary transform, Eqs. (34) go over into two decoupled equations (18) for two different parity states with $\varphi = \pm 1$ being the eigenvalues of (38). Thus properly normalized solutions of Eqs. (34) and (18) are related by the transform $\Phi = \mathbf{U}\Phi_0\mathbf{U}^\dagger$, where Φ is a 2×2 matrix composed of two independent solutions to Eqs. (34) and $\Phi_0 (= \text{diag}(\Phi_+, \Phi_-))$ is that for Eqs. (18). Since both Φ and Φ_0 are fixed by the asymptotics corresponding to the K -matrix formalism, the same transformation relates the K -matrices. Note that the transformation (35) for the K matrix is the same as that derived in Ref. [17] for the adiabatic potential curves.

The partial cross sections for total angular momentum J and total spin S are given by

$$\sigma_{ij}^{JS} = \frac{4\pi}{k_i^2} W_{JS} \left| \left(\frac{\mathbf{K}^{JS}}{1 - i\mathbf{K}^{JS}} \right)_{ij} \right|^2 \quad (39a)$$

$$= \frac{4\pi}{k_i^2} W_{JS} \frac{\delta_{ij} D_{JS}^2 + (K_{ij}^{JS})^2}{(D_{JS} - 1)^2 + (K_{11}^{JS} + K_{22}^{JS})^2} \quad (39b)$$

where

$$D_{JS} = K_{11}^{JS} K_{22}^{JS} - (K_{12}^{JS})^2 \quad (40)$$

and

$$W_{JS} = \frac{(2J+1)(2S+1)}{(2F+1)(2s_{\text{nuc}}+1)} \quad (41)$$

The total cross section is

$$\sigma_{ij} = \sum_{J,S} W_{JS} \sigma_{ij}^{JS} \quad (42)$$

V. NUMERICAL PROCEDURE

The numerical solution of the scattering equations is achieved using quintic spline expansions and a collocation procedure on each of the three variables t , r , and θ . The explicit form of the quintic splines can be found in Ref. [14]. They are composed of three basic piecewise fifth-order polynomials called the cardinal basis $\phi_{i\sigma}(\sigma = 0, 1, 2)$ and are nonzero only on adjoining intervals (r_{i-1}, r_{i+1}) , where $r_0 (= 0), r_1, r_2, \dots, r_k$ are the natural knots of the variable r . They satisfy the conditions [15]

$$\partial_r^\sigma \phi_{i\sigma'}(r_i) = \delta_{\sigma,\sigma'}, \quad \sigma, \sigma' = 0, 1, 2; \quad i = 0, 1, 2, \dots, k. \quad (43)$$

These properties ensure the continuity of the wave function, as well as its first and second derivatives, across the natural knots.

The total number of splines needed to cover all the intervals in the variable r is $3k + 3$. Three of the splines are eliminated in the first and the last intervals to satisfy boundary conditions. Therefore for the variable r the expansion involves $3k$ splines with $3k$ unknown

coefficients. The collocation procedure with three Gaussian quadrature points per interval provides the $3k$ equations required to determine the unknown coefficient.

We adopt the notation

$$(s_1, s_2, \dots, s_M) \equiv (\phi_{i\sigma}, \sigma = 0, 1, 2; i = 0, 1, \dots, k) \quad (44)$$

where $M = 3k$. The scattering amplitude in the three-dimensional spline expansion is expanded as

$$F(t, r, \theta) = \sum_{l=1}^L \sum_{m=1}^M \sum_{n=1}^N f_{lmn} s_l(t) s_m(r) s_n(\theta) \quad (45)$$

where L , M , and N each equals $3k$ but k can be different for different variables. Upon substitution of (45) into Eq. (22), this procedure reduces the problem to a set of linear inhomogeneous equations for the coefficient f_{lmn} .

In S-wave scattering, $F(t, 1, \theta)$ is independent of t and θ . The phase shift δ can be obtained using Eqs. (27).

VI. RESULTS AND CONCLUSIONS

One of the principal motivations for the present work was to check the problematic convergence of the $p\mu + p$ cross sections at low energy. The previous calculations of Bracci *et al* [9] were done with a large (still incomplete, of course) adiabatic expansion using the customary reduced mass; those of Cohen [13] were done with two improved-adiabatic states using a compensatory reduced mass. Of all the muonic hydrogen atoms it is only in the case of $p\mu + p$ collisions that the large and the (compensated) small cross-section calculations differ significantly. The present and two previous results, in terms of the reactance matrix K , are presented in Table I. In most cases the present values lie in between the previous pair but generally closer to the large expansion. We conclude that those calculations [9] are reasonably well converged and are reliable for general use. They, as well as those in Ref. [13], are carried out for all partial waves and spin states.

The unusual sensitivity of the $p\mu + p$ cross sections to the physical representation is likely due to the existence of a virtual state of even parity close to threshold [18]. The position of the virtual state is sensitive to the mass ratio m_p/m_μ as well as to mixing with higher states, and its proximity to threshold allows it to greatly affect the low-energy cross sections.

At sufficiently high energies the hyperfine splitting is expected to be negligible. Setting the splitting to zero implies a condition of exact resonance, which allows the scattering to be treated by two uncoupled Faddeev equations (formulation of Sec. II) instead of two coupled equations (formulation of Sec. III). As is evident by comparing the formulations in Sec. II and Sec. III, this condition considerably simplifies the calculation. Results for $p\mu + p$ are given in Table II in this approximation. The phase shifts designated by subscripts + and - correspond to the decoupled states, which are of *gerade* and *ungerade* spatial symmetry. The K -matrix elements, easily obtained from these phase shifts using Eqs. (35)–(37a), are also given.

In Table III and in Figs. 1–3 the cross sections with and without hyperfine splitting are compared for $p\mu + p$ collisions. The two are in fair agreement at energies several times the hyperfine splitting [given in Eq. (1)] but differ greatly at lower energies. Evidently the neglect of the hyperfine splitting becomes a reasonable approximation for the inelastic cross section at lower collision energy than for the elastic cross sections. Already at $E \approx \Delta E$ (with respect to the excited state) it is within about 20% of the accurate value.

Another important factor governing the threshold behavior of the cross sections is the virtual state of the $pp\mu$ system, mentioned above, which is very close to the $F = 0$ threshold. It manifests itself in large values of all cross sections at very low energies (Figs. 1–3), and in typical resonance-like structures of the reactance matrix elements shown in Figs. 4–6, with a sharp slope at $E = 0$. It can be clearly seen that the hyperfine splitting somewhat damps the resonant behavior of the elastic cross sections as it does the reactance matrix elements. The reason is that turning on the hyperfine splitting is equivalent to adding a repulsive potential to the three-body Hamiltonian, which pushes the virtual state away from the threshold. That is also why the hyperfine splitting effects, which are negligible in the cross sections at

$E > 2$ eV, are yet distinguishable in the diagonal elements of the reactance matrix at rather higher energies; even at $E \gg \Delta E$, the hyperfine splitting effects are strongly magnified by changing the position of the virtual state.

ACKNOWLEDGMENTS

This work was supported by National Science Foundation Grant No. PHY-9013072, the San Diego Supercomputer Center, and the U.S. Department of Energy.

REFERENCES

- [1] Faddeev L D 1960 *Zh. Eksp. Teor. Fiz.* **39** 1459 (*Sov. Phys.—JETP* **12** 1014)
- [2] Merkuriev S P 1977 *Theor. Math. Phys.* **32** 187
 — 1980 *Ann. Phys. (N.Y.)* **130** 395
- [3] Kvitsinsky A A, Kostykin V V and Merkuriev S P 1990 *Fiz. Elem. Chastits At. Yadra* **21** 1301 (*Sov. J. Part. Nucl.* **21** 553)
- [4] Kvitsinsky A A, Carbonell J and Gignoux C 1992 *Phys. Rev. A* **46** 1310
- [5] Kvitsinsky A A and Hu C-Y 1993 *Phys. Rev. A* **47** 994
- [6] Hu C-Y and Kvitsinsky A A 1994 *Phys. Rev. A* **50** 1924
- [7] Kvitsinsky A A, Wu A and Hu C-Y 1995 *J. Phys. B: At. Mol. Opt. Phys.* to be published
- [8] Melezhik V S 1988 *Muon Catal. Fusion* **2** 117
- [9] Bracci L, Chiccoli C, Fiorentini G, Melezhik V S, Pasini P, Ponomarev L I and Wozniak J 1989 *Muon Catal. Fusion* **4** 247
- [10] Bracci L, Chiccoli C, Pasini P, Fiorentini G, Melezhik V S and Wozniak J 1990 *Nuovo Cimento* **105B** 459
- [11] Kino Y and Kamimura M 1993 *Hyperfine Interact.* **82** 45
- [12] Bubak M and Faifman M P 1987 *Communications of the Joint Institute for Nuclear Research* No. E4-87-464 (Dubna: JINR)
- [13] Cohen J S 1991 *Phys. Rev. A* **43** 4668
- [14] Hu C-Y and Kvitsinsky A A 1993 *Hyperfine Interact.* **82** 59
- [15] Prenter P M 1975 *Splines and Variational Method* (New York: Wiley)
- [16] Cohen J S 1991 *Phys. Rev. A* **44** 2836

[17] Gershtein S S 1958 *Zh. Eksp. Teor. Fiz.* **34** 463 (*Sov. Phys.—JETP* **7** 318)

[18] Zel'dovich Ya B and Gershtein S S 1960 *Usp. Fiz. Nauk* **71** 581 (*Sov. Phys. Usp.* **3** 593)

FIGURES

FIG. 1. Elastic cross section (in units of 10^{-20} cm^2) for $p\mu(\uparrow\downarrow) + p$, calculated with and without the hyperfine splitting.

FIG. 2. Hyperfine-quenching cross section (in units of 10^{-20} cm^2) for $p\mu(\uparrow\uparrow) + p \rightarrow p\mu(\uparrow\downarrow) + p$, calculated with and without the hyperfine splitting.

FIG. 3. Elastic cross section (in units of 10^{-20} cm^2) for $p\mu(\uparrow\uparrow) + p$ ($S = \frac{1}{2}$ only), calculated with and without the hyperfine splitting.

FIG. 4. The reactance matrix element K_{11} calculated with and without the hyperfine splitting.

FIG. 5. The reactance matrix element K_{12} calculated with and without the hyperfine splitting.

FIG. 6. The reactance matrix element K_{22} calculated with and without the hyperfine splitting.

TABLES

TABLE I. K -matrix elements for $p\mu + p$ scattering with $S = \frac{1}{2}$ and $J = 0$. Index 1 is for the $F = 0$ state; 2 is for $F = 1$. The energy is relative to the $F = 1$ state.

E (eV)		$K_{11}^{0\frac{1}{2}}$	$K_{12}^{0\frac{1}{2}} (= K_{21}^{0\frac{1}{2}})$	$K_{22}^{0\frac{1}{2}}$
0.005	Present	0.07184	0.10036	0.05914
	Ref. [9]	0.06528	0.09476	0.05694
	Ref. [13]	0.084	0.108	0.066
0.01	Present	0.07098	0.1186	0.08237
	Ref. [9]	0.06570	0.1132	0.08010
	Ref. [13]	0.085	0.129	0.092
0.02	Present	0.07215	0.1423	0.1159
	Ref. [9]	0.06663	0.1358	0.1122
	Ref. [13]	0.086	0.155	0.130
0.05	Present	0.07683	0.1850	0.1828
	Ref. [9]	0.06897	0.1748	0.1732
	Ref. [13]	0.090	0.199	0.201
0.1	Present	0.07568	0.2193	0.2425
	Ref. [9]	0.07187	0.2144	0.2366
	Ref. [13]	0.094	0.243	0.276
0.2	Present	0.08330	0.276	0.3361
	Ref. [9]	0.07539	0.2662	0.3163
	Ref. [13]	0.100	0.299	0.370
0.5	Present	0.08157	0.3586	0.4555
	Ref. [9]	0.07644	0.3546	0.4391
	Ref. [13]	0.103	0.392	0.509
1.0	Present	0.06371	0.4270	0.5330
	Ref. [9]	0.05966	0.4279	0.5205

	Ref. [13]	0.086	0.464	0.595
2.0	Present	0.01205	0.4866	0.5612
	Ref. [9]	0.01288	0.4919	0.5564
	Ref. [13]	0.033	0.521	0.620
5.0	Present	-0.1535	0.5302	0.4543
	Ref. [9]	-0.1515	0.5356	0.4525
	Ref. [13]	-0.137	0.556	0.500
10.0	Present	-0.3899	0.5670	0.2628
	Ref. [9]	-0.4008	0.5652	0.2492
	Ref. [13]	-0.381	0.578	0.284

TABLE II. The $J = 0$ phase shifts (in rad) and corresponding $S = \frac{1}{2}$ K -matrix elements for $p\mu + p$ scattering without hyperfine interaction. Index 1 is for the $F = 0$ state; 2 is for $F = 1$.

E (eV)	$\delta_+^{(0)}$	$\delta_-^{(0)}$	$K_{11}^{0\frac{1}{2}}$	$K_{12}^{0\frac{1}{2}} (= K_{21}^{0\frac{1}{2}})$	$K_{22}^{0\frac{1}{2}}$
0.01	0.1240	-0.0147	0.02012	0.06033	0.08978
0.02	0.1736	-0.0208	0.02820	0.08494	0.1263
0.05	0.2665	-0.0331	0.04339	0.1326	0.1965
0.10	0.3602	-0.0473	0.05868	0.1836	0.2707
0.20	0.4699	-0.0679	0.07592	0.2494	0.3639
0.50	0.6145	-0.1127	0.09154	0.3546	0.5009
1.00	0.6935	-0.1667	0.08157	0.4328	0.5813
2.00	0.7248	-0.2496	0.03021	0.4938	0.6004
5.00	0.6705	-0.4198	-0.1365	0.5367	0.4832
10.00	0.5383	-0.6138	-0.3792	0.5637	0.2717

TABLE III. Partial cross sections (in units of 10^{-20} cm^2) for $p\mu + p$ ($S = \frac{1}{2}$, $J = 0$) with and without hyperfine splitting (hfs). Index 1 designates $F = 0$; 2 designates $F = 1$. Energies are measured relative to the the $F = 1$ state. Entries are present results except where otherwise indicated.

$E \text{ (eV)}$	$\sigma_{11}^{0\frac{1}{2}}$		$\sigma_{21}^{0\frac{1}{2}}$			$\sigma_{22}^{0\frac{1}{2}}$		
	No hfs	With hfs	No hfs	With hfs		No hfs	With hfs	
				Present	Ref. [9]		Present	Ref. [9]
0.01	19.92	12.67	177.60	670.37	626.5	393.50	326.58	316.9
0.02	19.43	12.39	173.41	473.76	443.3	383.57	317.59	306.0
0.05	18.11	12.17	161.97	306.16	282.5	356.51	302.57	280.9
0.10	16.29	10.00	145.96	205.22	202.1	318.65	254.71	249.8
0.20	13.65	9.43	121.95	148.12	143.8	261.99	224.16	207.4
0.50	9.64	7.37	82.14	86.15	87.41	168.14	144.61	139.9
1.00	7.48	6.53	53.40	53.96	55.79	101.91	90.59	89.46
2.00	6.77	6.54	31.81	31.87	33.14	53.67	49.51	49.87
5.00	7.30	7.32	14.62	14.55	15.02	18.21	17.05	17.34
10.00	7.83	7.90	7.76	7.80	7.89	6.12	6.03	5.88

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6