[28]Experience shows that problems of this type are not very sensitive to the detailed form of the closed-channel function, provided that the regularity condition (Eq. B7) is satisfied. In fact, if all the coefficients $(a, b, \ldots, \bar{a}, \bar{b}, \ldots)$ in Eq. (B10) are omitted, the phase shifts are unaffected, although the asymptotic oscillations of g_L are not correctly represented.

[29]T. F. O'Malley, L. Rosenberg, and L. Spruch, Phys. Rev. 125, 1300 (1962).

Faddeev Equations for Atomic Problems and Solutions for the (e,H) System*

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Solutions of the Faddeev equations for Coulomb potentials are investigated. A method which is of practical use for solving the Faddeev equations below the three-particle breakup threshold is developed. As an example, the method is applied to the (e, H) system in which the H^- bound state and the lowest members of the resonances in both the singlet and the triplet $J = 0$ series are calculated. The results are in good agreement with the experimental measurements and previous calculations which used conventional methods.

I. INTRODUCTION

The nonrelativistic three-body problem with two-body interactions has been formulated by Faddeev[1,2] in a way that allows straightforward computations. For short-range forces, the Faddeev equations have been applied successfully to a number of problems.[3-13] It is the purpose of this paper to show that the Faddeev equations are equally applicable to atomic problems as long as the total energy is below the three-body breakup threshold – for example, the calculation of three-body bound states and resonance energies and wave functions below the ionization energy. The significant advantage of the Faddeev equation over conventional methods is that the wave functions are calculated systematically along with the energy levels. No trial wave function is needed in the computation. Although this paper only contains a few illustrative examples all dealing with the e-H problem, we believe that the Faddeev equation has a considerably wider range of applicability. A brief account of this work was presented recently at the Leningrad Conference.[14]

In Sec. II, we give a simple derivation of the Faddeev equation, and review the method of reduction with respect to angular momentum. The method of solution is presented in Sec. III and applied to the H^- problem in Sec. IV. A discussion of possible extensions is given in Sec. V.

II. THE FADDEEV EQUATIONS

A. Formal Derivation

The scattering matrix $T(s)$ for the three-particle system with two-body interactions is a solution of the equation

$$T(s) = V + VG_0(s)T(s), \tag{2.1}$$

with $V = \sum_i V_i \; (V_i \equiv V_{jk})$, (2.2)

$$G_0(s) = (s - H_0)^{-1}, \tag{2.3}$$

where the three particles are labeled by i, j, and k, and $G_0(s)$ is the free three-particle Green's function. The "off-shell" scattering matrix $T_i(s)$ arising from the two-body potential V_i above is given by the Lippmann-Schwinger equation

$$T_i(s) = V_i + V_i G_0(s) T_i(s) . \tag{2.4}$$

Since V_i acts only on two particles, the third particle is therefore left as a spectator in Eq. (2.4). Equation (2.4), in effect, is equivalent to the equation for two-particle scattering matrix; the presence of the spectator particle gives rise to merely a shift in the energy scale.

Now we decompose the three-particle scattering matrix $T(s)$ into three components

$$T(s) = T^{(1)}(s) + T^{(2)}(s) + T^{(3)}(s) , \tag{2.5}$$

where $$T^{(i)}(s) = V_i + V_i G_0(s) T(s) . \tag{2.6}$$

As it stands, Eq. (2.6) is a set of integral equations with each $T^{(i)}$ coupled to all three operators $T^{(j)}$, $j = 1$, 2, and 3. The main difference between these equations and the Faddeev equations is that, in the latter, each $T^{(i)}$ is only coupled to two $T^{(j)}$'s with $j \neq i$, and as a result, the kernel of the integral equation is less singular. We give here a simple derivation of the Faddeev equations:

Define the expression

$$\Omega = T^{(i)}(s) - T_i(s) - \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s) . \tag{2.7}$$

One can readily show by utilizing Eqs. (2.4)–(2.6) that

$$\Omega = V_i + \sum_{j=1}^{3} V_i G_0 T^{(j)} - V_i - V_i G_0 T_i - \sum_{j \neq i}^{3} V_i G_0 T^{(j)} - \sum_{j \neq i}^{3} V_i G_0 T_i G_0 T^{(j)} = V_i G_0 \Omega . \tag{2.8}$$

Since $V_i G_0(s)$ is not the identity operator, Eq. (2.8) implies that $\Omega = 0$ for each i. We then obtain for $T^{(i)}(s)$ the equations

$$T^{(i)}(s) = T_i(s) + \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s), \quad i = 1, 2, 3, \tag{2.9}$$

which are the well-known Faddeev equations.[1] In the matrix form:

$$\begin{pmatrix} T^{(1)}(s) \\ T^{(2)}(s) \\ T^{(3)}(s) \end{pmatrix} = \begin{pmatrix} T_1(s) \\ T_2(s) \\ T_3(s) \end{pmatrix} + \begin{pmatrix} 0 & T_1(s) & T_1(s) \\ T_2(s) & 0 & T_2(s) \\ T_3(s) & T_3(s) & 0 \end{pmatrix} G_0(s) \begin{pmatrix} T^{(1)}(s) \\ T^{(2)}(s) \\ T^{(3)}(s) \end{pmatrix} . \tag{2.10}$$

This is a coupled set of integral equations in five variables. Since no approximation is made on this formal transformation, the solution of Eq. (2.10) yields $T^{(1)}$, $T^{(2)}$, and $T^{(3)}$ whose sum is the exact solution of the original equation (2.1).

The Faddeev equations can also be interpreted diagrammatically. Let us represent T_1 by the sum of the diagrams as shown in Fig. 1 and similarly for T_2 and T_3. For the T's with a superscript, we use the symbols shown in Fig. 2. The Faddeev equations are then given by Fig. 3. One can easily see that the iterative solution of the three equations in Fig. 3 using the equation in Fig. 1 reproduces all the diagrams in perturbation theory. Our formal derivation given earlier simply shows that the Eqs. in Fig. 3 are valid even if the perturbation series fails to converge. In the diagrammatic representation, it is physically evident that $T^{(1)}$ is that part of the full three-body T matrix where particles 2 and 3 undergo a final-state interaction. Since T_i already represent a complete sequence of two-body interactions, each $T^{(i)}$ can only couple to $T^{(j)}$, $j \neq i$. As mentioned earlier, this decoupling of $T^{(i)}$ from itself results in a less singular kernel as compared to the original equation (2.6). This is due to the fact that each T_i is associated with a δ function corresponding to the momentum conservation of the ith particle, and the decoupling removes the repeated δ functions.

B. Three-Body Kinematics

To reduce the Faddeev equations, a suitable set of basis variables must first be chosen. For this purpose, the momentum representation is adopted. Let the masses and asymptotic momenta of the three particles be denoted by m_1, m_2, and m_3, and $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$, respectively. An appropriate set of basis variables may be constructed by taking certain combinations of the momenta in the center-of-mass system of the three particles. For $T^{(1)}$, the suitable basis variables are the pair of independent momentum

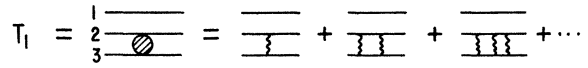

FIG. 1 Diagrams for the two-body scattering matrix T_i. The wavy lines represent the two-particle potential V_1.

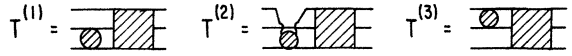

FIG. 2 Symbols representing the three-body scattering matrix $T^{(i)}$ with a pair of particles undergoes a final-state interaction.

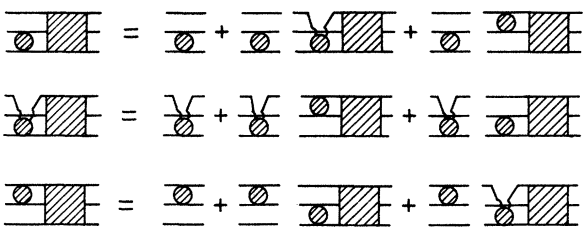

FIG. 3 Diagrammatical representation of the Faddeev equations. The gap between two diagrams represents a a noninteracting three-body Green's function.

variables.[3]

$$\vec{p}_1=[m_3\vec{k}_2-m_2\vec{k}_3]/[2m_2m_3(m_2+m_3)]^{1/2},\quad \vec{q}_1=[m_1(\vec{k}_2+\vec{k}_3)-(m_2+m_3)\vec{k}_1]/[2m_1(m_2+m_3)(m_1+m_2+m_3)]^{1/2}, \tag{2.11}$$

and their conjugated pairs $\vec{p}_2\vec{q}_2$ and $\vec{p}_3\vec{q}_3$ which are obtained by a cyclic interchange of subscripts in Eqs. (2.11) are the appropriate sets for $T^{(2)}$ and $T^{(3)}$ respectively.

The nonrelativistic kinetic energy in the center-of-mass frame may be written in any pair of basis variables;

$$H_0=p_1^2+q_1^2=p_2^2+q_2^2=p_3^2+q_3^2. \tag{2.12}$$

Consequently, the corresponding state vector $|\vec{k}_1\vec{k}_2\vec{k}_3\rangle$ may be represented in several equivalent forms

$$|\vec{k}_1\vec{k}_2\vec{k}_3\rangle=|\vec{p}_1\vec{q}_1\rangle_1=|\vec{p}_2\vec{q}_2\rangle_2=|p_3q_3\rangle_3, \tag{2.13}$$

where the extra subscript keeps track of the proper pair of basis variables.

These sets of basis momentum variables are linearly dependent on each other. The relations are summarized below.

$$\vec{p}_1=-\alpha_{12}\vec{p}_2-\beta_{12}\vec{q}_2=-\alpha_{13}\vec{p}_3+\beta_{13}\vec{q}_3,\quad \vec{q}_1=\beta_{12}\vec{p}_2-\alpha_{12}\vec{q}_2=-\beta_{13}\vec{p}_3-\alpha_{13}\vec{q}_3, \tag{2.14a}$$

$$\vec{p}_2=-\alpha_{21}\vec{p}_1+\beta_{21}\vec{q}_1=-\alpha_{23}\vec{p}_3-\beta_{23}\vec{q}_3,\quad \vec{q}_2=-\beta_{21}\vec{p}_1-\alpha_{21}\vec{q}_1=\beta_{23}\vec{p}_3-\alpha_{23}\vec{q}_3, \tag{2.14b}$$

$$\vec{p}_3=-\alpha_{32}\vec{p}_2+\beta_{32}\vec{q}_2=-\alpha_{31}\vec{p}_1-\beta_{31}\vec{q}_1,\quad \vec{q}_3=-\beta_{32}\vec{p}_2-\alpha_{32}\vec{q}_2=\beta_{31}\vec{p}_1-\alpha_{31}\vec{q}_1, \tag{2.14c}$$

where $$\alpha_{ij}\equiv[m_im_j/(m_i+m_k)(m_j+m_k)]^{1/2},\quad \beta_{ij}\equiv(1-\alpha_{ij}^2)^{1/2} \tag{2.15}$$

We will frequently interchange these basis momentum variables among different sets for convenience.

C. Separation of Angular Momentum

A separation of the angular momentum states in the Faddeev equations can be carried out using the relative angular momentum of two particles, which is combined with the angular momentum of the third particle in the over-all center-of-mass system.[8,15] In this decoupling scheme, the state vector $[\vec{p}_i,\vec{q}_i\rangle_i$ may be expanded in terms of a set of orthonormal partial-wave states $|p_i l m_l, q_i L m_L\rangle_i$. Since the total angular momentum J is conserved, we may in general consider the states to be diagonal in J. These states are given by

$$|pqJMlL\rangle_i=(-)^{L-l-M}(2J+1)^{\frac{1}{2}}\sum_{m_lm_L}\begin{pmatrix}J & l & L\\ -M & m_l & m_L\end{pmatrix}|plm_l,qLm_L\rangle_i, \tag{2.16}$$

with

$$|plm_l,qLm_L\rangle_i=Y_{lm_l}(\hat{p})Y_{Lm_L}(\hat{q})|\vec{p},\vec{q}\rangle_i, \tag{2.17}$$

$${}_i\langle plm_l,qLm_L|p'l'm_{l'},q'L'm_{L'}\rangle_i=(pq)^{-2}\,\delta(p-p')\,\delta(q-q')\,\delta_{ll'}\,\delta_{LL'}\,\delta_{m_lm_{l'}}\,\delta_{m_Lm_{L'}}, \tag{2.18}$$

where the Wigner $3j$ symbol is adopted for the Clebsch-Gordan coefficients.

The Faddeev equations [Eqs. (2.9)] may be written in this representation as

$$\Psi_\alpha^{(i)}(p,q,s) = \Phi_\alpha^{(i)}(p,q,s) + \tfrac{1}{4}\sum_{\alpha_j}\sum_{j\neq i}\int_0^\infty dp_j^{\,2}\int_0^\infty dq_j^{\,2}\,\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j)[p_jq_j/(p_j^{\,2}+q_j^{\,2}-s)] \times \Psi_{\alpha_j}^{(j)}(p_j,q_j,s)\,, \tag{2.19}$$

$$\text{with}\quad \Psi_\alpha^{(i)}(p,q,s) \equiv {}_i\langle pq\alpha\,|\,T^{(i)}(s)\,|\vec{k}_1\vec{k}_2\vec{k}_3\rangle, \tag{2.20}$$

$$\Phi_\alpha^{(i)}(p,q,s) \equiv {}_i\langle pq\alpha\,|\,T_i(s)\,|\vec{k}_1\vec{k}_2\vec{k}_3\rangle, \tag{2.21}$$

$$\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j) \equiv {}_i\langle pq\alpha\,|\,T_i(s)\,|\,p_jq_j\alpha_j\rangle_j\,, \tag{2.22}$$

where for convenience the discrete quantum numbers ($JMlL$) are collectively denoted by α. The physical interpretation of the equations is straightforward. The quantity $\Psi_{\alpha_i}^{(i)}(p_iq_is)$ represents the contribution to the three-particle scattering amplitude in which particles j and $k(j\neq k\neq i)$ undergo final-state interaction with relative angular momentum l_i. The quantity $\Phi_{\alpha_i}^{(i)}(p_i\,q_i\,s)$ represents the scattering amplitude in which particle i acts as a spectator. The initial state which is denoted by $|\vec{k}_1\vec{k}_2\vec{k}_3\rangle$ is arbitrary. The quantity p is proportional to the magnitude of the relative momentum between particles j and k, and the quantity q is proportional to the magnitude of the momentum of particle i in the three-particle center-of-mass frame.

Utilizing Eqs. (2.16)–(2.18), we obtain for the kernel $\mathcal{K}_j^{(i)}$ [defined in Eq. (2.22)] the expression

$$\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j) = (-)^{L+L'-l-l'}\sum_{\substack{m_lm_L\\ m_{l'}m_{L'}}}\begin{pmatrix} J & l & L\\ -M & m_l & m_L\end{pmatrix}\begin{pmatrix} J & l' & L'\\ -M & m_{l'} & m_{L'}\end{pmatrix} \times\int d\hat{p}_j\,d\hat{q}_j\,d\hat{p}_i\,d\hat{q}_i\;{}_i\langle\vec{p}\,\vec{q}\,|\,T_i(s)\,|\,\vec{p}_j\,\vec{q}_j\rangle_j\,(2J+1)Y^*_{lm_l}(\hat{p}_i)Y^*_{Lm_L}(\hat{q}_i)Y_{l'm_{l'}}(\hat{p}_j) \times Y_{L'm_{L'}}(\hat{q}_j)\,. \tag{2.23}$$

Since T_i involves only two-body potential V_i [see Eq. (2.4)], the matrix element ${}_i\langle\vec{p}\,\vec{q}\,|\,T_i(s)\,|\vec{p}_i\,\vec{q}_j\rangle_j$ in Eq. (2.23) may be reduced to a two-particle matrix element. According to Eqs. (2.3), (2.12), and (2.13), we have

$${}_i\langle\vec{p}\,\vec{q}\,|\,T_i(s)\,|\vec{p}_j\,\vec{q}_j\rangle_j = {}_i\langle\vec{p}\,\vec{q}\,|\,T_i(s)\,|\,p_iq_i\rangle_i = \delta(\vec{q}-\vec{q}_i)\,\langle\vec{p}\,|\,\tilde{T}_i(s-q^2)\,|\vec{p}_i\rangle\,, \tag{2.24}$$

$$\text{with}\quad \delta(\vec{q}-\vec{q}_i) = 2q^{-1}\delta(q^2-q_i^{\,2})\,\delta(\cos\theta_{\vec{q}}-\cos\theta_{\vec{q}_i})\,\delta(\varphi_{\vec{q}}-\varphi_{\vec{q}_i})\,, \tag{2.25}$$

where $\tilde{T}_i$ is the two-particle scattering matrix in the Hilbert space of the two-particle states. We may make use of the decomposition

$$\langle\vec{p}\,|\,\tilde{T}_i(s-q^2)\,|\vec{p}_i\rangle = -\frac{1}{2\pi^2}\sum_{l=0}^{\infty}(2l+1)\,P_l(\cos\theta_{\vec{p}\,\vec{p}_i})\,t_l^{(i)}(p,p_i;s-q^2)\,, \tag{2.26}$$

where the scattering amplitude between particles j and k with angular momentum l is normalized according to the equation

$$t_l^{(i)}(p,p;p^2) = e^{i\delta_l}(\sin\delta_l)/p\,. \tag{2.27}$$

Here p^2 is the two-body center-of-mass energy.

When Eqs. (2.24)–(2.26) are utilized, the kernel in the Faddeev equations may be written as[8]

$$\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j) = \int_{-1}^{1} d\cos\theta_{\vec{q}_j\vec{p}_j}\,A_{\alpha\alpha_j}(\theta_{\vec{p}_i\vec{p}_j},\theta_{\vec{q}_i\vec{p}_j},\theta_{\vec{q}_j\vec{p}_j})\,\delta(q^2-q_i^{\,2})t_l^{(i)}(p,p_i;s-q^2) \tag{2.28}$$

$$\text{with } A_{\alpha\alpha'}(\theta_{\vec{q}_j\vec{p}_j})=\frac{(-)^{L+L'-l-l'+1}}{q}16\pi^{\frac{1}{2}}(2l'+1)^{\frac{1}{2}}\delta_{JJ'}\delta_{MM'}\sum_{\bar{m}_l\bar{m}_L\bar{m}_{L'}}\begin{pmatrix} l & L & J \\ m_l & m_L & -m_{L'}\end{pmatrix}\begin{pmatrix} l' & L' & J' \\ 0 & \bar{m}_{L'} & -\bar{m}_{L'}\end{pmatrix}$$

$$\times Y^*_{l\bar{m}_l}(\theta_{\vec{p}_i\vec{p}_j},0)Y^*_{L\bar{m}_L}(\theta_{\vec{q}_i\vec{p}_j},0)Y_{L'\bar{m}_{L'}}(\theta_{\vec{q}_j\vec{p}_j},0)\,, \tag{2.29}$$

where $\theta_{\vec{q}_j\vec{p}_j}$, for example, is the angle between momentum variables $\vec{q}_j$ and $\vec{p}_j$. It should be noted that these angles are related through the relations between different sets of pair momentum variables [see Eqs. (2.14)].

The above result was derived for any angular momentum state J of the three-particle system. For convenience, we will consider explicitly only states corresponding to zero total angular momentum. For this $J=0$ case, $\alpha=(00ll)\equiv l$, and Eq. (2.29) becomes

$$A_{ll'}(\theta_{\vec{q}_j\vec{p}_j})=\frac{2(-)^{l+l'}}{\pi q}(2l+1)^{\frac{1}{2}}(2l'+1)^{\frac{1}{2}}p_l(\cos\theta_{\vec{q}_i\vec{p}_i})p_{l'}(\cos\theta_{\vec{q}_j\vec{p}_j}), \tag{2.30}$$

with $p_i^2=p_j^2+q_j^2-q^2$ and

$$\cos\theta_{\vec{q}_i\vec{p}_i}=(ij)\frac{[\alpha_{ij}^2(q_j^2-q^2)+\beta_{ij}^2(q^2-p_j^2)]}{2\alpha_{ij}\beta_{ij}qp_i}\,, \tag{2.31}$$

$$\cos\theta_{\vec{p}_j\vec{q}_j}=(ij)\frac{[\beta_{ij}^2p_j^2+\alpha_{ij}^2q_j^2-q^2]}{2\alpha_{ij}\beta_{ij}p_jq_j}\,, \tag{2.32}$$

where (ij) denotes that $(12)=(23)=(31)=1$ and $(21)=(32)=(13)=-1$.

Substituting Eq. (2.28) with $A_{ll'}$ given by Eq. (2.30) back into Eq. (2.19), and integrating over the angles, we obtain for the Faddeev equations

$$\Psi_l^{(i)}(p,q,s)=\Phi_l^{(i)}(p,q,s)+\sum_{j\neq i}\sum_{l'=0}\int_0^\infty dq_j^2\int_{L_{ij}}^{U_{ij}}dp_j^2$$
$$\times\frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{\frac{1}{2}}P_l(\cos\theta_{\vec{p}_i\vec{q}_i})P_{l'}(\cos\theta_{\vec{p}_j\vec{q}_j})}{4\pi\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)}$$
$$\times t_l^{(i)}(p,p_i;s-q^2)\Psi_{l'}^{(j)}(p_j,q_j,s)\,,\quad i=1,2,3 \tag{2.33}$$

$$\text{with } U_{ij}=(\alpha_{ij}q_j+q)^2/\beta_{ij}^2\,,\quad L_{ij}=(\alpha_{ij}q_j-q)^2/\beta_{ij}^2\,. \tag{2.34}$$

It is clear that if $t_l^{(i)}(p,p_i;s-q^2)$ is expanded in a sum of terms separable in p and p_i, then the p dependence of $\Psi_l^{(i)}(p,q,s)$ becomes explicit (p does not appear in the kinematic functions or the limits of integrations), and the coupled integral equations in two variables [Eq. (2.33)] can be reduced to equations of one variable.[10,12] We will consider the application of these equations to three-particle atomic systems in which the interaction proceeds through two-body Coulomb potentials between each pair of particles.

III. THE METHOD OF SOLUTION

A. Eigenfunction Expansion for "Off-Shell" Amplitude

As mentioned before, the partial-wave Faddeev equations of two variables may be reduced to equations of one variable if the "off-shell" two-body scattering amplitudes t_l are represented in sums of separable terms. In general, if the two-body potentials $V_l^{(i)}$ for a system are given, the two-body amplitude $t_l^{(i)}$ can be obtained from the solution of the Lippmann-Schwinger equation

$$t_l^{(i)}(p,p';E)=V_l^{(i)}(p,p')+\pi^{-1}\int_0^\infty dp''^2\,p''V_l^{(i)}(p,p'')t_l^{(i)}(p'',p';E)/(p''^2-E)\,. \tag{3.1}$$

Since the argument E is replaced by $(s-q^2)$ in the Faddeev equations, it is negative-definite provided the three-particle energy s is below the three-particle threshold ($s=0$). For negative values of E, the $(p''^2-E)^{-1}$ term in Eq. (3.1) is nonsingular, and it is well known that the solution for $t_l^{(i)}$ can be expressed

in terms of eigenfunctions of the homogeneous portion of Eq. (3.1).

The solution $\phi_{nl}^{(i)}$ of the homogeneous Lippmann-Schwinger equation and the corresponding eigenvalues $\lambda_{nl}^{(i)}$ are defined by

$$\lambda_{nl}^{(i)}(E)\phi_{nl}^{(i)}(p,E)=\pi^{-1}\int_0^\infty dp''^2\,[p''V^{(i)}(p,p'')/(p''^2-E)]\,\phi_{nl}^{(i)}(p'',E), \tag{3.2}$$

with the orthonormality property

$$\pi^{-1}\int_0^\infty dp''^2\,p''\phi_{nl}^{(i)}(p'',E)\phi_{ml}^{(i)}(p'',E)/(p''^2-E)=\delta_{nm}\,. \tag{3.3}$$

Since $\phi_{nl}^{(i)}$ constitutes a complete set, the two-body amplitude $t_l^{(i)}$ can be expanded in the form

$$t_l^{(i)}(p,p';E)=\sum_{n=0}^{\infty} C_{nl}^{(i)}(p',E)\phi_{nl}^{(i)}(p,E)\,. \tag{3.4}$$

Substitution of (3.4) into Eq. (3.1) yields, with the help of Eqs. (3.2) and (3.3),

$$t_l^{(i)}(p,p';E)=\sum_{n=0}^{\infty}\{\lambda_{nl}^{(i)}(E)/[1-\lambda_{nl}^{(i)}(E)]\}\,\phi_{nl}^{(i)}(p,E)\,\phi_{nl}^{(i)}(p',E)\,. \tag{3.5}$$

This is the desired representation for $t_l^{(i)}$ in the sums of separable terms.

In momentum representation, the Coulomb potential is

$$V_l^{(i)}(p,p')=-(Z_i\mu_i^{\frac{1}{2}}/\sqrt{2}\,pp')Q_l(p^2+p'^2)/2pp'\,, \tag{3.6}$$

where the Q_l's are the Legendre functions of the second kind, μ_i is the reduced mass, and Z_i is the product of the charges (i.e., Z_jZ_k) of the two particles. For this potential the eigenfunction $\phi_{nl}^{(i)}$ and the eigenvalue $\lambda_{nl}^{(i)}$ are both known analytically.[16] We have

$$\phi_{nl}^{(i)}(p,E)=[N_{nl}(E)p^l/(p^2-E)^{l+1}]\,C_{n-l-1}^{\,l+1}[(p^2+E)/(p^2-E)],\quad n>l \tag{3.7}$$

and $$\lambda_{nl}^{(i)}(E)=-Z_i\mu_i^{\frac{1}{2}}/n\sqrt{-2E}\,, \tag{3.8}$$

where $n>l$ and the normalization constant is

$$N_{nl}(E)=[2^{4l+3}n(n-l-1)!/\Gamma(n+l+1)]^{\frac{1}{2}}\,l!\,(-E)^{(2l+3)/4}\,. \tag{3.9}$$

The $C_{m-1}^{\,l+1}(x)$'s in Eq. (3.7) are the Gegenhauer polynomials[17]

$$C_{m-1}^{l+1}(x)=\frac{\Gamma(m+2l+1)}{\Gamma(m)\Gamma(2l+2)}\,F\left(m+2l+1,1-m;\,l+\tfrac{3}{2};\,\tfrac{1}{2}(1-x)\right)=\sum_{\gamma=0}^{m-1}a_\gamma^{(l+1)}(m)\left(\frac{x-1}{2}^{\gamma}\right), \tag{3.10}$$

with $$a_\gamma^{(l+1)}(m)=[2(m+2l+\gamma)(m-\gamma)/\gamma(2l+2\gamma+1)]\,a_{\gamma-1}^{(l+1)}(m)\,, \tag{3.11}$$

where the recursion relation for the a's starts with

$$a_0^{(l+1)}(m)\equiv(m+2l)!/(2l+1)!\,(m-1)!\,. \tag{3.12}$$

B. Coupled Single-Variable Integral Equations

Utilizing the separable representation [Eq. (3.5)] for the off-shell two-particle amplitude, the p dependence of $\Psi_\alpha^{(i)}(p,q,s)$ can now be made explicit. Let us return to the Faddeev equations for total $J=0$. From Eq. (2.33), it is clear with the help of Eq. (3.5) that $\Psi_l^{(i)}(p,q,s)$ can be expressed as

$$\Psi_l^{(i)}(p,q,s)=\Phi_l^{(i)}(p,q,s)+\sum_n\{\lambda_{nl}^{(i)}\;(s-q^2)/[1-\lambda_{nl}^{(i)}(s-q^2)]\}\phi_{nl}^{(i)}\;(p,s-q^2)\chi_{nl}^{(i)}(q,s)\,. \tag{3.13}$$

Substituting Eq. (3.13) into Eq. (2.33), we obtain a set of coupled single-variable integral equations for $\chi_{nl}^{(i)}(q,s)$:

$$\chi_{nl}^{(i)}(q,s)=\eta_{nl}^{(i)}(q,s)+\sum_{n',l';j\neq i}\int_0^\infty dq_j^{\,2}\,\mathcal{K}_{nl,nl'}^{(i,j)}(q,q_j;s)\chi_{n'l'}^{(j)}(q_j,s),\quad i=1,2,3 \tag{3.14}$$

with $$\eta_{nl}^{(i)}(q,s)=\sum_{l',j\neq i}\int_0^\infty dq_j^{\,2}\int_{L_{ij}}^{U_{ij}} dp_j^{\,2}\,\frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{\frac{1}{2}}}{4\pi\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)}P_l(\cos\theta_{\vec{p}_i\vec{q}_i})P_{l'}(\cos\theta_{\vec{p}_j\vec{q}_j})$$

$$\times\phi_{nl}^{(i)}(p_i,s-q^2)\phi_{l'}^{(j)}(p_j,q_j), \tag{3.15}$$

$$\mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j;s)=\int_{L_{ij}}^{U_{ij}} dp_j^{\,2}\,\frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{\frac{1}{2}}P_l(\cos\theta_{\vec{p}_i\vec{q}_i})P_{l'}(\cos\theta_{\vec{p}_i\vec{q}_j})}{4\pi\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)[1-\lambda_{n'l'}^{(j)}(s-q_j^2)]}$$

$$\times\phi_{nl}^{(i)}(p_i,s-q^2)\lambda_{n'l'}^{(j)}(s-q_j^2)\phi_{n'l'}^{(j)}(P_j,s-q_j^2). \tag{3.16}$$

Equations (3.14) are the basic working equations. We will now examine their physical implications.

Let us first examine the singularities of the kernel $\mathcal{K}$ given by Eq. (2.16). For negative values of s, two-particle bound states of the system (if they exist) play an important role in the analytic structure of the kernel $\mathcal{K}$. Denote the two-particle bound-state energy by $-\epsilon$. For each such two-particle state, there is a corresponding eigenvalue λ which equals to unity at $-\epsilon$. The denominator $1-\lambda_{n'l'}^{(j)}(s-q^2)$ in the kernel then vanishes at $q^2=s+\epsilon$ for $s>-\epsilon$, therefore creating a branch point for $\chi_{nl}^{(i)}(q,s)$ at $s=-\epsilon$. Three-particle bound states can only occur below the branch points. The region between the lowest and the next branch points is the energy region for purely elastic scattering of a particle by a two-particle system in its ground state. A single inelastic process occurs above the second threshold, and so forth. By solving the Faddeev equations, we can obtain bound-state and resonance energies and wave functions below the three-particle breakup threshold.

Now if there is no two-particle bound state between any pair of particles in the three-particle system, the behavior of the kernel $\mathcal{K}$ becomes less complicated, since in this case the kernel is pure real below $s=0$. Again, Eqs. (3.14) can be solved in a straightforward manner for both the energies and wave functions of any possible three-particle bound states.

It should be noted, however, that if the total energy s is positive (i.e., above the three-particle breakup threshold), then there is a region $0<q^2<s$ where the two-particle energy $s-q^2$ is positive and the expansion for the off-shell two-particle amplitude [Eq. (3.5)] in general fails to converge. The method discussed above becomes unsuitable. This includes the problems of three-particle breakup such as, for example, the ionization of hydrogen atoms by electron impact.

We remark here that, for the Coulomb interaction, the two-body T matrix $t_l(p,p',E)$ is singular at $p^2=E$, $p'^2=E$ or $p=p'$ for all E. The first two regions are inaccessible below the three-particle threshold (ionization energy), because E is negative-definite while p and p' are positive. The region $p=p'$ is accessible but the kernel $\mathcal{K}_{nl,n'l'}(q,q_j;s)$ is already the result of an integration over p_j^2. Since the singularity at $p=p'$ is only logarithmatic, the kernel no longer contains such a logarithmatic singularity. This, we believe, is the reason why the three particle atomic problem can be handled by the Faddeev equations without further modification, as long as the total energy is below the three-particle breakup threshold.

So far the initial states of the three-particle system are left unspecified. This is possible because the kernel of the integral equation is independent of the initial state, and the energy spectrum of the three-body system is determined entirely by the kernel. The specification of the initial state and the corresponding inhomogeneous terms are, however, of importance for the wave function of the scattering problem. We now show how this term may be calculated.

For a physical scattering process, one usually has an initial state consisting of two interacting subsystems; in the present case, a particle plus a two-particle subsystem in certain bound state. For definiteness, we consider an initial state consisting of particle 1 and a bound state of (2,3) with energy s_0 and angular momentum l_0. The corresponding inhomogeneous term takes the form [see Eqs. (2.21), (2.24), and (2.26)]

$$\Phi_{l_0}^{(1)}(p,q,s)\underset{q_0^2\to(s-s_0)}{=}-\frac{4}{\pi q}t_{l_0}^{(1)}(p,p_0,s-q_0^2)\delta(q^2-q_0^2), \tag{3.17}$$

where p_0 and q_0 are the p and q of the initial state. Since $t_{l_0}^{(1)}$ has a pole at $s - q_0^2 = s_0$, $\Phi_{l_0}^{(1)}(p,q,s)$ can be rewritten as

$$\Phi_{l_0}^{(1)}(p,q,s) \underset{q_0^2 \to (s-s_0)}{=} \frac{4}{\pi q}[\delta(q^2 - s + s_0)/\lambda_{n_0 l_0}^{(1)\prime}(s_0)(s - q_0^2 - s_0)]\,\phi_{n_0 l_0}^{(1)}(p,s_0)\phi_{n_0 l_0}^{(1)}(p_0,s_0)\,, \tag{3.18}$$

where λ' is the derivative of λ with respect to s.

Now multiply both sides of Eq. (2.33) by $(s - q_0^2 - s_0)/\phi_{n_0 l_0}^{(1)}(p_0,s_0)$ and then take the limit $q_0^2 \to s - s_0$. It is easily seen that all the inhomogeneous terms vanish except for $\Phi_{l_0}^{(1)}$ and that the wave function of the initial (2,3) bound state $\phi_{n_0 l_0}^{(1)}(p_0,s_0)$ is factored out of the equation. Substitution of $\Phi_{l_0}^{(1)}$ from Eq. (3.18) into Eq. (3.15) gives an explicit inhomogeneous term $\eta_{nl}^{(i)}$. Equation (3.14) can now be solved by standard numerical methods. For s above the lowest branch point the kernel must be taken as the limit of s approaching the real axis from above. One can either use numerical methods for complex arithematics or the Fredholm reduction given by Noyes[18] and by Kowalski.[19]

C. Spin and Identical Particles

So far, we have not considered spin in this formulation of the Faddeev equations. For nonrelativistic atomic problems, there is no spin-orbit coupling and the effect of the spin simply appears as a multiplicative factor in the kernel[8]:

$$\mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j;s) \to \mathcal{K}_{nlS,n'l'S'}^{(i,j)}(q,q_j;s,S_0) = (-1)^{S_i+S_j+S_k+S_0}[(2S+1)(2S'+1)]^{\frac{1}{2}} \begin{Bmatrix} S_j & S_k & S \\ S_i & S_0 & S' \end{Bmatrix} \times \mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j,s)\,, \tag{3.19}$$

where S_0 is the total spin of the three-particle system; S the spin of the pair (j,k); S' the spin of the pair (k,i); S_i, S_j, and S_k the spins of the individual particles; and $\{\ \}$ denotes the $6j$ symbol. Of course, the T-matrix elements $\chi_{nl}^{(i)}$ should now carry an additional spin index S denoting the spin of the pair (j,k).

As for identical particles, the statistics require that the two-body partial wave T matrix $t_l^{(i)}(p,p';E,S)$ be identically zero for certain l. In particular, for two spin-$\frac{1}{2}$ identical fermions, t is zero for even l if $S = 1$ and for odd l if $S = 0$. As long as all the two-body T-matrix elements satisfy the requirement of statistics, the solution of the Faddeev equations also satisfies the statistic. The number of equations is reduced because some of the kernels become equivalent.

IV. APPLICATION TO THE (e,H) SYSTEM

It is well-known that for the (e,H) system, there exists only one three-particle bound state corresponding to the ground ^1S H^- state. All the other three-particle states are unstable. They correspond to the resonant states which may be generated in the laboratory in an electron-hydrogen (atom) scattering experiment.[20,21] Theoretically it can be shown[22,23] that associated with each excited two-particle threshold (corresponding to the excited states of H atom) there exist a number of resonances supported by a potential which asymptotically goes to zero primarily as r^{-2}. Reasonably accurate determinations of the position and the width of a few of the lower members of the resonances have been recently carried out both theoretically[24–29] and experimentally.[21] For the bound H^- state on the other hand, an accurate value for the H^- detachment potential has been known for some time. A calculation of this singlet H^- state and the lowest members of the resonances in both the singlet and the triplet $J = 0$ series would therefore provide some insight into the feasibility of the method outlined in Sec. III.

A. The ^1S H^- Bound State

Since the ^1S H^- state has a zero total angular momentum (i.e., $J = 0$), Eq. (3.4) may be used for the calculation of this state. One can readily show for singlet spin multiplicity that the electron-proton interaction amplitudes for electrons 1 and 2 must satisfy the relation

$$\chi_{nl}^{(1)}(q,s) = (-)^l \chi_{nl}^{(2)}(q,s)\,, \tag{4.1}$$

and the electron-electron amplitude the relation

$$\chi_{nl}^{(3)}(q,s) = 0 \quad \text{for odd } l. \tag{4.2}$$

Equation (4.2) is simply the statement of the Pauli principle which excludes the possibility for two electrons in the singlet spin state to have odd parity. Equation (4.1) allows for the reduction of the coupled equations [Eq. (3.14)] into a pair of coupled equations. The spin factor for the kernel is unity in this case.

We write Eq. (3.14) in the matrix notation

$$\underline{\chi}(q,s)=\underline{\eta}(q,s)+\int_0^\infty dq_j^{\,2}\,\underline{\mathcal{K}}(q,q_j;s)\underline{\chi}(q_j,s)\,, \tag{4.3}$$

$$\text{with}\quad \underline{\chi}^{\dagger}(q,s)=[\chi_0^{(1)}(q,s),\chi_0^{(3)}(q,s),\chi_1^{(1)}(q,s),\chi_1^{(3)}(q,s),\chi_2^{(1)}(q,s),\chi_2^{(3)}(q,s),\ldots], \tag{4.4}$$

where each element $\chi_l^{(i)}(q,s)$ is a row with a dimension which equals the number of terms included in the off-shell two-particle amplitude $t_l^{(i)}$ [see Eq. (3.5)]. Equation (4.3) may be solved for $\chi(s)$ by digitizing the continuous variables q and q_j and inverting the matrix $(I-\underline{\mathcal{K}})$

$$\underline{\chi}(s)=[I-\underline{\mathcal{K}}(s)]^{-1}\underline{\eta}(s)\,. \tag{4.5}$$

To calculate the bound H^- state, we need to determine the pole in the inverse operator $[I-\underline{\mathcal{K}}(s)]^{-1}$. The pole may be located by locating the energy s at which the determinant of the $I-\underline{\mathcal{K}}(s)$matrix is zero.

For Coulomb interactions, the matrix elements in $\underline{\mathcal{K}}$ may be obtained analytically since both the eigenfunctions $\phi_{nl}^{(i)}$ and eigenvalues $\lambda_{nl}^{(i)}$ of the homogeneous Lippmann-Schwinger equation [Eq. (3.2)] are known explicitly [see Eqs. (3.7) and (3.8)]. It can be shown that when these explicit expressions are utilized with the help of Eq. (3.10), all the integrals needed for the evaluation of the matrix element in $\underline{\mathcal{K}}$ can be expressed in terms of the basic integrals

$$I_n(q,q_i;s)\equiv\int_{(\sqrt{2}q-q_i)^2}^{(\sqrt{2}q+q_i)^2}\frac{dp_i^{\,2}}{(p_i^{\,2}+q_i^{\,2}-s)^{n+1}}\,, \tag{4.6}$$

where we have made use of the large disparity between the electron and proton masses (i.e., $m_1/m_3=m_2/m_3\cong 0$). These integrals satisfy the recursion relation

$$I_{n+1}=[n/(n+1)]\{[(\xi+\zeta)^{n+1}-(\xi-\zeta)^{n+1}]/[(\xi+\zeta)^n-(\xi-\zeta)^n]\}\,[I_n/(\xi^2-\zeta^2)],\quad n\geq 1\,, \tag{4.7}$$

$$\text{with}\quad \xi=(2q^2+2q_i^{\,2}-s)\,,\quad \zeta=2\sqrt{2}\,qq_i\,, \tag{4.8}$$

where the recursion relation for the I's starts with

$$I_1=4\sqrt{2}\,qq_i/[(2q^2+2q_i^{\,2}-s)^2-8q^2q_i^{\,2}]\,. \tag{4.9}$$

As discussed before, the three-particle bound states can only occur below the branch point corresponding to the elastic threshold. In this energy region $s<-1$ Ry (-13.605 eV), the matrix $(I-\mathcal{K})$ is pure real. After Eqs. (4.1) and (4.2) are utilized in Eqs. (4.3), the resultant matrix integral equations are then solved by matrix inversion [Eq. (4.5)]. By taking only the first term in the $t_l^{(i)}$ expansion [Eq. (3.5)], we found that the H^- state appears at -1.0516 Ry below the three-particle breakup threshold. This corresponds to a detachment potential of -0.0516 Ry (i.e., 0.702 eV) for H^- in comparison with the accurate value of -0.0555 Ry of Peheris.[30] The agreement is most remarkable in view of the fact that only a single $1s$ term in the $t_l^{(i)}$ expansion is used in the calculation. This then implies that all the remaining terms contribute less than 7%.

To demonstrate that all the remaining terms in the $t_l^{(i)}$ expansion contribute less than 7% is, however, a somewhat difficult task. The expansion converges in an oscillatory manner and involves large cancellations. For example, the addition of the $2s$ term pushes the H^- state up very close to the elastic threshold. The $2s$ term effect is cancelled by the $3s$ term. The net result due to the inclusion of the $2s$ and $3s$ terms is to move the H^- state down to -1.061 Ry. On the other hand, the addition of $2p$ and $3p$ terms would lower further the H^- state to -1.064 Ry, and the addition of a $3d$ and $4s$ terms then pushes the H^- state up to -1.063 Ry. It is clear from the numerical result that the oscillations become smaller for higher terms in the $t_l^{(i)}$ expansion. However, our results seem to converge to a value lower than the accepted value. This is probably due to systematic errors in our numerical calculations. We will return to the convergence problem in Sec. V. Perhaps it is worthwhile to note that there is a substantial continuum component in each term of the $t_l^{(i)}$ expansion because this is a Stermian function expansion, so that the symbols $1s$, $2s$, $2p$, etc. should be interpreted accordingly.

Recently, a calculation of the H^- bound state has been carried out by Vesselova.[31] In this calculation the two-body interaction amplitude between the electrons $t_l^{(3)}$ was taken to be zero. As a test of our program we have considered the $t_l^{(3)}=0$ case and obtained, as expected, an energy spectrum which is simply the superposition of two sets of hydrogenic levels.

B. The Resonant H^- States

As the total energy s of the system moves above the elastic threshold, we encounter the electron-hydrogen scattering problem. The corresponding matrix $(I-\underline{\mathcal{K}})$ now becomes complex and contains branch points arising from bound states of H atom. These branch points must be treated properly in solving Eq. (4.3) for resonant states and in calculating the complex poles in $(I-\underline{\mathcal{K}})^{-1}$. As an example, we will determine the two lowest $J=0$ resonances with singlet and triplet spin states in the elastic region. We choose this example for simplicity since in the elastic energy region the branch point of concern is reduced to just the one associated with the ground hydrogen state.

For the calculation of the singlet $J=0$ resonances, one may again solve Eq. (4.3) numerically. Due to the presence of the branch points, it is difficult to maintain a desired accuracy by the standard numerical method of complex integration. However, the accuracy may be significantly improved by the Fredholm reduction method[18,19] in which the branch points are removed from the matrix to be inverted. For the present problem, the only branch point of concern is that associated with the ground H state in $\chi_0^{(1)}(q,s)$ [Eq. (4.4)]. We will now show how such a method may be adopted for the present problem.

Write for $\underline{\chi}(q,s)$ the expression

$$\underline{\chi}(q,s)=u(s)\underline{\Upsilon}(q,s) \tag{4.10}$$

where $u(s)=\chi(\sqrt{s_0},s)$ and

$$\underline{\Upsilon}^{\dagger}(s)=[\Upsilon_0^{(1)\dagger}(q,s),\ \Upsilon_0^{(3)\dagger}(q,s),\ \Upsilon_1^{(1)\dagger}(q,s),\ \Upsilon_1^{(3)\dagger}(q,s),\ \Upsilon_2^{(1)\dagger}(q,s),\ \Upsilon_2^{(3)\dagger}(q,s),\ldots], \tag{4.11}$$

where $s_0\equiv s+1$, $u(s_0)$ is a scalar function, and the $\Upsilon_l^{(i)}(q,s)$'s are columns with elements $\Upsilon_{nl}^{(i)}(q,s)$. For the purpose of calculating resonance poles, we may replace Eq. (4.3) by

$$u(s)\underline{\Upsilon}(q,s)=\underline{\mathcal{K}}_{10}^{(1)}(q,\sqrt{s_0},s)+u(s)\int_0^{\infty}dq_j^{\,2}\underline{\mathcal{K}}(q,q_j,s)\underline{\Upsilon}(q_j,s) \tag{4.12}$$

where we have replaced $\underline{\eta}(q,s)$[see Eq. (4.3)] by $\underline{\mathcal{K}}_{10}^{(1)}(q,s_0;s)$ since poles in $\chi(s)$ are independent of the inhomogeneous term $\eta(q,s)$[see Eq. (4.5)]. The symbol $\underline{\mathcal{K}}_{10}^{(1)}$ stands for $\underline{\mathcal{K}}_{10,nl}^{(1,i)}$ where i, n, and l are the suppressed indices of Υ. This quantity ${}_{10}^{(1)}(q,s_0;s)$ in Eq. (4.12) is chosen to make the kernel of the integral equation for Υ nonsingular at $q^2=s_0$. By definition of u, $\Upsilon_{10}^{(1)}(\sqrt{s_0},s)$ is normalized to unity. Solving Eq. (4.12) for $u(s)$ at $q^2=s_0$, we obtain

$$u(s)=\mathcal{K}_{10,10}^{(1,1)}(\sqrt{s_0},\sqrt{s_0};s)\Big/\Big(1-\sum_{\substack{j,n,l\\ n>l}}\int_0^{\infty}dq_j^{\,2}\,\mathcal{K}_{10,nl}^{(l,j)}(\sqrt{s_0},q_j;s)\,\Upsilon_{nl}^{(j)}(q_j,s)\Big)\,. \tag{4.13}$$

Substitution of $u(s)$ from Eq. (4.13) back into Eq. (4.12) yields

$$\underline{\Upsilon}(q,s)=\frac{\underline{\mathcal{K}}_{10}^{(1)}(q,\sqrt{s_0},s)}{\mathcal{K}_{10,10}^{(1,1)}(\sqrt{s_0},\sqrt{s_0};s)}+\int_0^{\infty}dq_1^{\,2}\left\{\underline{\mathcal{K}}(q,q_j;s)-\frac{\underline{\mathcal{K}}_{10}^{(1)}(q,\sqrt{s_0};s)}{\mathcal{K}_{10,10}^{(1,1)}(\sqrt{s_0},\sqrt{s_0};s)}\underline{\mathcal{K}}_{10}^{(1)\dagger}(\sqrt{s_0},q_j;s)\right\}\underline{\Upsilon}(q_j,s)\,. \tag{4.14}$$

Now, the kernel does not have a pole at $q_j^{\,2}=s_0$, and Eq. (4.14) contains no branch point for $s<-0.25$ Ry. It may be solved in a straightforward manner for $\underline{\Upsilon}(q,s)$. Having obtained $\underline{\Upsilon}(q,s)$, $u(s)$ can be calculated by evaluating the principal part integral in Eq. (4.13), and the poles of $u(s)$ are then poles of χ.

Unlike the case for the bound state, retaining only the $1s$ term in the $t_l^{(i)}$ expansion [Eq. (3.5)] fails to give any resonance. A resonance pole is found when either the $2s$ or the $2p$ term is included in the $t_l^{(i)}$ expansion. This is expected since the H^- resonances are closed-channel resonances[22] lying very close to the excitation threshold. The positions of the pole obtained in the $1s$-$2s$ and $1s$-$2p$ expansions are at -0.286 and -0.291 Ry below the three-particle breakup threshold, respectively. The position of the lowest H^- resonance in the $J=0$ singlet series has been found to be at -0.2973 Ry both experimentally[21] and theoretically.[22–29] This seems to indicate that neither the $2s$ nor the $2p$ term alone is sufficiently attractive to lower the pole to -0.2973 Ry. From these results one may also conclude that the $2p$ term is more attractive than the $2s$ term.

The combined effect of the $2s$ and $2p$ terms, on the other hand, is much too attractive. The pole is lowered in the $1s$-$2s$-$2p$ approximation to -0.326 Ry. It requires the $3s$ term to push the pole up to -0.3004 Ry. The addition of the $3p$ and $3d$ terms move the pole further up to -0.298 Ry, which is closer to the value of -0.2973 Ry calculated in the closed-coupling approximation with correlated wave functions. Though there is a definite indication of convergence towards the value of -0.2973 Ry, the convergence is again oscillatory and not rapid. It is perhaps worthwhile to emphasize that the present calculation is term-by-term exact. No variational or stationary parameters were used in the calculation.

The calculated width for the lowest $J=0$ singlet resonance in the $1s$-$2s$-$2p$-$3s$ approximation is 0.0025 Ry (0.034 eV) which is in reasonable agreement with previous calculations.[24,25,28,29] The measured width for this resonance is 0.043 eV.[21] In Fig. 4 the profile of the elastic scattering cross section in the neigh-

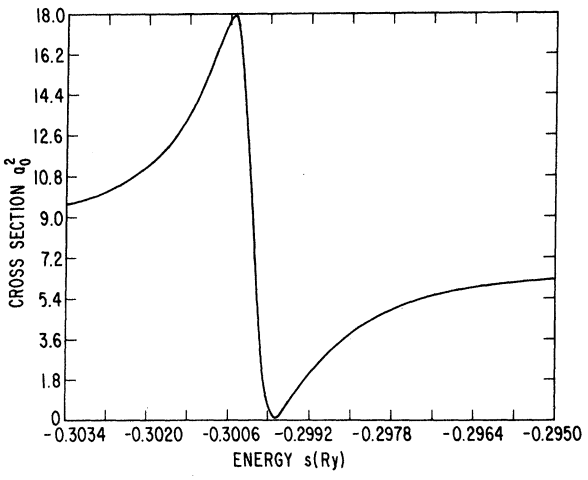

FIG. 4 Energy dependence of the singlet $J=0$ elastic scattering cross section in the neighborhood of the resonance in the $1s$-$2s$-$2p$-$3s$ approximation.

borhood of the $J=0$ singlet resonance is given. It is seen that the interference between direct and resonance scattering is important. Due to the absence of other channels, the cross section actually dips through zero at $s=-0.2997$ Ry.

For the triplet case, the electron-proton interaction amplitudes for electrons 1 and 2 must satisfy, instead of Eq. (4.1), the relation

$$\chi_{nl}^{(1)}(q,s)=(-)^{l+1}\chi_{nl}^{(2)}(q,s), \tag{4.15}$$

and the electron-electron interaction must satisfy, instead of Eq. (4.2), the relation

$$\chi_{nl}^{(3)}(q,s)=0, \quad \text{for even } l. \tag{4.16}$$

Equation (4.16) is again the statement of the Pauli principle which excludes the possibility for two electrons in the triplet spin state to have even parity. Equation (4.15) allows for the reduction of Eq. (3.14) into a different pair of coupled equations for the triplet case. The spin factor for the kernel is again unity.

The behavior of the solution for the triplet case is similar in nature to the singlet case. We obtain in the $1s$-$2s$-$2p$-$3s$-$3p$ approximation a resonance pole at -0.257 Ry below the three-particle breakup threshold with a width of $\sim 2\times10^{-5}$ Ry (2.72×10^{-4} eV) which are in reasonable agreement with the previously calculated values.[25,29]

V. CONCLUDING REMARKS

The method presented in Sec. III provides a practical way of solving the Faddeev equation for Coulomb potentials below three-particle breakup threshold. It is seen, from the example in Sec. IV, that by retaining only a few leading terms in the series a reasonably accurate value is obtained. The interesting problem is then to investigate the convergence of the remaining terms in the series. This is, however, a somewhat difficult task, since, as was pointed out in Sec. IV, the expansion converges in an oscillatory manner and involves large cancellations. The net sum of all the terms, considered as a whole, constitutes, nevertheless, a small correction. It is then feasible that a perturbation scheme in which the sum of the contribution of the remaining terms is treated as a perturbation may be developed. In this concluding section, we outline such a perturbative scheme.

Let us consider the problem of determining the poles in the inverse operator in Eq. (4.5) by examining the energy dependence of the determinant Det $\{I-\mathcal{K}(s)\}$. We can partition the matrix as

$$I-\underline{\mathcal{K}}(s)=\underline{B}+\underline{\mathcal{E}}=\underline{B}\{I+\underline{B}^{-1}\underline{\mathcal{E}}\}, \tag{5.1}$$

where $\underline{B}$ is a square matrix consisting of elements obtained in a truncated expansion including the leading terms in the series and $\mathcal{E}$ is the remainder. Utilizing the relation between the determinant and the trace of the logarithm of the corresponding matrix,

$$\mathrm{Det}\underline{A}=\exp\{\mathrm{Tr}(\ln\underline{A})\}, \tag{5.2}$$

we have

$$\mathrm{Det}\{I-\underline{\mathcal{K}}(s)\}=\mathrm{Det}\underline{B}\exp\{\mathrm{Tr}[\ln(1+\underline{B}^{-1}\underline{\mathcal{E}})]\}=\mathrm{Det}\underline{B}\{1+\mathrm{Tr}\underline{B}^{-1}\underline{\mathcal{E}}-\tfrac{1}{2}\mathrm{Tr}(\underline{B}^{-1}\underline{\mathcal{E}}\underline{B}^{-1}\underline{\mathcal{E}})+\cdots\}. \tag{5.3}$$

Defining $\underline{C}=\underline{B}^{-1}$, we have

$$\mathrm{Det}\{I-\underline{\mathcal{K}}(s)\}=\mathrm{Det}\underline{B}\Big[1+\sum_{\alpha=m+1}^{n}\epsilon_{\alpha\alpha}-\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\sum_{\gamma=m+1}^{n}c_{\alpha\beta}\epsilon_{\beta\gamma}\epsilon_{\gamma\alpha}-\tfrac{1}{2}\sum_{\alpha=m+1}^{n}\sum_{\lambda=m+1}^{n}\epsilon_{\lambda\alpha}\epsilon_{\alpha\lambda}$$

$$+\frac{1}{2}\Big(\sum_{\alpha=m+1}^{n}\epsilon_{\alpha\alpha}\Big)^2+\cdots\Big], \tag{5.4}$$

where ϵ_{ij} and c_{ij} are the elements of matrices $\underline{\mathcal{E}}$ and $\underline{C}$ respectively, n is the order of the matrix while m is the order of the submatrix corresponding to the truncated expansion. This then provides a systematic way of investigating the convergence problem.

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