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Faddeev Equations for Atomic Problems. II. Determination of Collision Amplitudes*

Joseph C. Y. Chen, Kwong T. Chung, and Paul J. Kramer
Department of Physics and Institute for Pure and Applied Physical Sciences, University of California, San Diego, La Jolla, California 92037

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The method for solving the Faddeev equations for atomic problems proposed in Paper I of this series is reexamined using a new separable representation for the off-shell two-body amplitude. Specific details for the determination of the collision amplitudes are worked out. A new set of reduced equations with proper inhomogeneous terms are obtained for cases with identical particles (electrons). As an illustrative example, the phase shift for low energy electron scattering by a hydrogen atom is calculated and compared with that calculated from conventional methods. In Appendix A, the possibility of applying the Faddeev equations to heavy-particle reactions using approximate or phenomenological atom-atom pair interactions is investigated.

I. INTRODUCTION

In a recent paper,[1] we have investigated the applicability of the Faddeev equations[2] to atomic problems with Coulomb potentials.[3] A practical method for reducing the Faddeev equations to a set of single-variable integral equations was introduced. This set of equations can be solved in a straightforward manner. As an illustrative example, the method was 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 were calculated. In the application we left the boundary conditions, associated with the physical process open, since all we need for the calculation of three-body bound states and resonances is to locate the poles in the kernel of the set of integral equations which are independent of the inhomogeneous terms. The boundary conditions must, however, be explicitly imposed if, in addition, one wishes to calculate the collision amplitudes and wavefunctions. In the present paper we extend the method to the calculation of collision amplitudes and wave functions.

The Faddeev equations and the method of Paper I for solving these equations are outlined in Sec. II in a form suitable to the present application. (A few misprints in Paper I are corrected.[4]) In Paper I, the off-shell two-body scattering amplitudes are represented in terms of Sturmian functions in sums of separable terms. Though very encouraging results were obtained for the (e, H) system using only a few leading terms, the Sturmian-function representation converges in an oscillatory manner and involves large cancellations. In view of this numerical difficulty the Coulomb-function representation recently proposed by Chen and Ishihara[5] is adopted. A new set of single-variable integral equations is given in a mixed-mode representation. In this representation, the Coulomb functions are used for pairs where the interaction potential is attractive. For pairs where the interaction potential is repulsive and the continuum contribution is dominating, the Sturmian functions are used.

In Sec. III, we consider the problem of putting these sets of equations back on the energy shell corresponding to the physical problem of interest and the problem of calculating collision amplitudes. In the case where two of the three particles are identical, we show (in Sec. IV) that the set of integral equations may be further reduced, just as in the case for the calculation of bound-state and resonance poles, to a single equation and a pair of coupled equations. As an illustrative example, the phase shift for low-energy electron scattering by hydrogen atoms is calculated in Sec. V. The result is compared with that obtained by the variational,[6] the close-coupling,[7] and the extended polarized-orbital[8] methods. Detailed investigations of the convergence problem and the relations between the Sturmian- and Coulomb-function representations are given elsewhere in Paper III[9] of this series.

In Appendix A, the interesting possibility of applying Faddeev equations to atomic reactions, using approximate or phenomenological potentials, is investigated. It is shown that our procedure can be adopted with simple modifications to atomic reactions if suitable potentials between each pair of atoms are available. For reactions involving a three-body force, the Faddeev equation must be modified to account for the additional three-body interaction. A simple proof of Newton's modification[10] of the Faddeev equations in the presence of a three-body force is given. In this case, an additional equation involving the three-body force is coupled into the Faddeev equations. If the three-body force is small, a perturbative scheme may be adopted. In Appendix B, an alternative set of single-variable integral equations in the mixed-mode representation is given.

II. THREE-BODY THEORY

A. The Faddeev Equations

The collision matrix $T(s)$ for a three-body system is a solution of the equation[11]

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

where $G_0(s) = (s - H_0)^{-1}$ (2.2)

and where s and V are the total energy and total interaction potential of the three-body system, respectively, and $G_0(s)$ is the free three-body Green's function. If the total interaction V consists of a sum over only two-body interactions V_{ij} $(i > j = 1, 2, 3)$, then

$$V = \textstyle\sum_i V_i \; (V_i = V_{jk}) . \tag{2.3}$$

Faddeev[2] has shown, using a method which is related to the multiple scattering theory of Watson,[12] that the three-body collision matrix can be conveniently expressed as a sum of three terms corresponding to the three alternative pairs of particles undergoing a final-state interaction (see Appendix A for cases with a three-body force):

$$T(s) = T^{(1)}(s) + T^{(2)}(s) + T^{(3)}(s) . \tag{2.4}$$

The $T^{(i)}$ satisfy the well-known Faddeev equations

$$T^{(i)}(s) = T_i(s) + \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s), \quad i = 1, 2, 3, \tag{2.5}$$

where the scattering matrix $T_i(s)$ arising from the two-body potential V_i is given by the Lippman-Schwinger equations[11]

$$T_i(s) = V_i + V_i G_0(s) T_i(s) . \tag{2.6}$$

The absence of direct coupling of $T^{(i)}$ with itself in the Faddeev equations results in a less singular kernel.

In momentum representation, the nonrelativistic kinetic energy in the c. m. frame may be written

$$H_0 = p_1^2 + q_1^2 = p_2^2 + q_2^2 = p_3^2 + q_3^2 , \tag{2.7}$$

$$\text{with } \vec{p}_i = \frac{m_k \vec{k}_j - m_j \vec{k}_k}{[2m_j m_k(m_j + m_k)]^{1/2}} , \quad \vec{q}_i = \frac{m_i(\vec{k}_j + \vec{k}_k) - (m_j + m_k)\vec{k}_i}{[2m_i(m_j + m_k)(m_i + m_j + m_k)]^{1/2}} , \tag{2.8}$$

where m_1, m_2, and m_3, and $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ are the masses and asymptotic momenta of the three particles, respectively. Consequently, the corresponding state vector $|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle$ may be written in any of the three pairs of basis variables

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle = |\vec{p}_1, \vec{q}_1\rangle_1 = |\vec{p}_2, \vec{q}_2\rangle_2 = |\vec{p}_3, \vec{q}_3\rangle_3 . \tag{2.9}$$

These sets of basis momenta [defined by Eq. (2.8)] in cyclic order of i, j, and k are linearly dependent [see Eqs. (I2.14)].

Since the total angular momentum J and its projection M is conserved, we consider these states to be diagonal in J and M. The separation of the angular momentum states in the Faddeev equations can then be carried out[13] using the relative angular momentum l between two particles, which is combined with the angular momentum L of the third particle in the over-all center-of-mass system. We have [see Eq. (I2.19)]

$$\Psi_{\alpha}^{(i)}(p,q,s)=\Phi_{\alpha}^{(i)}(p,q,s)-\tfrac{1}{4}\sum_{\alpha_j}\sum_{j\neq i}\int_0^\infty dp_j^{\,2}\int_0^\infty dq_j^{\,2}\,\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j)[p_jq_j/(p_j^{\,2}+q_j^{\,2}-s)] \times\Psi_{\alpha_j}^{(j)}(p_j,q_j,s), \qquad (2.10)$$

$$\text{with } \Psi_{\alpha}^{(i)}(p,q,s)\equiv{}_i\langle p,q,\alpha\,|\,T^{(i)}(s)\,|\,\vec{k}_1,\vec{k}_2,\vec{k}_3\rangle, \qquad (2.11)$$

$$\Phi_{\alpha}^{(i)}(p,q,s)\equiv{}_i\langle p,q,\alpha\,|\,T_i(s)\,|\,\vec{k}_1,\vec{k}_2,\vec{k}_3\rangle\ , \qquad (2.12)$$

$$\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j)\equiv{}_i\langle p,q,\alpha\,|\,T_i(s)\,|\,p_jq_j\alpha_j\rangle_j\ , \qquad (2.13)$$

where for convenience the discrete quantum numbers $(JMlL)$ are collectively denoted by α.

Since T_i involves only the two-body potential V_i, the matrix element ${}_i\langle\vec{p}\vec{q}\,|\,T_i(s)\,|\,\vec{p}_i\vec{q}_i\rangle_j$ in the kernel $\mathcal{K}_j^{(i)}$ may be reduced to a two-particle matrix element. The kernel in the Faddeev equations may be written as[13]

$$\mathcal{K}_j^{(i)}(pq\alpha\,|\,p_jq_j\alpha_j)=\int_{-1}^{1}d\cos\theta_{\vec{p}_j\vec{q}_j}\,A_{\alpha\alpha_j}(\theta_{\vec{p}_i\vec{p}_j},\theta_{\vec{p}_j\vec{q}_i},\theta_{\vec{p}_j\vec{q}_j})\,\delta(q^2-q_i^{\,2})\,t_l^{(i)}(p,p_i;s-q^2)\,, \qquad (2.14)$$

with

$$A_{\alpha\alpha'}(\theta_{\vec{p}_i\vec{p}_j},\theta_{\vec{p}_j\vec{q}_i},\theta_{\vec{p}_j\vec{q}_j})=(-)^{L+L'-l-l'+M}\,\frac{16\pi^{1/2}}{q}(2l'+1)^{1/2}\,\delta_{JJ'}\delta_{MM'}$$

$$\times\sum_{m_lm_Lm_{L'}}\begin{pmatrix} l & L & J\\ m_l & m_L & -m_{L'}\end{pmatrix}\begin{pmatrix} l' & L' & J'\\ 0 & m_{L'} & -m_{L'}\end{pmatrix}Y^*_{lm_l}(\theta_{\vec{p}_i\vec{p}_j},0)\,Y^*_{Lm_L}(\theta_{\vec{p}_j\vec{q}_i},0)\,Y_{L'm_{L'}}(\theta_{\vec{q}_j\vec{p}_j},0), \qquad (2.15)$$

where $\theta_{\vec{p}_i\vec{p}_j}$, for example, is the angle between momentum variables $\vec{p}_i$ and $\vec{p}_j$. With $p_i^{\,2}=p_j^{\,2}+q_j^{\,2}-q^2$, we have

$$\cos\theta_{\vec{p}_i\vec{q}_i}=\omega_i=(ij)[\alpha_{ij}^{\,2}(q_j^{\,2}-q^2)+\beta_{ij}^{\,2}(q^2-p_j^{\,2})]/2\alpha_{ij}\beta_{ij}qp_i\ , \qquad (2.16)$$

$$\cos\theta_{\vec{p}_j\vec{q}_j}=\overline{\omega}_j=(ij)[\beta_{ij}^{\,2}p_j^{\,2}+\alpha_{ij}^{\,2}q_j^{\,2}-q^2]/2\alpha_{ij}\beta_{ij}p_jq_j\ , \qquad (2.17)$$

$$\text{where}\quad \alpha_{ij}\equiv[m_im_j/(m_i+m_k)(m_j+m_k)]^{1/2}\quad\text{and}\quad\beta_{ij}\equiv(1-\alpha_{ij}^{\,2})^{1/2}\,, \qquad (2.18)$$

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

The scattering amplitude $t_l^{(i)}(p,p_i;s-q^2)$, between particle j and k with angular momentum l, is the solution of the Lippmann-Schwinger equations

$$t_l^{(i)}(p,p';E)=V_l^{(i)}(p,p')-\pi^{-1}\int_0^\infty dp''^{2}p''\,V_l^{(i)}(p,p'')\,t_l^{(i)}(p'',p';E)/(p''^{2}-E)\,, \qquad (2.19)$$

with the Coulomb potential[14]

$$V_l^{(i)}(p,p')=(\tfrac{1}{2}\mu_i)^{1/2}(Z_i/pp')\,Q_l[(p^2+p'^2)/2pp']\,, \qquad (2.20)$$

where the Q_l are the Legendre functions of the second kind, μ_i is the reduced mass for the (j,k) two-body system, and Z_i is the product of the charges (i.e., Z_jZ_k) of the two particles. The scattering amplitude is normalized[14] on the energy shell according to the equation

$$t_l^{(i)}(p,p;p^2)=-e^{i\delta_l}(\sin\delta_l)/p\,. \qquad (2.21)$$

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

The partial-wave Faddeev equations with the kernel given by Eqs. (2.14) and (2.15) are effectively a set of coupled two-variable integral equations. 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, and the two-variable integral equations can be reduced to equations with one variable. We will consider such a reduction in the next two subsections, using two possible separable representations of t_l in terms of the Sturmian and Coulomb functions.

B. Variable Reduction in Sturmian-Function Representation

The reduction of the partial-wave Faddeev equations in two variables to a set of single-variable equations has been carried out in Paper I, using the Sturmian-function expansion for the off-shell two-body amplitude in sums of separable terms,

$$t_l(p,p';E)=\sum_\lambda[1-\gamma_{\lambda l}(E)]^{-1}\phi_{\lambda l}(p,E)\phi_{\lambda l}(p',E). \tag{2.22}$$

The Sturmian functions

$$\phi_{\lambda l}(p,E)=\left\{\frac{2^{4l+3}\lambda(\lambda-l-1)!}{\Gamma(\lambda+l+1)}\right\}^{1/2} l!(-E)^{(2l+3)/4}\,\frac{p^l}{(p^2-E)^{l+1}}\,C_{\lambda-l-1}{}^{l+1}\left(\frac{p^2+E}{p^2-E}\right), \tag{2.23}$$

which satisfy the orthonormality property

$$\pi^{-1}\int_0^\infty dp^2\,p\,\phi_{\lambda l}(p,E)\phi_{\lambda' l}(p,E)/(p^2-E)=\delta_{\lambda\lambda'}\,, \tag{2.24}$$

are solutions of the homogeneous Lippmann-Schwinger equations with eigenvalues $[\gamma_{\lambda l}]^{-1}$:

$$[\gamma_{\lambda l}(E)]^{-1}\phi_{\lambda l}(p,E)=-\pi^{-1}\int_0^\infty dp'^2[p'/(p'^2-E)]\,V_l(p,p')\phi_{\lambda l}(p',E), \tag{2.25}$$

with

$$\gamma_{\lambda l}(E)=-\lambda(-2E/\mu)^{1/2}/Z\,, \tag{2.26}$$

where $C_{\lambda-l-1}{}^{l+1}$ are the Gegenbauer polynomials.

Utilizing the separable Sturmian-function (S-F) expansion [Eq. (2.22)] for t_l, the p dependence of $\Psi_\alpha{}^{(i)}(p,q,s)$ can be made explicit. For simplicity, let us consider now the $J=M=0$ case. In this case, $\alpha=(JMlL)=(00ll)\equiv l$ and the off-shell three-body collision amplitude $\Psi_l{}^{(i)}(p,q,s)$, from Eqs. (2.10) with the ith pair of particles undergoing final-state interaction, can be expressed with the help of Eq. (2.22) as

$$\Psi_l^{(i)}(p,q,s)=\Phi_l^{(i)}(p,q,s)+\sum_\lambda[\gamma_{\lambda l}^{(i)}(s-q^2)-1]^{-1}\,\phi_{\lambda l}^{(i)}(p,s-q^2)\chi_{\lambda l}^{(i)}(q,s). \tag{2.27}$$

The functions $\chi_{\lambda l}{}^{(i)}$ can be determined from the set of coupled single-variable integral equations [see Eqs. (I3.14) to (I3.16)]:

$$\chi_{\lambda l}^{(i)}(q,s)=\eta_{\lambda l}^{(i)}(q,s)+\sum_{\lambda',l',j\neq i}\int_0^\infty dq_j{}^2\,\mathcal{K}_{\lambda l,\lambda' l'}^{(i,j)}(q,q_j;s)\chi_{\lambda' l'}^{(j)}(q_j,s),\quad i=1,2,3, \tag{2.28}$$

with

$$\mathcal{K}_{\lambda l,\lambda' l'}^{(i,j)}(q,q_j;s)=-\int_{L_{ij}}^{U_{ij}}dp_j{}^2B_{ll'}{}^{(i,j)}(q,p_j,q_j;s)[1-\gamma_{\lambda' l'}{}^{(j)}(s-q_j{}^2)]^{-1}\phi_{\lambda l}{}^{(i)}(p_i,s-q^2)\phi_{\lambda' l'}{}^{(j)}$$
$$\times(p_j,s-q_j{}^2); \tag{2.29}$$

$$\eta_{\lambda l}^{(i)}(q,s)=\sum_{l',j\neq i}\int_0^\infty dq_j{}^2\int_{L_{ij}}^{U_{ij}}dp_j{}^2B_{ll'}{}^{(i,j)}(q,p_j,q_j;s)\phi_{\lambda l}{}^{(i)}(p_i,s-q^2)\Phi_{l'}{}^{(j)}(p_j,q_j,s); \tag{2.30}$$

$$B_{ll'}{}^{(i,j)}(q,p_jq_j;s)\equiv\{(-)^{l+l'}[(2l+1)(2l'+1)]^{1/2}/4\pi\alpha_{ij}\beta_{ij}q(p_j{}^2+q_j{}^2-s)\}P_l(\omega_i)P_{l'}(\overline{\omega}_j); \tag{2.31}$$

where the limits of integration are given by the equations

$$U_{ij}=(\alpha_{ij}q_j+q)^2/\beta_{ij}{}^2,\quad L_{ij}=(\alpha_{ij}q_j-q)^2/\beta_{ij}{}^2\;. \tag{2.32}$$

From the example of applying Eq. (2.28) to the (e,H) system for the calculation of three-body bound-state and resonance poles we have found in Paper I that the S-F expansion, though it gives encouraging results for the first few leading terms, converges in an oscillatory manner and involves large cancellations. In the next subsection, the alternative, separable representation for the two-body scattering amplitude $t_l^{(i)}$, in terms of Coulomb functions, will be considered.

C. Variable Reduction in Mixed-Mode Representation

The off-shell two-body scattering amplitude for a Coulomb potential may be represented in terms of Coulomb functions as a sum of separable terms[5,15]

$$t_l(p,p';E) = V_l(p,p') + \tfrac{1}{2}\pi{\sum_n}'[(p^2-\epsilon_n)(p'^2-\epsilon_n)/(E-\epsilon_n)]\psi_{nl}(np)\psi_{nl}(np'), \tag{2.33}$$

with the Coulomb potential given by any of the following expressions:

$$V_l(p,p') = -\tfrac{1}{2}\pi{\sum_n}'(p^2-\epsilon_n)\psi_{nl}(np)\psi_{nl}(np'), \tag{2.34a}$$

$$= -\tfrac{1}{2}\pi{\sum_n}'(p'^2-\epsilon_n)\psi_{nl}(np)\psi_{nl}(np'), \tag{2.34b}$$

$$= -\tfrac{1}{4}\pi{\sum_n}'[(p^2-\epsilon_n)+(p'^2-\epsilon_n)]\psi_{nl}(np)\psi_{nl}(np'), \tag{2.34c}$$

where the prime on the summation sign indicates that we sum over (if V_l is attractive) the discrete states and integrate over the continuum states.

The Coulomb functions are solutions of the Schrödinger equation

$$(p^2-\epsilon_n)\psi_{nl}(np) = -\pi^{-1}\int_0^\infty dp'\,{}^2p'\,V_l(pp')\psi_{nl}(np'), \tag{2.35}$$

with the orthonormality property

$$\int_0^\infty \psi_{nl}(np)\psi_{n'l}(n'p)p^2dp = \delta_{nn'} . \tag{2.36}$$

For discrete states, we have $\epsilon_n^{(i)} = -Z_i{}^2\mu_i/(2n^2)$ (2.37)

and $$\psi_{nl}(np) = \left\{\frac{2^{4l+5}n(n-l-1)!}{\pi(n+l)!}\right\}^{1/2} l!(-\epsilon_n)^{(2l+5)/4}\frac{pl}{[p^2-\epsilon_n]^{l+2}}C_{n-l-1}^{l+1}\left(\frac{p^2+\epsilon_n}{p^2-\epsilon_n}\right). \tag{2.38}$$

The separable Coulomb-function (C-F) representation for t_l in general converges uniformly and is not, in principle, limited to negative energies as is the case for the S-F expansion.[16] Consequently the single-variable integral equation obtained using the C-F representation for t_l should, in principle, be capable of dealing with problems with positive total energies; this includes the problem of three-body breakup, such as, for example, the ionization of hydrogen atoms by electron impact.

The convergence property of the C-F representation of t_l [Eqs. (2.33) and (2.34)] for attractive V_l has been investigated and compared with that of the S-F expansion [Eq. (2.22)] in some detail.[17] In general, the C-F representation converges uniformly and rapidly to a limit which is displaced from the exact value unless continuum states are explicitly included. The displacements which depend sensitively upon the arguments p and p' account for the continuum contribution. For most cases the continuum contribution is usually only a few percent. This suggests that, for pairs of particles with attractive interaction, the C-F representation, including only discrete states, should constitute a reasonable approximation for $t_l^{(i)}$, especially at low energies. This then permits us to reduce the partial-wave Faddeev equations to a set of single-variable equations, in the mixed-mode representation suitable for dealing with problems at total energies below the three-body breakup threshold. In this mixed-mode representation we adopt the C-F representation for pairs of particles with attractive potential and for pairs of particles with repulsive interactions, where the continuum contribution that dominates the S-F expansion is used.

When the expressions for $t_l^{(i)}$ given by Eqs. (2.33) to (2.34) are utilized for pairs of particles with attractive potential, several sets of new single-variable equations can be obtained from the partial-wave Faddeev equations. We consider here the set obtained by using Eq. (2.34a) for V_l. Though Eq. (2.34c) for V_l preserves, term-by-term, the symmetry in interchanging p and p', it increases the number of final coupled single-variable equations [see Appendix B] and is, therefore, less desirable from a practical point of view in solving these equations.

Utilizing Eqs. (2.33) and (2.34a), we obtain, for $\Psi_l^{(i)}(p,q,s)$ with pairs of particles undergoing an attractive final-state interaction, the expression

$$\Psi_l^{(i)}(p,q,s)=\Phi_l^{(i)}(p,q,s)+\frac{\pi}{2}\sum_n{}' \frac{p^2-\epsilon_n^{(i)}}{s-\epsilon_n^{(i)}-q^2}\,\psi_{nl}^{(i)}(np)\chi_{nl}^{(i)}(q,s)\,. \tag{2.39}$$

For the off-shell three-body collision amplitude with pairs of particles undergoing repulsive final-state interaction, we use the Sturmian-function expansion [Eq. (2.22)] and obtain

$$\Psi_l^{(j)}(p,q,s)=\Phi_l^{(j)}(p,q,s)+\sum_\lambda [\gamma_\lambda^{(j)}(s-q^2)-1]^{-1}\,\phi_{\lambda l}^{(j)}(p,s-q^2)\chi_{\lambda l}^{(j)}(q,s)\,. \tag{2.40}$$

The functions $\chi_{nl}^{(i)}$ and $\chi_{\lambda l}^{(j)}$ can be determined from the set of coupled single-variable equations:

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

$$+\sum_{\lambda'l'}\int_0^\infty dq_3^2\,\mathcal{K}_{nl,\lambda'l'}^{(i,3)}(q,q_3;s)\chi_{\lambda'l'}^{(3)}(q_3,s),\quad i=1,2; \tag{2.41a}$$

$$\chi_{\lambda l}^{(3)}(q,s)=\eta_{\lambda l}^{(3)}(q,s)+\sum_{n'l'}{}'\sum_{j\neq 3}\int_0^\infty dq_j^2\,\mathcal{K}_{\lambda l,n'l'}^{(3,j)}(q,q_j;s)\chi_{n'l'}^{(j)}(q_j,s); \tag{2.41b}$$

with

$$\mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j;s)=-\frac{\pi}{2}\int_{L_{ij}}^{U_{ij}}dp_j^2\,B_{ll'}^{(i,j)}(q,p_j,q_j;s)\frac{(p_j^2+q_j^2-s)(p_j^2-\epsilon_{n'}^{(j)})}{s-\epsilon_{n'}^{(j)}-q_j^2}\,\psi_{nl}^{(i)}(np_i)\psi_{n'l'}^{(j)}(n'p_j); \tag{2.42a}$$

$$\mathcal{K}_{nl,\lambda'l'}^{(i,3)}(q,q_j;s)=\int_{L_{i3}}^{U_{i3}}dp_3^2\,B_{ll'}^{(i,3)}(q,p_3,q_3;s)\,\frac{p_3^2+q_3^2-s}{1-\gamma_{\lambda'l'}^{(3)}(s-q_3^2)}\,\psi_{nl}^{(i)}(np_i)\phi_{\lambda'l'}^{(3)}(p_3,s-q_3^2); \tag{2.42b}$$

$$\mathcal{K}_{\lambda l,n'l'}^{(3,j)}(q,q_j;s)=\frac{\pi}{2}\int_{L_{3j}}^{U_{3j}}dp_j^2\,B_{ll'}^{(3,j)}(q,p_j,q_j;s)\frac{p_j^2-\epsilon_{n'}^{(j)}}{s-\epsilon_{n'}^{(j)}-q_j^2}\,\phi_{\lambda l}^{(3)}(p_3,s-q^2)\psi_{n'l'}^{(j)}(n'p_j)\,, \tag{2.42c}$$

$$\eta_{nl}^{(i)}(q,s)=-\sum_{l',j\neq i}\int_0^\infty dq_j^2\int_{L_{ij}}^{U_{ij}}dp_j^2\,B_{ll'}^{(i,j)}(q,p_j,q_j;s)(p_j^2+q_j^2-s)\psi_{nl}^{(i)}(np_i)\Phi_{l'}^{(j)}(p_j,q_j,s),\quad i=1,2; \tag{2.43a}$$

$$\eta_{\lambda l}^{(3)}(q,s)=\sum_{l',j\neq 3}\int_0^\infty dq_j^2\int_{L_{3j}}^{U_{3j}}dp_j^2\,B_{ll'}^{(3,j)}(q,p_j,q_j;s)\phi_{\lambda l}^{(3)}(p_3,s-q^2)\Phi_{l'}^{(j)}(p_j,q_j,s), \tag{2.43b}$$

where we have chosen, for definiteness, the third pair (i.e., particles 1 and 2) as having a repulsive interaction potential while pairs 1 and 2 have an attractive interaction potential.

Equations (2.40) can be rewritten in the form of Eq. (2.28)

$$\chi_{\nu l}^{(i)}(q,s)=\eta_{\nu l}^{(i)}(q,s)+\sum_{\nu',l',j\neq i}{}'\int_0^\infty dq_j^2\,\mathcal{K}_{\nu l,\nu'l'}^{(i,j)}(q,q_j;s)\chi_{\nu'l'}^{(j)}(q_j,s), \tag{2.44}$$

where it is understood that the inhomogeneous terms and the kernels take their appropriate expressions as given by Eqs. (2.42) and (2.43) and that the prime on the summation sign indicates an integration, when appropriate, over the continuum states. If the Coulomb-function representation is adopted for all the two-body off-shell amplitudes, equations similar to Eqs. (2.44) would again be obtained in which all the kernels and the inhomogeneous terms are given by Eqs. (2.41a) and (2.42a), respectively.

III. DETERMINATION OF THE COLLISION AMPLITUDE

In our development, we have so far left the initial states $|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle$ of the three-body system unspecified. For the purpose of determining the bound and resonance states, this is sufficient since the energy spectrum of the three-body system is determined entirely by the kernel of the integral equations which is independent of the initial state. The specification of the initial state and the corresponding inhomogeneous terms as well as of the final states is of importance for the calculation of the collision amplitude and wave function of the collision problem. We now consider the problem of specifying the appropriate initial and final states for physical collision processes.

A. Specification of the Initial Physical State

For a physical collision process, one usually has an initial state consisting of two interacting subsystems, such as an incident particle plus a two-body subsystem in a certain bound state. We have, for the initial state,

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle_i = |p_0, q_0, \alpha_0\rangle_i \,, \tag{3.1}$$

where $\vec{p}_0$ is proportional to the magnitude of the relative momentum between the two particles in the two-body subsystem, and $\vec{q}_0$ is proportional to the magnitude of the momentum of the incident particle in the three-body center-of-mass frame. The corresponding inhomogeneous term $\Phi_\alpha^{(i)}(p,q,s)$ [see Eq. (2.12)] takes the form

$$\begin{aligned}\Phi_\alpha^{(i)}(p,q,s) &\equiv {}_i\langle p,q,\alpha|T_i(s)|p_0,q_0,\alpha_0\rangle_j \\ &= -\int_{-1}^{1} d\cos\theta_{\vec{p}_{0j}\vec{q}_{0j}} A_{\alpha\alpha_{0j}}(\theta_{\vec{p}_i\vec{p}_{0j}}, \theta_{\vec{q}_i\vec{p}_{0j}}, \theta_{\vec{p}_{0j}\vec{q}_{0j}})\delta(q^2 - q_i^2)t_l^{(i)}(p,p_i;s-q^2)\,, \end{aligned}\tag{3.2}$$

where $A_{\alpha\alpha_{0j}}$ is given by Eq. (2.15).

For definiteness, we consider an initial state consisting of particle "1" and a bound state of (2,3) with energy s_0, angular momentum l_0, and principal quantum number λ_0. The corresponding inhomogeneous term for $J=M=0$ then takes the form [see Eq. (I3.17)]

$$\Phi_{l_0}^{(1)}(p,q,s) = \frac{4}{\pi q} t_{l_0}^{(1)}(p,p_0;s-q_0^2)\delta(q^2-q_0^2), \quad \text{for } q_0^2 \to (s-s_0), \tag{3.3}$$

where $t_{l_0}^{(1)}$ is the two-body t matrix of the initial two-body subsystem. Since the initial two-body subsystem is in a bound state with energy s_0, $t_{l_0}^{(1)}$ has a pole at $s-q^2=s_0$. $\Phi l_0^{(1)}(p,q,s)$ can be rewritten in the Sturmian functions as

$$\Phi_{l_0}^{(1)}(p,q,s) = -\frac{4Z_1[2\mu_1(-s_0)]^{1/2}}{\pi\lambda_0 q} \frac{\delta(q^2-s+s_0)}{s-q_0^2-s_0} \phi_{\lambda_0 l_0}^{(1)}(p,s_0)\,\phi_{\lambda_0 l_0}^{(1)}(p_0,s_0), \quad \text{for } q_0^2 \to (s-s_0), \tag{3.4}$$

and in the Coulomb functions with $s_0 = \epsilon_{n_0}^{(1)}$ as

$$\Phi_{l_0}^{(1)}(p,q,s) = \frac{2}{q}\left[\frac{\delta(q^2-s+s_0)}{s-q_0^2-\epsilon_{n_0}^{(1)}}\right](p^2-\epsilon_{n_0}^{(1)})(p_0^2-\epsilon_{n_0}^{(1)})\psi_{n_0}^{(1)}(n_0 p)\psi_{n_0 l_0}^{(1)}(n_0 p_0); \quad \text{for } q_0^2 \to (s-s_0), \tag{3.5}$$

where we have taken λ_0 and n_0 to denot the initial (2, 3) two-body state having an energy s_0 in Sturmian and Coulomb function representations, respectively.

B. Specification of the Final Physical States

Having specified the initial physical state, we are now in a position to determine the collision amplitude by simply putting the Faddeev equations back on the energy shell for the desired corresponding final physical states. As an example, we consider the rearrangement collision in which the incident particle (i.e., particle "1") picks up particle "3" from the initial subsystem (2,3) leaves behind particle "2," and forms a new two-body subsystem (1,3) in the final state with energy s_f and angular momentum l_f. The collision amplitude for such a rearrangement process can be obtained from Eqs. (2.27) or Eqs. (2.39) by taking the appropriate energy limits that correspond to the energies associated with the initial and final states.

Let the rearrangement collision matrix element be denoted by $\mathcal{T}_{0\to f}$, we then have from $\Psi_l^{(2)}$ (which corresponds to the off-shell three-body collision amplitude with particles "1" and "3" undergoing a final-state interaction [see Eq. (2.10)] the expression for $\mathcal{T}(0\to f)$:

$$\mathcal{T}_{0\to f}=\lim_{q^2\to s-s_f}\left\{\frac{s-q^2-s_f}{\phi_{\lambda_f l_f}{}^{(2)}(p,s-q^2)}\lim_{q_0{}^2\to s-s_0}\left(\frac{s-q_0{}^2-s_0}{\phi_{\lambda_0 l_0}{}^{(1)}(p_0,s-q_0{}^2)}\Psi_{l_f}{}^{(2)}(p,q,s)\right)\right\}, \tag{3.6}$$

where the first limit $q_0{}^2\to s-s_0$ which operates only on the inhomogeneous terms puts the collision amplitude back on the initial energy shell, and the second limit puts the collision amplitude back on the final energy shell. In this expression for $\mathcal{T}_{0\to f}$, the initial (2,3) bound state $\phi^{(1)}$ and the final (1,3) bound state $\phi^{(2)}$ are properly factored out.[18]

Utilizing Eqs. (2.27) we obtain

$$\mathcal{T}_{0\to f}=\frac{Z_2}{\lambda_f}[2\mu_2(-s_f)]^{1/2}\chi_{\lambda_f l_f}{}^{(2)}(K_f,s;K_0)^{1/2}, \quad \text{with } K_0=(s-s_0)^{1/2}, \quad K_f=(s-s_f)^{1/2}, \tag{3.7}$$

where $\chi^{(2)}$ is the solution of Eq. (2.28). The argument K_0 in $\chi_{\lambda_f l_f}{}^{(2)}$ is introduced to indicate that the limit $q_0{}^2\to s-s_0$ for the initial state has been carried out. The inhomogeneous terms [i.e., the $\eta_{\lambda l}{}^{(2)}(q,s)$] in Eq. (2.28) for the χ_{nl} are given, after taking the $q_0{}^2\to s-s_0$ limit, by the equation

$$\eta_{\lambda l}{}^{(2)}(q,s)=-\frac{4Z_2[2\mu_2(-s_0)]^{1/2}}{\pi\lambda_0 K_0}\int_{L_{21}(q,K_0)}^{U_{21}(q,K_0)}dp_1{}^2B_{ll_0}{}^{(2,1)}(q,p_1,K_0;s)\phi_{\lambda l}{}^{(2)}((p_1{}^2+s-s_0-q^2)^{1/2},s-q^2)$$
$$\times\phi_{\lambda_0 l_0}{}^{(1)}(p_1,s_0), \tag{3.8}$$

with [see Eqs. (2.31)]

$$U_{21}(q,K_0)=(\alpha_{21}K_0+q)^2/\beta_{21}{}^2, \quad L_{21}(q,K_0)=(\alpha_{21}K_0-q)^2/\beta_{21}{}^2, \tag{3.9}$$

where, on taking the limit $q_0{}^2\to s-s_0$ the $\Phi_{\lambda l}{}^{(3)}$ inhomogeneous terms [as well as $\Phi_{\lambda l}{}^{(2)}$ in Eq. (3.7)] dropped out.

In terms of Coulomb functions, the rearrangement collision matrix element for the pick-up process takes the form[18]

$$\mathcal{T}_{0\to f}=\lim_{q^2\to s-s_f}\left[\frac{s-q^2-\epsilon_{n_f}{}^{(2)}}{(p^2-\epsilon_{n_f}{}^{(2)})\psi_{n_f l_f}{}^{(2)}(n_f p)}\lim_{q_0{}^2\to s-s_0}\left(\frac{s-q^2-\epsilon_{n_0}{}^{(1)}}{(p_0{}^2-\epsilon_{n_0}{}^{(1)})\psi_{n_0 l_0}{}^{(1)}(n_0 p_0)}\Psi_{l_f}{}^{(2)}(p,q,s)\right)\right] \tag{3.10}$$

similarly we obtain, with the help of Eqs. (2.39),

$$\mathcal{T}_{0\to f}=\tfrac{1}{2}\pi\chi_{n_f l_f}{}^{(2)}(K_f,s;K_0) \tag{3.11}$$

with $\eta_{nl}{}^{(2)}(q,s)$ given by

$$\eta_{nl}{}^{(2)}(q,s)=-\frac{2}{K_0}\int_{L_{21}(q,K_0)}^{U_{21}(q,K_0)}dp_1{}^2B_{ll_0}{}^{(2,1)}(q,p_1,K_0;s)(p_1{}^2-s_0)(p_1{}^2-\epsilon_{n_0}{}^{(1)})\psi_{n_0 l_0}{}^{(1)}(n_0 p_1)\psi_{nl}{}^{(2)}$$
$$\times(n(p_1{}^2+s-s_0-q^2)^{1/2}), \tag{3.12}$$

where, of course, $s_0=\epsilon_{n_0}{}^{(1)}$ and $s_f=\epsilon_{n_f}{}^{(2)}$.

It is a simple matter to relate the collision matrix element $\mathcal{T}_{0\to f}$ to the cross section. The differential cross section for the pick-up reaction is given in terms of the usual collision amplitude $f_{0\to f}$ as[11]

$$d\sigma_{0\to f}/d\Omega=(\kappa_f/\kappa_0)|f_{0\to f}(\Omega)|^2, \tag{3.13}$$

$$\text{with} \quad \kappa_f{}^2/2\mu_f+s_f=\kappa_0{}^2/2\mu_0+s_0, \quad \mu_f=m_2(m_1+m_3)/(m_1+m_2+m_3), \tag{3.14}$$

where κ_0 and κ_f are the relative wave numbers between the initial subsystems [i.e., "1," and (2,3)], respectively, and μ_0 and μ_f are the reduced mass of the initial and final subsystems. For the $J=0$ case considered here we have

$$f_{0\to f}(\Omega)=-4\pi(2\mu_f)^{-1/2}\mathcal{T}_{0\to f}\,, \tag{3.15}$$

where the factor $4\pi/(2\mu_f)^{1/2}$ in Eq. (3.15) results from our normalization of the T matrix on the energy shell.

Similarly, the elastic scattering matrix element $\mathcal{T}_{0\to0}$ may be obtained by taking $q^2\to s-s_0$ and $q_0{}^2\to s-s_0$ limits for $\Psi_{l_0}{}^{(1)}$. This can be done without additional calculations since, once the set of coupled equations [Eqs. (2.28) or Eqs. (2.44)] is solved for a given energy, we obtain all $\Psi_l{}^{(1)}$, $\Psi_l{}^{(2)}$, and $\Psi_l{}^{(3)}$, as well as the energy spectrum of the three-body system. Consequently, the collision matrix elements for all the accessible processes are determined by taking appropriate energy limits. Utilizing these collision matrix elements, we may present our results in terms of eigenphase shifts.

C. Determination of Eigenphase Shift

From the solutions of the coupled equations for the χ's, the collision matrix elements for all the accessible processes may be obtained by taking appropriate energy limits as outlined in Sec. III B. The S matrix for the interacting system may then be constructed from these matrix elements. Let us return to the example of the pick-up process discussed in Sec. III B and assume that we are in an energy region where the pick-up process is the only inelastic collision accessible for the system, with the initial subsystems consisting of an incident particle "1" and a two-body system (2,3) in a bound state. The S matrix takes the expression

$$S=\begin{pmatrix}1-i\rho_0\mathcal{T}_{0\to0} & -i\rho_f\mathcal{T}_{0\to f}\\ -i\rho_0\mathcal{T}_{f\to0} & 1-i\rho_f\mathcal{T}_{f\to f}\end{pmatrix}, \tag{3.16}$$

$$\text{with } \rho_0=2\kappa_0/(2\mu_0)^{1/2},\quad \rho_f=2\kappa_f/(2\mu_f)^{1/2}, \tag{3.17}$$

where $\mathcal{T}_{0\to0}$ and $\mathcal{T}_{0\to f}$ are the collision matrix elements for the scattering process $1+(2,3)\to1+(2,3)$ and pick-up process $1+(2,3)\to(1,3)+2$, respectively, and where $\mathcal{T}_{f\to0}$ and $\mathcal{T}_{f\to f}$ are the elements for the reverse processes, $(1,3)+2\to1+(2,3)$ and $(1,3)+2\to(1,3)+2$, respectively.

The example discussed here corresponds exactly, for example, to the physical problem of the collision of positron by a hydrogen atom at energies below the first excitation threshold of the target hydrogen. In this case, $\mathcal{T}_{0\to0}$ corresponds to the elastic scattering and $\mathcal{T}_{0\to f}$ corresponds to the positronium formation, while $\mathcal{T}_{f\to f}$ and $\mathcal{T}_{f\to0}$ correspond to the reverse processes of positronium scattering and electron capture by a proton.

These matrix elements are expressed in terms of the χ's as follows:

$$\mathcal{T}_{0\to0}=(Z_1/\lambda_0)[2\mu_1(-s_0)]^{1/2}\chi_{\lambda_0l_0}{}^{(1)}(K_0,s;K_0)\,, \tag{3.18}$$

$$\mathcal{T}_{f\to0}=(Z_1/\lambda_0)[2\mu_1(-s_0)]^{1/2}\chi_{\lambda_0l_0}{}^{(1)}(K_0,s;K_f)\,, \tag{3.19}$$

$$\text{and}\quad \mathcal{T}_{f\to f}=(Z_2/\lambda_0)[2\mu_2(-s_f)]^{1/2}\chi_{\lambda_fl_f}{}^{(2)}(K_f,s;K_f)\,, \tag{3.20}$$

where the additional (last) argument in the χ's is introduced to indicate that the corresponding limit for the initial state has been taken. The expression for $\mathcal{T}_{0\to f}$ is given by Eq. (3.7). Similar expressions for these collision matrix elements, such as Eq. (3.11), can be obtained from Eq. (2.39) in terms of Coulomb functions in exactly the same manner.

The symmetric, and unitary S matrix given by Eq. (3.16), may be diagonalized by a real, orthogonal matrix[11,19]

$$O=\begin{pmatrix}\cos\zeta & \sin\zeta\\ -\sin\zeta & \cos\zeta\end{pmatrix}, \tag{3.21}$$

to give $$OSO^{-1}=\begin{pmatrix} e^{2i\delta_1} & 0 \\ 0 & e^{2i\delta_2} \end{pmatrix}, \tag{3.22}$$

where δ_1 and δ_2 are the eigenphase shifts and ξ is the connecting parameter.

In terms of the eigenphase shifts and the connecting parameter, the collision matrix elements take the form

$$\mathcal{T}_{0\to 0}=(i/\rho_0)[\cos^2\xi e^{2i\delta_1}+\sin^2\xi\, e^{2i\delta_2}-1], \tag{3.23}$$

$$\mathcal{T}_{0\to f}=(i/2\rho_f)\sin(2\xi)[e^{2i\delta_1}-e^{2i\delta_2}], \tag{3.24}$$

$$\mathcal{T}_{f\to 0}=(i/2\rho_0)\sin(2\xi)[e^{2i\delta_1}-e^{-2i\delta_2}], \tag{3.25}$$

$$\mathcal{T}_{f\to f}=(i/\rho_f)[\sin^2\xi\, e^{2i\delta_1}+\cos^2\xi\, e^{2i\delta_2}-1]. \tag{3.26}$$

If more than two channels are open, the dimension of the S matrix will, of course, increase. More connecting parameters are required in the real, orthogonal matrix O to diagonalize the S matrix. In general if there are n channels to be considered, there will be n eigenphase shifts. One would therefore need $n(n-1)/2$ connecting parameters to characterize the O matrix for the diagonalization of the S matrix.

IV. REDUCTION FOR IDENTICAL PARTICLES

The equations in Secs. II and III can be further simplified for cases with identical particles. As an example we consider the problem of electron scattering by a hydrogen atom (or helium ion). This is a system with two identical electrons having spin one half. For definiteness let us label the two electrons by "1" and "2" and the proton by "3." The equations derived in Sec. III C can be immediately taken over for the inelastic direct and exchange scatterings in the (e, H) system. In this case, we have $\epsilon_0=\epsilon_f$. The scattering matrix elements for the direct and exchange scattering are given, respectively, by Eq. (3.18) and Eq. (3.7) if the incident electron is "1" and, respectively, by Eq. (3.20) and Eq. (3.19) if the incident electron is "2." Because of the identity of the electrons, there is no physical means of telling which was the incident electron. The two scattering amplitudes as well as the two exchange amplitudes should therefore be equivalent.

The S matrix may easily be diagonalized, giving two solutions, as, for example, in Sturmian-function representation

$$\mathcal{T}^{(+)}=\mathcal{T}_d+\mathcal{T}_{\text{ex}}=(Z_1/\lambda_0)[2\mu_1(-s_0)]^{1/2}[\chi_{\lambda_0 l_0}{}^{(1)}(K_0,s;K_0)+\chi_{\lambda_0 l_0}{}^{(2)}(K_0,s;K_0)]; \tag{4.1}$$

$$\mathcal{T}^{(-)}=\mathcal{T}_d-\mathcal{T}_{\text{ex}}=(Z_1/\lambda_0)[2\mu_1(-s_0)]^{1/2}[\chi_{\lambda_0 l_0}{}^{(1)}(K_0,s;K_0)-\chi_{\lambda_0 l_0}{}^{(2)}(K_0,s;K_0)], \tag{4.2}$$

which correspond to the familiar singlet and triplet scattering matrix elements. From this result it is apparent that, for singlet scattering, one need only calculate the sum of the direct and exchange amplitudes and, for triplet scattering, only the difference of the direct and exchange amplitudes. The fact that the S matrix for a nonrelativistic two-electron system is diagonal in spin states is actually a very general result[11] (not limited to elastic scattering). We now show that a set of reduced equations for the sum, as well as for the difference, of the direct and exchange scattering matrix elements may be derived for the singlet and triplet scatterings.

Utilizing the symmetry relations [see Eqs. (2.16) and (2.17)]

$$P_l(\omega_2)P_{l'}(\bar{\omega}_1)=(-)^{l+l'}P_l(\omega_1)P_{l'}(\bar{\omega}_2), \tag{4.3}$$

$$P_l(\omega_2)P_{l'}(\bar{\omega}_3)=(-)^{l+l'}P_l(\omega_1)P_{l'}(\bar{\omega}_3), \tag{4.4}$$

$$P_l(\omega_3)P_{l'}(\bar{\omega}_2)=(-)^{l+l'}P_l(\omega_3)P_{l'}(\bar{\omega}_1). \tag{4.5}$$

The set of single-variable equations [Eqs. (2.28) or Eqs. (2.44)] may be rewritten

$$\chi_{\nu l}^{(1)}(q,s)=\eta_{\nu l}^{(1)}(q,s)+\sum_{\nu' l'}\int_0^\infty dq_2{}^2\varkappa_{\nu l,\nu' l'}^{(1,2)}(q,q_2;s)\chi_{\nu' l'}{}^{(2)}(q_2,s)+\sum_{\nu' l'}\int_0^\infty dq_3{}^2\varkappa_{\nu l,\nu' l'}^{(1,3)}(q,q_3;s)$$
$$\times\chi_{\nu' l'}{}^{(3)}(q_3,s)\,, \tag{4.6}$$

$$\chi_{\nu l}^{(2)}(q,s)=\eta_{\nu l}^{(2)}(q,s)+\sum_{\nu' l'}(-)^{l+l'}\int_0^\infty dq_2{}^2\varkappa_{\nu l,\nu' l'}^{(1,2)}(q,q_2;s)\chi_{\nu' l'}{}^{(1)}(q_2,s)+\sum_{\nu' l'}(-)^{l+l'}\int_0^\infty dq_3{}^2\varkappa_{\nu l,\nu' l'}^{(1,3)}$$
$$\times(q,q_3;s)\chi_{\nu' l'}{}^{(3)}(q_3,s), \tag{4.7}$$

$$\chi_{\nu l}^{(3)}(q,s)=\eta_{\nu l}^{(3)}(q,s)+\sum_{\nu' l'}\int_0^\infty dq_2{}^2\varkappa_{\nu l,\nu' l'}^{(3,1)}(q,q_2;s)[\chi_{\nu' l'}{}^{(1)}(q_2,s)+(-)^{l+l'}\chi_{\nu' l'}{}^{(2)}(q_2,s)]\,, \tag{4.8}$$

Multiplying Eq. (4.7) by $(-)^l$, adding the resultant to Eq. (4.6), and also subtracting the resultant from Eq. (4.6), we obtain

$$u_{\nu l}{}^{(1,2)}(q,s)=\xi_{\nu l}{}^{(1,2)}(q,s)+\sum_{\nu' l'}(-)^{l'}\int_0^\infty dq'^2\varkappa_{\nu l,\nu' l'}^{(1,2)}(q,q';s)u_{\nu' l'}{}^{(1,2)}(q',s)+\sum_{\nu' l'}[1+(-)^{l'}]\int_0^\infty dq'^2$$
$$\times\varkappa_{\nu l,\nu' l'}^{(1,3)}(q,q';s)\chi_{\nu' l'}{}^{(3)}(q',s)\,, \tag{4.9}$$

$$v_{\nu l}{}^{(1,2)}(q,s)=\zeta_{\nu l}{}^{(1,2)}(q,s)+\sum_{\nu' l'}(-)^{l'+1}\int_0^\infty dq'^2\varkappa_{\nu l,\nu' l'}^{(1,2)}(q,q';s)v_{\nu' l'}{}^{(1,2)}(q',s)+\sum_{\nu' l'}[1-(-)^{l'}]\int_0^\infty dq'^2$$
$$\times\varkappa_{\nu l,\nu' l'}^{(1,3)}(q,q';s)\chi_{\nu' l'}{}^{(3)}(q',s)\,, \tag{4.10}$$

$$\chi_{\nu l}{}^{(3)}(q,s)=\eta_{\nu l}{}^{(3)}(q,s)+\tfrac{1}{2}[1+(-)^l]\sum_{\nu' l'}\int_0^\infty dq'^2\varkappa_{\nu l,\nu' l'}^{(3,1)}(q,q';s)u_{\nu' l'}{}^{(1,2)}(q',s)+\tfrac{1}{2}[1-(-)^l]\sum_{\nu' l'}\int_0^\infty dq'^2$$
$$\times\varkappa_{\nu l,\nu' l'}^{(3,1)}(q,q';s)v_{\nu' l'}{}^{(1,2)}(q',s)\,, \tag{4.11}$$

with $u_{\nu l}{}^{(1,2)}(q,s)\equiv\chi_{\nu l}{}^{(1)}(q,s)+(-)^l\chi_{\nu l}{}^{(2)}(q,s)\,,$ (4.12)

$$v_{\nu l}{}^{(1,2)}(q,s)\equiv\chi_{\nu l}{}^{(1)}(q,s)-(-)^l\chi_{\nu l}{}^{(2)}(q,s)\,, \tag{4.13}$$

$$\xi_{\nu l}{}^{(1,2)}(q,s)\equiv\eta_{\nu l}{}^{(1)}(q,s)+(-)^l\eta_{\nu l}{}^{(2)}(q,s)\,, \tag{4.14}$$

$$\zeta_{\nu l}{}^{(1,2)}(q,s)\equiv\eta_{\nu l}{}^{(1)}(q,s)-(-)^l\eta_{\nu l}{}^{(2)}(q,s)\,, \tag{4.15}$$

where we have rewritten Eq. (4.8) in terms of $u_{\nu l}{}^{(1,2)}$ and $v_{\nu l}{}^{(1,2)}$ as Eq. (4.11).

Since the Pauli principle excludes the possibility for two electrons in the singlet-spin states to have odd parity, we have

$$\chi_{\nu l}{}^{(3)}(q,s)=0,\quad\text{and odd } l\,. \tag{4.16}$$

Equation (4.16), together with the fact that when l' is even the factor $[1-(-)^{l'}]$ eliminates the $\chi_{\nu' l'}{}^{(3)}$ term in Eq. (4.10), uncouples $v_{\nu l}{}^{(1,2)}$ and $\chi_{\nu l}{}^{(3)}$ in the set of coupled equations. We then have, for singlet scattering, the reduced set of single-variable integral equations:

$$\begin{pmatrix} u_{\nu l}{}^{(1,2)}(q,s) \\ \chi_{\nu l}{}^{(3)}(q,s) \end{pmatrix}=\begin{pmatrix} \xi_{\nu l}{}^{(1,2)}(q,s) \\ \eta_{\nu l}{}^{(3)}(q,s) \end{pmatrix}+\sum_{\nu' l'}\int_0^\infty dq'^2$$

$$\times\begin{pmatrix} (-)^{l'}\mathcal{K}^{(1,2)}_{\nu l,\nu' l'}(q,q';s) & 2\mathcal{K}^{(1,3)}_{\nu l,\nu' l'}(q,q';s) \\ \mathcal{K}^{(3,1)}_{\nu l,\nu' l'}(q,q';s) & 0 \end{pmatrix}\begin{pmatrix} u_{\nu' l'}{}^{(1,2)}(q,s) \\ \chi_{\nu' l'}{}^{(3)}(q,s) \end{pmatrix} \quad , \tag{4.17}$$

$$v_{\nu l}{}^{(1,2)}(q,s)=\zeta_{\nu l}{}^{(1,2)}(q,s)+\sum_{\nu' l'}(-)^{l'+1}\int_0^\infty dq'^2\mathcal{K}^{(1,2)}_{\nu l,\nu' l'}(q,q';s)v_{\nu' l'}{}^{(1,2)}(q',s)\,. \tag{4.18}$$

Similarly, since the Pauli principle excludes the possibility for two electrons in the triplet-spin states to have even parity, we have

$$\chi_{\nu l}{}^{(3)}(q,s)=0, \quad \text{for even } l\,. \tag{4.19}$$

Equation (4.19), together with the fact that when l' is odd the factor $[1+(-)^{l'}]$ eliminates the $\chi_{\nu' l'}{}^{(3)}$ terms in Eq. (4.9), decouples the functions $u_{\nu l}{}^{(1,2)}$ with $\chi_{\nu l}{}^{(3)}$ in the set of equations. We then have, for triplet scattering, the reduced set of single-variable integral equations:

$$u_{\nu l}{}^{(1,2)}(q,s)=\xi_{\nu l}{}^{(1,2)}(q,s)+\sum_{\nu' l'}(-)^{l'}\int_0^\infty dq'^2\,\mathcal{K}^{(1,2)}_{\nu l,\nu' l'}(q,q';s)u_{\nu' l'}{}^{(1,2)}(q',s)\,, \tag{4.20}$$

$$\begin{pmatrix} \chi_{\nu l}{}^{(3)}(q,s) \\ v_{\nu l}{}^{(1,2)}(q,s) \end{pmatrix}=\begin{pmatrix} \eta_{\nu l}{}^{(3)}(q,s) \\ \zeta_{\nu l}{}^{(1,2)}(q,s) \end{pmatrix}+\sum_{\nu' l'}\int_0^\infty dq'^2\begin{pmatrix} 0 & \mathcal{K}^{(3,1)}_{\nu l,\nu' l'}(q,q';s) \\ 2\mathcal{K}^{(1,3)}_{\nu l,\nu' l'}(q,q';s) & (-)^{l'+1}\mathcal{K}^{(1,2)}_{\nu l,\nu' l'}(q,q';s) \end{pmatrix}$$

$$\times\begin{pmatrix} \chi_{\nu' l'}{}^{(3)}(q',s) \\ v_{\nu' l'}{}^{(1,2)}(q',s) \end{pmatrix} \quad . \tag{4.21}$$

These are interesting results, since they simplify the actual calculation considerably. [It is of interest to observe that Eqs. (4.17) and (4.21), except for the inhomogeneous terms, are identical to the equations used in Paper I for the calculation of three-body bound and resonance states with $\chi_{\lambda l}{}^{(1)}$ and $\chi_{\lambda l}{}^{(2)}$ replaced by $u_{\lambda l}{}^{(1,2)}$ and $v_{\lambda l}{}^{(1,2)}$, respectively.]

For singlet scatterings into even-l states, instead of having to solve the three coupled sets of equations [Eq. (2.28) or Eq. (2.44)], one needs to solve only Eq. (4.17) which has just two coupled sets of equations. For singlet scattering into odd-l final states one needs to solve only a single set of equations [Eq. (4.18)]. We have for $J=M=0$ singlet-scattering matrix elements, for example, in the Sturmian-function representation:

$$\mathcal{T}_{0\to f}{}^{(\uparrow\downarrow)}=(Z_1/\lambda_f)[2\mu_1(-s_f)]^{1/2}u_{\lambda_f l_f}{}^{(1,2)}(K_f,s;K_0), \quad \text{for } l_f \text{ even}\,, \tag{4.22}$$

$$\mathcal{T}_{0\to f}{}^{(\uparrow\downarrow)}=(Z_1/\lambda_f)[2\mu_1(-s_f)]^{1/2}v_{\lambda_f l_f}{}^{(1,2)}(K_f,s;K_0), \quad \text{for } l_f \text{ odd}, \tag{4.23}$$

where the ↑ and ↓ arrows denote spin up and spin down for the two electrons, respectively, and where the $u_{\lambda_f l_f}$ and the $v_{\lambda_f l_f}$ are obtained from the solution of Eqs. (4.17) and (4.18), respectively.

The scattering matrix elements corresponding to the two possible final states resulting from direct and exchange scatterings can be easily recovered by forming linear combinations of $u_{\lambda_f l_f}{}^{(1,2)}$ and $v_{\lambda_f l_f}{}^{(1,2)}$ We have, for direct scattering,

$$\mathcal{T}_{0\to f}{}^{(\uparrow\downarrow\to\uparrow\downarrow)}=(Z_1/2\lambda_f)[2\mu_1(-s_f)]^{1/2}[u_{\lambda_f l_f}{}^{(1,2)}(K_f,s;K_0)+v_{\lambda_f l_f}{}^{(1,2)}(K_f,s;K_0)]\,, \tag{4.24}$$

and, for exchange scattering,

$$\mathcal{T}_{0\to f}{}^{(\uparrow\downarrow\to\downarrow\uparrow)}=(-)^{l_f}(Z_1/2\lambda_f)[2\mu_1(-s_f)]^{1/2}[u_{\lambda_f l_f}{}^{(1,2)}(K_f,s;K_0)-v_{\lambda_f l_f}{}^{(1,2)}(K_f,s;K_0)]\,. \tag{4.25}$$

The two scattering processes can be directly studied experimentally, using polarized electron beams. In the first case, the scattered electron retains its spin orientation, and in the second case the scattered electron has its spin flipped.

For triplet scatterings we solve Eqs. (3.38a) or (3.38b), depending on whether the final state has odd- or even-l_f, respectively. We have

$$\mathcal{T}_{0\to f}(\uparrow\uparrow) = (Z_1/\lambda_f)[2\mu_1(-s_f)]^{1/2} u_{\lambda_f l_f}{}^{(1,2)}(K_f, s; K_0), \quad \text{for } l_f \text{ odd}, \tag{4.26}$$

$$\mathcal{T}_{0\to f}(\uparrow\uparrow) = (Z_1/\lambda_f)[2\mu_1(-s_f)]^{1/2} v_{\lambda_f l_f}{}^{(1,2)}(K_f, s; K_0), \quad \text{for } l_f \text{ even}. \tag{4.27}$$

Here the $u_{\lambda_f l_f}$ and the $v_{\lambda_f l_f}$ are now obtained from the solutions of Eqs. (4.20) and (4.21), respectively.

V. LOW-ENERGY (*e*,H) SCATTERING

As a simple illustrative application, we consider here the calculation of a phase shift for low-energy electron scattering by hydrogen atoms. For the present we confine our interest to energies below the first resonance in the elastic channel. (These resonances in the elastic channel have been calculated using Faddeev equations in Paper I.) A very accurate variational calculation of the phase shift for this system has been carried out in this energy region by Schwartz[6] for both the singlet and triplet scatterings.

For the calculation of singlet phase shift, we may use either the full three coupled sets of equations: Eq. (2.28) [or Eq. (2.44)], for $\chi_{10}^{(1)}$ and $\chi_{10}^{(2)}$; or the reduced equations Eq. (4.17), for $u_{10}^{(1,2)}$. Calculation has been carried out using both the full and the reduced equations. The results from the two sets of equations, of course, agree and are shown in Fig. 1, together with the variational result of Schwartz. Similarly, the result for triplet phase shifts obtained from Eq. (4.18) agrees with that from the full equation and is shown in Fig. 2 together with the variational results.

There are several methods for solving such coupled single-variable integral equations. In the present calculation the matrix inversion method was adopted. For numerical accuracy, the branch points associated with the ground target state were removed from the matrix to be inverted, by the Fredholm reduction method as described in Paper I. The matrix inversion was carried out by straightforward digitizing the continuous variable q and q' for each fixed value of the three-body energy s. To check the accuracy, we have also solved this set of equations by a stationary variational method.[9] The variational results converge to the results obtained by the matrix inversion.

The present calculations were carried out by retaining only the first term [i.e., the $(\lambda l = 10)$ $1s$ term] in the Sturmian-function expansion. The inclusion of more states does not pose any difficulty. There are, however, practical difficulties with the matrix inversion method due to the limitations of computer storage, because the dimension of the matrix to be inverted after digitizing increases rapidly with increasing number of states to be included. However, this practical difficulty does not appear to be serious for the stationary variational method.

The agreement of the present calculation with the Schwartz variational result is remarkable for the singlet case but not at all for the triplet case. This result is understandable for the triplet case since, by retaining only the $1s$ term, we have, from the fact that $\chi_{10}^{(3)} = 0$, neglected electron-electron correlations. The presence of the second electron is felt only through the Pauli exclusion principle. The remarkable agreement for the singlet case obtained by using only a single term is interesting but should not be taken too seriously, as it was pointed out in Paper I that the Sturmian-function expansion converges in an oscillatory manner and involves cancellations. The purpose of the present investigation is to demonstrate our method of determining the phase shift.

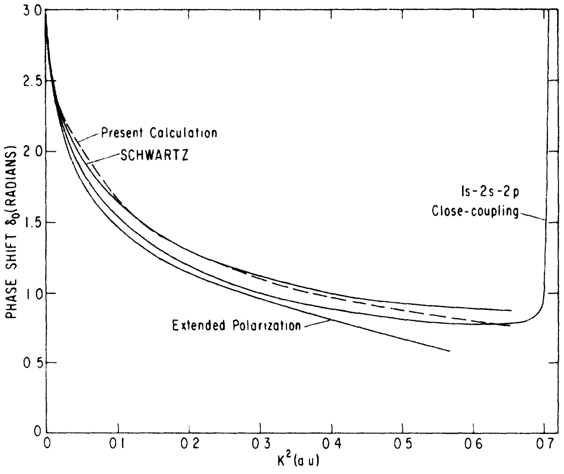

FIG. 1. Singlet s-wave phase shift for the (e, H) system: Schwartz (variational, Ref. 6); $1s$-$2s$-$2p$ closed coupling (Ref. 7); extended polarization (Ref. 8).

The problem of convergence and comparison of the Sturmian-function expansion and the Coulomb-function representation are given elsewhere in Paper III[9] of this series.

As expected the 1s term alone fails to predict the resonances near the first excitation threshold. These resonances can be accounted for[9] when more terms are included as shown in Paper I. The scattering length obtained in the present 1s-term calculation is $6.337a_0$ and $3.112a_0$ for the singlet and triplet scatterings, respectively. The corresponding values obtained by the variational method are $5.965a_0$ and $1.769a_0$, respectively.[6]

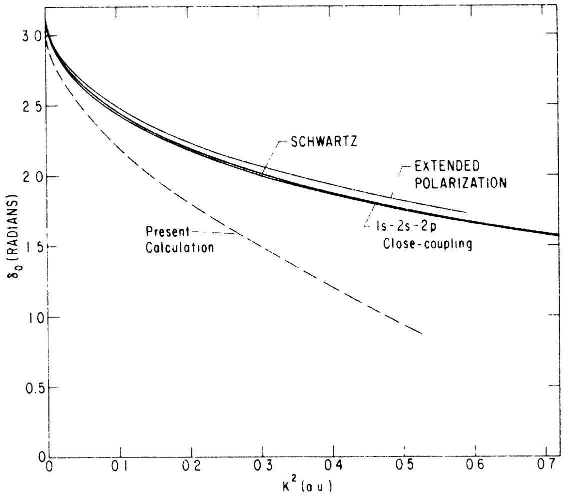

FIG. 2. Triplet s-wave phase shift for the (e, H) system: Schwartz (variational, Ref. 6); 1s-2s-2p closed coupling (Ref. 7); extended polarization (Ref. 8).

For comparison with other methods we have included in Figs. 1 and 2 recent results obtained from 1s-2s-2p close-coupling calculations by Burke and Schey[7] and the extended polarization potential by Callaway *et al.*[8] These are representative results for the target-state expansion and the polarized orbit methods. (For other calculations one should consult the original papers cited in these two references, in particular, the paper on the polarized orbit method by Temkin and Lamkin.[20]) It is seen from this comparison that the present procedure has interesting possibilities.

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APPENDIX A. APPLICATION TO HEAVY-PARTICLE REACTIONS

The method proposed in the previous sections may be applied equally well to problems involving composite particles such as atoms or molecules, with some simple modifications. For convenience we will refer to the composite particles as atoms. In dealing with reactions involving atoms in the framework of the three-body theory of Faddeev, atoms in different electronic states are considered as different atoms. For example, the collisional excitation process

$$A + B \rightarrow A + B^* , \tag{A.1}$$

in which atom B is excited into a different electronic state, may be considered as a three-body system consisting of A, B, and B^* (three atoms). Similarly, the exchange reaction

$$AB + C \rightarrow AC + B \tag{A.2}$$

may be considered as a three-body system, provided the three atoms A, B, and C remain in their respective electronic states asymptotically.

Now if the interaction potentials between each pair of atoms for such a three-body system are known reasonably accurately from, for example, calculations using the molecular-orbital method, the method for solving Faddeev equations given in Sec. II may be readily applied, since the separable expansion given by Eq. (2.20), or Eqs. (2.33) and (2.34), are valid for any central field potentials. However, in the present case the two-body eigenvalue problems [see Eqs. (2.25) or (2.35)] for each atom-atom pair potential, unlike for the Coulomb potential, may no longer be solved in closed form. Nevertheless, this provides no additional difficulties in principle since such two-body eigenvalue problems may always be solved numerically. The convergence of the partial-wave decomposition for heavy particle reactions may in certain cases give rise to some practical difficulties. If this is the case, the alternative method for representing the two-body off-shell amplitude becomes desirable.

In certain cases, the interaction potential for a three-atom system may not be adequately approximated by a sum of three atom-atom pair interactions, since there may be an additional intrinsic three-body potential in the system. For such a case, the Faddeev equations must be modified to account for the intrinsic three-body interactions. A modification of the Faddeev equations for systems with a three-body force was carried out by Newton.[10] Here we give a simple derivation of the modified Faddeev equations.

In the presence of an intrinsic three-body force, the total interaction V may be written

$$V=\sum_i V_i + U, \tag{A.3}$$

where the V_i are the atom-atom pair interactions and U is the intrinsic three-body interaction. In addition to the Lippmann-Schwinger equations for two-body potential V_i given by Eq. (2.6), we now also have an equation for the three-body potential U:

$$T_4(s) = UG_0(s)T_4(s). \tag{A.4}$$

Owing to the presence of U, one expects that certain portions of the three-atom collision matrix $T(s)$ will have all the three atoms undergoing a final-state interaction. We may now decompose the three-atom collision matrix into four components:

$$T(s)=T^{(1)}(s)+T^{(2)}(s)+T^{(3)}(s)+T^{(4)}(s), \tag{A.5}$$

with $$T^{(i)}(s)=V_i+V_iG_0(s)T(s), \quad i=1,2,3, \tag{A.6}$$

$$T^{(4)}(s)=U+UG_0(s)T(s), \tag{A.7}$$

where $T^{(1)}$, $T^{(2)}$, and $T^{(3)}$ correspond, as before, to portions of the three-body scattering matrix in which alternative pairs of atoms undergo a final-state interaction, and $T^{(4)}$ corresponds to that scattering matrix in which all the three atoms undergo a final-state interaction.

Define the expression

$$\Omega_i = T^{(i)} - T_i - \sum_{j\neq i} T_i G_0 T^{(j)}, \quad i=1,2,3,4. \tag{A.8}$$

One can readily show by utilizing Eqs. (2.6), (A.4), (A.6), and (A.7) that

$$\Omega_i = V_i G_0 \Omega_i, \quad i=1,2,3, \tag{A.9}$$

$$\Omega_4 = UG_0\Omega_4. \tag{A.10}$$

Since neither V_iG_0 nor UG_0 is an identity operator, Eqs. (A.9) and (A.10) imply that $\Omega_i=0$ for all i. We then obtain the Faddeev equations in the presence of three-body force:

$$\begin{pmatrix} T^{(1)}(s)\\ T^{(2)}(s)\\ T^{(3)}(s)\\ T^{(4)}(s)\end{pmatrix}=\begin{pmatrix} T_1(s)\\ T_2(s)\\ T_3(s)\\ T_4(s)\end{pmatrix}+\begin{pmatrix} 0 & T_1(s) & T_1(s) & T_1(s)\\ T_2(s) & 0 & T_2(s) & T_2(s)\\ T_3(s) & T_3(s) & 0 & T_3(s)\\ T_4(s) & T_4(s) & T_4(s) & 0\end{pmatrix} G_0(s) \begin{pmatrix} T^{(1)}(s)\\ T^{(2)}(s)\\ T^{(3)}(s)\\ T^{(4)}(s)\end{pmatrix} \tag{A.11}$$

This is the same set of equations as derived by Newton.[10]

The difficulty in solving these coupled equations arises primarily from solving Eq. (A.4). Since U is now a three-body potential, Eq. (A.4) unlike Eq. (2.6) can no longer be effectively reduced to a two-body equation. However, if the three-body potential is weak, a perturbation scheme may be adopted, in which one replaces $T_4(s)$ in the first-order approximation by U in the equation for $T^{(4)}(s)$, and then eliminates $T^{(4)}(s)$ by substituting back into the equations for the $T^{(i)}$ with $i=1$, 2, and 3.

APPENDIX B. AN ALTERNATIVE SET OF SINGLE-VARIABLE INTEGRAL EQUATIONS

In Eqs. (2.34) three alternative series representations of the Coulomb potential $V_l(p,p')$ [Eq. (2.20)] are given.[15] Though they are equivalent, when all the terms in the series are included, they have rather different convergence properties,[17] depending on their arguments p and p'. In Sec. II C, Eq. (2.34a) was adopted. No essential change in the formulation may result if Eq. (2.34b) is adopted instead. The third representation given by Eq. (2.34c) is a symmetrized version of Eqs. (2.34a) and (2.34b). In each term it preserves the symmetry of $V_l(p,p')$ in interchanging p and p'. Though in principle this is a desired feature, this symmetrized representation, when utilized, would result in a larger set of coupled equations.

When the symmetrized representation for $V_l(p,p')$ is utilized, the two-body off-shell scattering amplitude may be written

$$t_l(p,p';E)=\tfrac{1}{4}\pi\sum_n{}'[(p^2-\epsilon_n)(p'^2-E)/(E-\epsilon_n)+(p'^2-\epsilon_n)(p^2-E)/(E-\epsilon_n)]\,\psi_{nl}(np)\psi_{nl}(np')\,. \tag{B.1}$$

The off-shell three-body collision amplitude with a pair of particles undergoing attractive final state interaction may then be written

$$\Psi_l^{(i)}(p,q,s)=\Phi_l^{(i)}(p,q,s)+\frac{\pi}{4}\sum_n{}'\frac{p^2-\epsilon_n^{(i)}}{s-q^2-\epsilon_n^{(i)}}\psi_{nl}(np)\chi_{nl}^{(ia)}(q,s)+\frac{\pi}{4}\sum_n{}'\frac{p^2+q^2-s}{s-q^2-\epsilon_n^{(i)}}\psi_{nl}(np)\chi_{nl}^{(ib)}(q,s)\,, \tag{B.2}$$

For definiteness, we consider the same problem as that in Sec. II C in which the 3rd pair (i.e., particles 1 and 2) have a repulsive potential, and are represented by the Sturmian-function expansion. We then have Eq. (2.40) for $\Psi_l^{(3)}(p,q,s)$. The unknown functions $\chi_{nl}^{(ia)}$ and $\chi_{nl}^{(ib)}$ with $i=1$ and 2, and $\chi_{\lambda l}^{(3)}$ satisfy a set of coupled single-variable integral equations

$$\begin{aligned}\chi_{nl}^{(ia)}(q,s)={}&\eta_{nl}^{(ia)}(q,s)+\sum_{n'l'}{}'\sum_{j\neq i,j\neq 3}\int_0^\infty dq_j{}^2\,\mathcal{K}_{nl,n'l'}^{(ia,ja)}(q,q_j;s)\chi_{n'l'}^{(ja)}(q_j,s)\\&+\sum_{n'l'}{}'\sum_{j\neq i,j\neq 3}\int_0^\infty dq_j{}^2\,\mathcal{K}_{nl,n'l'}^{(ia,jb)}(q,q_j;s)\chi_{n'l'}^{(jb)}(q_j,s)+\sum_{\lambda'l'}\int_0^\infty dq_3{}^2\,\mathcal{K}_{nl,\lambda'l'}^{(ia,3)}(q,q_3;s)\chi_{\lambda'l'}^{(3)}(q_3,s)\,,\end{aligned} \tag{B.3a}$$

$$\begin{aligned}\chi_{nl}^{(ib)}(q,s)={}&\eta_{nl}^{(ib)}(q,s)+\sum_{n'l'}{}'\sum_{j\neq i,j\neq 3}\int_0^\infty dq_j{}^2\,\mathcal{K}_{nl,n'l'}^{(ib,ja)}(q,q_j;s)\chi_{n'l'}^{(ja)}(q_j,s)\\&+\sum_{n'l'}{}'\sum_{j\neq i,j\neq 3}\int_0^\infty dq_j{}^2\,\mathcal{K}_{nl,n'l'}^{(ib,jb)}(q,q_j;s)\chi_{n'l'}^{(jb)}(q_j,s)+\sum_{\lambda'l'}\int_0^\infty dq_3{}^2\,\mathcal{K}_{nl,n'l'}^{(ib,3)}(q,q_3;s)\chi_{\lambda'l'}^{(3)}(q_3,s)\,,\end{aligned} \tag{B.3b}$$

$$\begin{aligned}\chi_{\lambda l}^{(3)}(q,s)={}&\eta_{nl}^{(3)}(q,s)+\sum_{n'l'}{}'\sum_{j\neq 3}\int_0^\infty dq_j{}^2\,\mathcal{K}_{\lambda l,n'l'}^{(3,ja)}(q,q_j;s)\chi_{n'l'}^{(ja)}(q_j,s)\\&+\sum_{n'l'}{}'\sum_{j\neq 3}\int_0^\infty dq_j{}^2\,\mathcal{K}_{\lambda l,n'l'}^{(3,jb)}(q,q_j;s)\chi_{n'l'}^{(jb)}(q_j,s),\end{aligned} \tag{B.3c}$$

with

$$\mathcal{K}_{nl,n'l'}^{(ia,ja)}(q,q_j;s)=-\frac{\pi}{4}\int_{L_{ij}}^{U_{ij}}dp_j{}^2B_{ll'}^{(i,j)}(q,p_j,q_j;s)\frac{(p_j{}^2+q_j{}^2-s)(p_j{}^2-\epsilon_{n'}^{(j)})}{s-\epsilon_{n'}^{(j)}-q_j{}^2}\psi_{nl}^{(i)}(np_i)\psi_{n'l'}^{(j)}(n'p_j), \tag{B.4a}$$

$$\mathcal{K}_{nl,n'l'}^{(ia,jb)}(q,q_j;s)=-\frac{\pi}{4}\int_{L_{ij}}^{U_{ij}}dp_j{}^2B_{ll'}^{(i,j)}(q,p_j,q_j;s)\frac{(p_j{}^2+q_j{}^2-s)^2}{s-\epsilon_{n'}^{(j)}-q_j{}^2}\psi_{nl}^{(i)}(np_i)\psi_{n'l'}^{(j)}(n'p_j)\,, \tag{B.4b}$$

$$\mathcal{K}_{nl,\lambda'l'}^{(ia,3)}(q,q_j;s)=\int_{L_{i3}}^{U_{i3}}dp_3{}^2B_{ll'}^{(i,3)}(q,p_3,q_3;s)\frac{p_3{}^2+q_3{}^2-s}{1-\gamma_{\lambda'l'}^{(3)}(s-q_3{}^2)}\psi_{nl}^{(i)}(np_i)\phi_{\lambda'l'}^{(3)}(p_3,s-q_3{}^2)\,, \tag{B.4c}$$

$$\mathcal{K}_{nl,n'l'}^{(ib,ja)}(q,q_j;s)=-\frac{\pi}{4}\int_{L_{ij}}^{U_{ij}}dp_j{}^2B_{ll'}^{(i,j)}(q,p_j,q_j;s)\frac{(p_j{}^2+q_j{}^2-q^2-\epsilon_n^{(i)})(p_j{}^2-\epsilon_{n'}^{(j)})}{s-\epsilon_{n'}^{(j)}-q_j{}^2}$$

$$\times \psi_{nl}^{(i)}(np_i)\psi_{n'l'}^{(j)}(n'p_j), \tag{B.4d}$$

$$\mathcal{K}_{nl,n'l'}^{(ib,jb)}(q,q_j;s) = -\frac{\pi}{4}\int_{L_{ij}}^{U_{ij}} dp_j^{\,2} B_{ll'}^{(i,j)}(q,p_j,q_j;s)\frac{(p_j^{\,2}+q_j^{\,2}-q^2-\epsilon_n^{(i)})(p_j^{\,2}+q_j^{\,2}-s)}{s-\epsilon_{n'}^{(j)}-q_j^{\,2}}$$

$$\times \psi_{nl}^{(i)}(np_i)\psi_{n'l'}^{(j)}(n'p_j), \tag{B.4e}$$

$$\mathcal{K}_{nl,\lambda'l'}^{(ib,3)}(q,q_3;s) = \int_{L_{i3}}^{U_{i3}} dp_3^{\,2} B_{ll'}^{(i,3)}(q,p_j,q_j;s)\frac{(p_3^{\,2}+q_3^{\,2}-q^2-\epsilon_n^{(i)}}{1-\gamma_{\lambda'l'}(3)(s-q_3 2)}\psi_{nl}^{(i)}(np_i)\phi_{\lambda'l'}^{(3)}(p_3,s-q_3^{\,2}), \tag{B.4f}$$

$$\mathcal{K}_{\lambda l,n'l'}^{(3,ja)}(q,q_j;s) = \frac{\pi}{4}\int_{L_{3j}}^{U_{3j}} dp_j^{\,2} B_{ll'}^{(3,j)}(q,p_j,q_j;s)\frac{p_j^{\,2}-\epsilon_{n'}^{(j)}}{s-\epsilon_{n'}^{(j)}-q_j^{\,2}}\phi_{\lambda l}^{(3)}(p_3,s-q^2)\psi_{n'l'}^{(j)}(n'p_j), \tag{B.4g}$$

$$\mathcal{K}_{\lambda l,n'l'}^{(3,jb)}(q,q_j;s) = \frac{\pi}{4}\int_{L_{3j}}^{U_{3j}} dp_j^{\,2} B_{ll'}^{(3,j)}(q,p_j,q_j;s)\frac{p_j^{\,2}+q_j^{\,2}-s}{s-\epsilon_{n'}^{(j)}-q_j^{\,2}}\phi_{\lambda l}^{(3)}(p_3,s-q^2)\psi_{n'l'}^{(j)}(n'p_j), \tag{B.4h}$$

$$\eta_{nl}^{(ia)}(q,s) = -\sum_{l',j\neq i}\int_0^\infty dq_j^{\,2}\int_{L_{ij}}^{U_{ij}} dp_j^{\,2} B_{ll'}^{(i,j)}(q,p_j,q_j;s)(p_j^{\,2}+q_j^{\,2}-s)\psi_{nl}^{(i)}(np_i)\Phi_{l'}^{(j)}(p_j,q_j,s), \tag{B.5a}$$

$$\eta_{nl}^{(ib)}(q,s) = -\sum_{l',j\neq i}\int_0^\infty dq_j^{\,2}\int_{L_{ij}}^{U_{ij}} dp_j^{\,2} B_{ll'}^{(i,j)}(q,p_j,q_j;s)(p_j^{\,2}+q_j^{\,2}-q^2-\epsilon_n^{(i)})\psi_{nl}^{(i)}(np_i)\Phi_{l'}^{(j)}(p_j,q_j,s), \tag{B.5b}$$

$$\eta_{\lambda l}^{(3)}(q,s) = \sum_{l',j\neq i}\int_0^\infty dq_j^{\,2}\int_{L_{ij}}^{U_{ij}} dp_j^{\,2} B_{ll'}^{(3,j)}(q,p_j,q_j;s)\phi_{\lambda l}^{(3)}(p_3,s-q^2)\Phi_{l'}^{(j)}(p_j,q_j,s), \tag{B.5c}$$

where the $B_{ll'}^{(i,j)}$ are given by Eq. (2.31).

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[3] It is perhaps worthwhile to note that no practical difficulties were encountered with two-body Coulomb t matrix as defined in the conventional way, although West [G. B. West, J. Math. Phys. 8, 942 (1967)] has recently raised some formal problems associated with such two-body Coulomb t matrix.

[4] We call attention to the misprints in Eqs. (I2.13), (I2.19), (I2.24), (I2.29), (I2.30), (I3.2), (I3.6), (I3.10), (I3.14), (I3.15), (I3.16), (I4.11), (I4.13), and (I4.14). From equations in this paper, these misprints should become apparent (see also Ref. 14).

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[14] The expression of Coulomb potential $V_l^{(i)}$, and the normalization of the two-body amplitude $t_l^{(i)}$, are different from those in Paper I by a sign. These changes in sign make them agree with the convention adopted in atomic physics. The Coulomb potential $V_l^{(i)}$ is attractive if $Z_i = -|Z_i|$ and repulsive if $Z_i = |Z_i|$.

[15] It should be noted that the representation for $t_l(p,p'; E)$ given by Eqs. (2.33) and (2.34) is not limited to Coulomb potentials. This representation is in general valid for any central-field potential $V_l(p,p')$. It should also be noted that this representation is not a simple expansion in terms of the set of eigenfunctions $\{\psi_{nl}\}$ of Eq. (2.25) with $V_l(p,p')$ potential, since the coefficients depend explicitly on p and p'.

[16] Since Sturmian functions form a complete set for an arbitrary negative energy, one may, in principle, utilize the completeness property for expansion to deal with problems at energies lying above the three-body break-up threshold.

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[18] If the initial and final two-body bound states were not properly factored out due to, for example, improper normalization of these wave functions, the collision amplitude is then determined only within a multiplicative constant c. Care must be exercised to remove this constant. A simple procedure for determining such a multiplicative constant is to write the collision amplitudes in terms of eigenphase shifts and connecting parameters [see Eqs. (3.23) to (3.26)], including explicitly the multiplicative constants. The constants as well as eigenphase shifts and connecting parameters can then be determined by solving this set of equations.

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Studies of Negative-Ion-Molecule Reactions in the Energy Region from 0 to 3 eV†

J. A. D. Stockdale, R. N. Compton, and P. W. Reinhardt

Health Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

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A modulated retarding-potential-difference technique has been used to define the energy width of an electron beam located in the source region of a time-of-flight mass spectrometer. Negative ions with energies in the region 0–3 eV are produced by dissociative electron attachment to gas molecules in this source and are permitted to react for a controlled continuously variable length of time with neutral molecules to produce secondary negative-ion products. From the observed time development of the reactions, the reaction rate constant may be obtained, and the cross section then calculated if the primary-ion velocity is known. Results are presented for the reactions $O^- + NO_2 \rightarrow NO_2^- + O$, $H^- + H_2O \rightarrow OH^- + H_2$, and $D^- + D_2O \rightarrow OD^- + D_2$ at a number of primary ion energies, and for the reactions $O^- + N_2O \rightarrow NO^- + NO$, $HCOO^- + SF_6 \rightarrow SF_5^{-*} + (HCOOF)$, and $SF_6^- + HCl \rightarrow F_2Cl^- + (SF_4H)$ at single energy points.

I. INTRODUCTION

It has proved difficult to measure ion-molecule or charge-exchange cross sections as functions of the primary-ion energy in the region below a few eV. Drift-tube techniques[1] are confined in practice to energies $\lesssim 0.1$ eV and yield cross sections averaged over a range of ion energies. The flowing afterglow technique[2] is limited to thermal energies and collisional heating of the target neutrals. The components of the afterglow may make it difficult to compare directly rate constants obtained in this way with those from beam methods. The latter[3] have yielded most of the information which exists on the variation of cross sections with energy but are confined[4] to the energy region above a few eV because of difficulties in obtaining adequate energy resolution and beam intensity at