student is presently evaluating the matrix element between states of different azimuthal quantum number, using the Hunter and Pritchard wave functions (see Ref. 11).

[15]G. Herzberg, Spectra of Diatomic Molecules (D. Van Nostrand Co., Inc., New York, 1950), pp. 219–226.

[16]In the muonic molecules one need not worry about spin-orbit coupling except in perturbation theory even for non-σ states since the rotational splittings are of order: $\bar{\epsilon} \times$ Ryd and spin orbit is of order: $\alpha^2 \times$ Ryd. For the electron case, however, $\bar{\epsilon} \sim 10\alpha^2$, and spin-orbit coupling effects are significant.

[17]In general, for nonidentical nuclei, even in the adiabatic approximation one cannot choose such a simple form. Rather, a linear combination of odd and even P_μ components must be chosen (see Ref. 8).

PHYSICAL REVIEW VOLUME 186, NUMBER 1 5 OCTOBER 1969

Hydrogenic- and Sturmian-Function Expansions in Three-Body Atomic Problems*

Joseph C. Y. Chen and Takeshi Ishihara†

Department of Physics and Institute for Pure and Applied Physical Sciences, University of California, San Diego, La Jolla, California 92037

(Received 24 April 1969)

Hydrogenic-function and Sturmian-function expansions are examined in both the Schrödinger and Faddeev formulations for three-body atomic problems. A detailed comparison of their convergence behavior is made. The difficulty of Sturmian-function expansion in accounting for the strong coupling between degenerate target states at excitation thresholds does not arise in the Faddeev formulation. The difficulty with the uncontrolled continuum contribution in the hydrogenic-function expansion, however, persists in both formulations. An estimation of the continuum contribution in the hydrogenic-function expansion is made for off-shell amplitudes which appear in the Faddeev formulation.

I. INTRODUCTION

It is well known that a three-body scattering function which has a specified symmetry and angular momentum but which is otherwise arbitrary can always be expanded in terms of a complete set of two-body eigenfunctions. This then leads to a set of coupled integrodifferential equations for the three-body system. Since for most physical scattering processes, one encounters the scattering to two subsystems, consisting (for the present three-body system) of an incident particle and a two-body target subsystem in a certain bound state, the complete set of eigenfunctions of the two-body target subsystem constitutes, therefore, a natural set for the expansion.[1]

For atomic systems (with Coulomb potentials), the two-body target functions are hydrogenic functions which form a complete set only after continuum states are included. It was, therefore, generally felt that such a hydrogenic-function (HF) expansion would converge slowly since it involves continuum states. To avoid the continuum states, an alternative expansion in terms of Sturmian functions which form a complete set of discrete states has been proposed by Rotenberg.[2] It was hoped that the Sturmian-function (SF) expansion, containing no continuum states, would converge faster.

Subsequent investigation[3–9] of these two expansions in the Schrödinger formulation have found that both of these two expansions have undesirable limitations. It has been observed that the SF expansion converges in a oscillatory manner and cannot account for the strong coupling of the l-degenerate target states at excitation thresholds. The HF expansion, on the other hand, has the convergence problem associated with the uncontrolled error from continuum states. In addition, the straightforward expansion methods have also difficulties in relation to the correlation problems[8] and polarization interactions.[9]

A more serious drawback of the expansion method in the Schrödinger formulation is perhaps in the treatment of rearrangement collisions. For such a problem, there is no unique set of states available for the formulation of the close-coupling equations suitable for both scattering and rearrangement channels. The powerful projection operator method formulated by Feshbach[10] provides very

interesting possibilities for the treatment of rearrangement collisions. By decomposing the Feshbach projection operators into orthogonal channel projectors, a set of coupled equations adequate for both scattering and rearrangement collisions may be obtained explicitly.[11] For three-body collision systems, the exact expressions for the channel projectors for both the scattering and rearrangement channels has been constructed[11] and applied to the (e^+, H) collision system.[12] The coupled equations obtained in the projection operator formalism contains, however, a complicated nonlocal optical potential.[10-12] Methods for the evaluation of this potential in a systematic manner have yet to be developed.

Recently, an alternative formulation of the three-body problem was developed by Faddeev.[13] In this formulation, the three-body collision matrix is given by a set of three coupled equations in terms of two-body scattering matrices of the three alternative pairs of particles. This set of equations has no divergence problem and is adequate for treating both the scattering and rearrangement collisions. Now if the two-body scattering matrix may be represented by a sum of terms which are separable in momentum representation, in the initial and final momentum variables, the set of three coupled Faddeev equations with five variables may be reduced to three mutually coupled sets of single-variable integral equations.[14] This set of coupled single-variable integral equations, just like the set of single-variable integrodifferential equations obtained in the Schrödinger formulation, may be solved by straightforward methods.

A separable representation of the off-shell two-body scattering amplitude t_l may be obtained by expanding the scattering amplitude in terms of a complete set of SF.[14] This SF expansion for t_l, unlike the SF expansion for the scattering functions in the Schrödinger formulation,[2] provides adequate descriptions of the thresholds associated with the degenerate two-body states. This is because in the SF expansion for t_l the energy dependence of the SF is made explicit. At energies corresponding to the two-body bound-state energies where the amplitudes have poles, the SF become, within a constant factor, the eigenfunctions of the corresponding two-body states (see Sec. IV). Consequently, the set of coupled integral equations obtained in the Faddeev formulation accounts adequately for the degenerate two-body thresholds.

Application of this set of coupled equations to the (e, H) system has been carried out and found that the SF expansions for t_l converges in an oscillator manner and involves cancellations.[14] In the present work, we investigate the possibility of an alternative separable representation for the two-body off-shell amplitude and study in some detail the convergence properties of these expansions.

In Sec. II, the expansion method in the Schrödinger formulation is reviewed briefly with emphasis on the behavior of the resultant coupled equations at the degenerate threshold regions. The expansion method in the Faddeev formulation is given in Sec. III. In Sec. IV, we investigate the separable series representation for the off-shell two-body amplitudes t_l. An alternative separable series representation for t_l in terms of HF is derived.[15] A detailed study of the convergence behavior of the two series representation is carried out in Sec. V. The continuum contributions in the HF series are investigated.

II. EXPANSION IN SCHRÖDINGER FORMULATION

The Schrödinger equation for a nonrelativistic three-body system with two-body interactions may be written

$$(H - s)\Psi = 0 , \tag{2.1}$$

$$\text{with} \quad H = \sum_i (K_i + V_i) , \tag{2.2}$$

where K_i is the kinetic-energy operator and V_i ($V_i \equiv V_{jk}$) is the two-body potentials. For numerical convenience, the Schrödinger equation may be transferred into a set of coupled integrodifferential equations by expanding Ψ in terms of a complete set of two-body eigenfunctions χ_n

$$(K_{jk} + V_i - \epsilon_n^{(i)})\chi_n^{(i)} = 0 , \tag{2.3}$$

where K_{jk} is the relative kinetic-energy operator of particle j and k. The set of equations so obtained may be further reduced to a set of single-variable equations by angular decomposition[16] and then be solved systematically by standard methods.

For a three-body system involving Coulomb potentials, the natural set of eigenfunctions for expansion would be the set of HF. Such an HF expansion is particularly suitable for treating electron-atom scatterings. In this case, we have the antisymmetrized expansion

$$\Psi = \mathcal{A} \sum_n F_n(\vec{r}_1)\chi_n(\vec{r}_2) , \tag{2.4}$$

in which all scattering functions (i.e., the F_n) are properly associated with their corresponding target states. This HF expansion has, however, practical difficulties associated with the continuum-state contributions.[17] The HF expansion has nevertheless been applied to the (e, H) and (e, He^+) system by a number of workers.[3-5]

Burke and his associates[18] have shown, in a series of careful and detailed calculations, that the truncated HF expansion is capable of yielding

accurate results in the vicinity of the two-body excitation thresholds. At energies away from the threshold region the convergence problem becomes, however, serious. Recent calculations of the ^1D electron-hydrogen elastic scattering resonance below $n=2$ has shown[19] that the position of the resonance as calculated by the coupled equation depends critically upon the inclusion of higher-lying states of the target hydrogen atom. Recent experimental measurements have also found[20–22] that the truncated HF coupled equations (up to six states) predict values which are about 15% larger than that observed for the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation cross sections.

The difficulty with the convergence of the HF expansion is associated partly with the correlation and polarization problems[8,9] and partly with the omitted continuum states. Because of the latter difficulty, there is a renewed interest in the SF expansion [6,7] which was first applied to atomic collision problems by Rotenberg.[2]

The radiat SF may be obtained by solving the equation (in a.u.)

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2\gamma_\lambda(E)}{r} + 2E\right) S_{\lambda l}(Er) = 0 \tag{2.5}$$

for eigenvalue problems, where $\gamma_\lambda(E) = \lambda(-2E)^{1/2}$. In solving Eq. (2.5), the energy E is treated as a constant parameter. For negative E, the radial SF are found to be

$$S_{\lambda l}(Er) = \left(\frac{(\lambda-l-1)!}{2[(\lambda+l)!]^3}\right)^{1/2} e^{-(-2E)^{1/2}r} \times [2(-2E)^{1/2}r]^{l+1} L_{\lambda+l}^{2l+1}[2(-2E)^{1/2}r] \tag{2.6}$$

with the orthonormal properties

$$\int_0^\infty S_{\lambda l}(Er)\frac{2}{r} S_{\lambda' l}(Er)\,dr = \delta_{\lambda\lambda'} . \tag{2.7}$$

For each set of values for E and l, the SF form a complete discrete set.

If we take E to be $\epsilon_n = -\frac{1}{2}Z^2/n^2$ (the hydrogen energy spectrum), we have $\gamma_\lambda(\epsilon_n) = \lambda Z/n$. The SF $S_{\lambda l}(\epsilon_n r)$ then reduce to the hydrogenic radial wave functions $R_{nl}(r)$ (within a constant factor) whenever $\lambda = n$.

$$R_{nl}(r) = [(2Z)^{1/2}/n]\, S_{nl}(\epsilon_n r) . \tag{2.8}$$

This then implies that once E is chosen to be one of the hydrogenic energies, say ϵ_{n_1}, only one SF among the set $\{S_{\lambda l}\}$, namely, $S_{n'l}$ may correspond to the physical hydrogen states. Consequently, the SF expansion cannot, for such a choice of E, satisfy proper boundary conditions for excitation and deexcitation problems.

It has been shown by Gallaher and Wilets[7] that by taking

$$E = \epsilon_l = -Z^2/2(l+1)^2 , \tag{2.9}$$

the $1s$, $2p$, $3d$, etc., SF coincide with the HF within a factor $(2Z)^{1/2}/(l+1)$. This then permits us to treat scatterings involving the $1s$, $2p$, $3d$, etc., channels. By choosing different l dependence for E, one may make different SF coincide with the HF. By the choice of $E = -\frac{1}{2}Z^2/(l+2)^2$, for example, we recover the $2s$, $3p$, $4d$, etc., hydrogenic states. However, one cannot by such a choice for E, recover simultaneously all the degenerate l states associated with a given principal hydrogenic state.

This is, however, a serious limitation since these degenerate states are strongly coupled. For the (e, H) system, for example, Gailitis and Damburg[23] have shown that because of this degeneracy, a long-range dipole potential is created when these degenerate states are virtually excited. Such a long-range potential dominates the physics of the scattering problem especially at energies in the neighborhood of the two-body thresholds. The HF expansion though converges slowly; it, however, accounts adequately for the coupling of these degenerate states at the thresholds if the expansion is truncated properly. This is part of the reason why the close-coupling calculations have been successful.[18] An alternative approach which accounts for both channel couplings and continuum effects consists of a mixed-mode expansion in which the HF are used for the open-channel segment of the Hilbert space and the SF are used for the closed-channel segment of the Hilbert space.

III. EXPANSION IN FADDEEV FORMULATION

In this section, the expansion method for solving the Faddeev equations for three-body systems is outlined in a form suitable for the present application. For further details, we refer to the work of Ball, Chen, and Wang.[14]

In the Faddeev formulation of three-body problems, one starts from the integral equation of the Lippmann-Schwinger type. By decomposing the total T matrix (or collision wave function) into the sum of three components

$$T(s) = T^{(1)}(s) + T^{(2)}(s) + T^{(3)}(s) , \tag{3.1}$$

corresponding to the three alternative pairs of particles undergoing a final-state interaction,

Faddeev derived the coupled equations for three-body problems[13]

$$T^{(i)}(s) = T_i(s) + \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s) , \qquad i = 1, 2, 3 \qquad (3.2)$$

where s is the total energy of the three-body system. $G_0(s)$ is the Green's function for the three-body system in the absence of interaction. The two-body T matrix $T_i(s)$ arising from a two-body potential V_i is given by the Lippmann-Schwinger equations

$$T_i(s) = V_i + V_i G_0(s) T_i(s) . \qquad (3.3)$$

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

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

$$H_0 = p_1^2 + q_1^2 = p_2^2 + q_2^2 = p_3^2 + q_3^2 , \qquad (3.4)$$

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

$$\vec{q}_i = \frac{m_i (\vec{k}_j + \vec{k}_k) - (m_j + m_k)\vec{k}_i}{[2m_i (m_j + m_k)(m_i + m_j + m_k)]^{1/2}} , \qquad (3.5)$$

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

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle = |\vec{p}_1, \vec{q}_1\rangle_1 = |\vec{p}_2, \vec{q}_2\rangle_2 = |\vec{p}_3, \vec{q}_3\rangle_3 . \qquad (3.6)$$

These sets of basis momenta which are defined by Eq. (3.5) in cyclic order of i, j, k are linearly dependent.[24]

The angular decomposition of the Faddeev equations may be carried out in a number of ways.[25-27] Since the total angular momentum J and its projection M is conserved, we consider the states to be diagonal in J and M. The separation of the angular momentum states can be carried out using the relative angular momentum l between two particles which are combined with the angular momentum L of the third particle in the over-all c.m. system. We have[25]

$$\Psi_\alpha^{(i)}(p, q, s) = \Phi_\alpha^{(i)}(p, q, s) - \frac{1}{4} \sum_{\alpha_j} \sum_{j \neq i} \int_0^\infty dp_j^2 \int_0^\infty dq_j^2 \, \mathcal{K}_j^{(i)}(pq\alpha | p_j q_j \alpha_j) \times [p_j q_j / (p_j^2 + q_j^2 - s)] \Psi_{\alpha_j}^{(j)}(p_j, q_j, s) , \qquad (3.7)$$

with

$$\Psi_\alpha^{(i)}(p, q, s) = {}_i\langle p, q, \alpha | T^{(i)}(s) | \vec{k}_1, \vec{k}_2, \vec{k}_3 \rangle , \qquad (3.8)$$

$$\Phi_\alpha^{(i)}(p, q, s) = {}_i\langle p, q, \alpha | T_i(s) | \vec{k}_1, \vec{k}_2, \vec{k}_3 \rangle , \qquad (3.9)$$

$$\mathcal{K}_j^{(i)}(pq\alpha | p_j q_j \alpha_j) = \int_{-1}^{1} d\cos\theta_{\vec{p}_j \vec{q}_j} A_{\alpha\alpha_j}(\theta_{\vec{p}_i \vec{p}_j}, \theta_{\vec{p}_j \vec{q}_i}, \theta_{\vec{p}_j \vec{q}_j}) \times \delta(q^2 - q_i^2) t_l^{(i)}(p, p_i; s - q^2) , \qquad (3.10)$$

$$A_{\alpha\alpha'}(\theta_{\vec{p}_i \vec{p}_j}, \theta_{\vec{p}_j \vec{q}_i}, \theta_{\vec{p}_j \vec{q}_j}) = (-)^{L + L' - l - l'} \frac{16\pi^{1/2}}{q} (2l' + 1)^{1/2} \times \delta_{JJ'} \delta_{MM'} \sum_{m_l m_L m_{L'}} (-)^{m_L} \begin{pmatrix} l & L & J' \\ m_l & m_L & -m_{L'} \end{pmatrix} \times \begin{pmatrix} l' & L' & J' \\ 0 & m_{L'} & -m_{L'} \end{pmatrix} Y^*_{lm_l}(\theta_{\vec{p}_i \vec{p}_j}, 0) Y^*_{Lm_L}(\theta_{\vec{p}_j \vec{q}_i}, 0) \times Y_{L'm_{L'}}(\theta_{\vec{p}_j \vec{q}_j}, 0) , \qquad (3.11)$$

where $p_i^2 = p_j^2 + q_j^2 - q^2$ and $\theta_{\vec{p}_i \vec{p}_j}$, for example, is the angle between momentum variables $\vec{p}_i$ and $\vec{p}_j$. For convenience the discrete quantum number $(JMlL)$ are collectively denoted by α.

It has been observed that if the off-shell, partial-wave two-body scattering amplitude $t_l^{(i)}(p, p_i; s - q^2)$ may be represented in a sum of terms separable in p and p_i, then the p dependence of $\Psi_l^{(i)}(p, q, s)$ becomes explicit. The partial-wave Faddeev equations with two variables as given by Eqs. (3.7) can, therefore, be reduced to a set of single-variable integral equations.[14] This set of equations may then be solved systematically by standard methods for integral equations.

Let us suppose that the two-body t matrix $t(k, k', E)$ may be represented

$$t(k, k'; E) = \sum_\lambda C_\lambda(E) f_\lambda(k, E) g_\lambda(k', E) , \qquad (3.12)$$

where $C_\lambda(E)$ is function of E only. The functions f_λ and g_λ may or may not depend on E. If the f_λ and the g_λ are not the same functions, the symmetry with respect to the interchange of k and k' may be preserved for t_l term-by-term in the series by writing

$$t(k,k';E)=\frac{1}{2}\sum_\lambda C_\lambda(E)[f_\lambda(k,E)g_\lambda(k',E) + f_\lambda(k',E)g_\lambda(k,E)] . \quad (3.13)$$

It should be noted that the separable series representation for t_l need not be diagonal as assumed by Eqs. (3.12) and (3.13). The double-sum separable series for t_l are, however, more cumbersome to deal with numerically. We will show in Sec. IV that there are several such single-sum series for the off-shell two-body amplitude available.

Utilizing the assumed separable series representation as given by Eq. (3.12), Eq. (3.7) may be written

$$\Psi_\alpha^{(i)}(p,q,s)=\Phi_\alpha^{(i)}(p,q,s)+\sum_\lambda C_\lambda^{(i)} \times(s-q^2)f_\lambda^{(i)}(p,s-q^2)\chi_{\lambda\alpha}^{(i)}(q,s) . \quad (3.14)$$

The functions $\chi_{\lambda\alpha}^{(i)}$ can be determined from the set of coupled single-variable integral equations

$$\chi_{\lambda\alpha}^{(i)}(q,s)=\eta_{\lambda\alpha}^{(i)}(q,s)+\sum_{\lambda'\alpha_j,j\neq i}\int_0^\infty dq_j^{\,2} \times \mathcal{K}_{\lambda\alpha,\lambda'\alpha_j}^{(i,j)}(q,q_j;s)\chi_{\lambda'\alpha_j}(q_j,s) , \quad (3.15)$$

with

$$\mathcal{K}_{\lambda\alpha,\lambda'\alpha_j}^{(i,j)}(q,q_j;s)=-\tfrac{1}{4}\int_0^\infty dp_j^{\,2} B_{\alpha\alpha_j\lambda}^{(i)} \times(q,p_j,q_j;s)\frac{p_jq_j}{p_j^{\,2}+q_i^{\,2}-s} C_{\lambda'}^{(j)}(s-q_j^{\,2})f_{\lambda'}^{(j)} \times(p_j,s-q_j^{\,2}) , \quad (3.16)$$

$$\eta_{\lambda\alpha}^{(i)}(q,s)=\sum_{\alpha_j,j\neq i}\int_0^\infty dp_j^{\,2}\int_0^\infty dp_j^{\,2} \times B_{\alpha\alpha_j\lambda}^{(i)}(q,p_j,q_j;s) \times[p_jq_j/(p_j^{\,2}+q_j^{\,2}-s)]\Phi_{\alpha_j}^{(i)}(p_jq_j;s), \quad (3.17)$$

$$B_{\alpha\alpha_j\lambda}^{(i)}(q,p_j,q_j;s) =\int_{-1}^{1} d\cos\theta_{\vec{p}_j\vec{q}_j} A_{\alpha\alpha_j}(\theta_{\vec{p}_i\vec{p}_j},\theta_{\vec{p}_j\vec{q}_i},\theta_{\vec{p}_j\vec{q}_j}) \times\delta(q^2-q_i^{\,2})g_\lambda^{(i)}(p_i,s-q_j^{\,2}) . \quad (3.18)$$

This then demonstrates the fact that if the off-shell t_l may be represented in sums of separable terms, the set of two-variable Faddeev equations may be reduced to a set of single-variable integral equations.

This set of single-variable coupled integral equations [Eq. (3.15)] corresponds to the set of single-variable coupled integrodifferential equations obtained in the Schrödinger formulation. The convenient features of Eq. (3.15) lie in the fact that this set of equations provides adequate description for both bound and resonant three-body states and for both scattering and rearrangement collisions. The numerical practicability of this set of equations depends, of cource, again on the convergence of the expansion. Here, it depends on the convergence of the expansion for the off-shell two-body amplitudes.

IV. SEPARABLE SERIES REPRESENTATION FOR $t_l(k,k';E)$

There are several separable series which may be found for the off-shell two-body amplitudes. We first consider the separable series representation for $t_l(k,k';E)$ in terms of the set of eigenfunctions of the homogeneous two-body Lippmann-Schwinger equation. A new separable series representation for $t_l(k,k';E)$ is then introduced in terms of a set of eigenfunctions of the two-body Schrödinger equation in momentum representation. For the case with a Coulomb potential, these eigenfunctions are known analytically for both the homogeneous Lippmann-Schwinger equations and the Schrödinger equations in the momentum representation. They are the SF and HF, respectively. A comparison of the convergence properties of these two separable series for Coulomb potentials is given in Sec. V.

A. SF Representation

The partial-wave two-body amplitude $t_l(k,k';E)$ for potential V_l can be obtained from the solution of the Lippmann-Schwinger equation

$$t_l(k,k';E)=V_l(k,k';E)-\frac{2\mu}{\pi}\int_0^\infty dk''\frac{k''^2V_l(k,k'')}{k''^2-2\mu E}\,t_l(k'',k';E)\,, \tag{4.1}$$

where μ is the reduced mass for the two-body system. In writing Eq. (4.1) we take the two-body scattering amplitude to be normalized on the energy shell according to the equation

$$t_l(k,k;k^2/2\mu)=-\frac{1}{k^2}\,\frac{dE_k}{dk}\,\sin\delta_l e^{i\delta l}\,, \tag{4.2}$$

where δ_l is the standard phase shift and $dE_k/dk=\hbar^2k/\mu$ is the density of states.

A set of eigenfunctions $\phi_{\lambda l}(k,E)$ of the homogeneous Lippmann-Schwinger equation may be obtained by solving the eigenvalue problem

$$[\gamma_{\lambda l}(E)]^{-1}\phi_{\lambda l}(k,E)=-\frac{2\mu}{\pi}\int_0^\infty dk'\frac{k'^2}{k'^2-2\mu E}\,V_l(k,k')\phi_{\lambda l}(k',E)\,. \tag{4.3}$$

This set of $\phi_{\lambda l}(k,E)$ forms a complete orthonormal set for negative values of E with the orthonormality property

$$\frac{2\mu}{\pi}\int_0^\infty\frac{dk\,k^2}{k^2-2\mu E}\,\phi_{\lambda l}(k,E)\phi_{\lambda' l}(k,E)=\delta_{\lambda\lambda'}\,. \tag{4.4}$$

For negative values of E, the solution for $t_l(k,k';E)$ can be expressed in terms of the $\phi_{\lambda l}$. We have the separable series representation for $t_l(k,k';E)$[13]

$$t_l(k,k';E)=V_l(k,k')+\textstyle\sum_\lambda\phi_{\lambda l}(k,E)\phi_{\lambda l}(k',E)/\gamma_{\lambda l}(E)[1-\gamma_{\lambda l}(E)], \tag{4.5}$$

$$\text{with}\quad V_l(k,k')=-\textstyle\sum_\lambda\gamma_{\lambda l}(E)^{-1}\phi_{\lambda l}(k,E)\phi_{\lambda l}(k',E)\,, \tag{4.6}$$

Since the argument E is replaced by $s-q^2$ in the Faddeev equations [see Eqs. (3.10)], it is negative definite provided the three-body energy s is below the three-particle breakup threshold ($s=0$). The series representation [Eq. (4.5)] is therefore adequate for reducing Eqs. (3.7) to a set of single-variable equations of the type given by Eq. (3.15) for dealing with problems below the three-body breakup threshold.

At energies lying above the three-body breakup threshold, one may use the completeness property of the $\phi_{\lambda l}$ and expand t_l in a double-sum series

$$t_l(k,k';E)=\sum_{\lambda,\lambda'}a_{\lambda\lambda'}(E_0,E)\phi_{\lambda l}(k,E_0)\phi_{\lambda' l}(k',E_0)\,, \tag{4.7}$$

where E_0 is an arbitrary negative number and the $a_{\lambda\lambda'}(E_0,E)$ are the expansion coefficients to be determined. The double-sum expansion, however, is rather cumbersome numerically.

For Coulomb potentials, we have

$$V_l(k,k')=(Ze^2/kk')Q_l[(k^2+k'^2)/2kk']\,, \tag{4.8}$$

where Q_l is the Legendre function of the second kind and Z is the product of the charges of the two particles. We adopt the convention: $Z=-|Z|$ attractive and $Z=|Z|$ repulsive. In this case, the eigenvalue problem for the homogeneous Lippmann-Schwinger equation [Eq. (4.3)] may be solved analytically. We have

$$\gamma_{\lambda l}(E)=-\lambda(-2\mu E)^{1/2}/Z\mu\,, \tag{4.9}$$

and

$$\phi_{\lambda l}(k,E)=\left(\frac{2^{4l+3}\lambda(\lambda-l-1)!}{\mu\Gamma(\lambda+l+1)}\right)l!(-2\mu E)^{(2l+3)/4}\frac{k^l}{(k^2-2\mu E)^{l+1}}\,C_{\lambda-l-1}^{l+1}\left(\frac{k^2+2\mu E}{k^2-2\mu E}\right), \tag{4.10}$$

where $C_{\lambda-l-1}^{l+1}$ is the Gegenbauer polynomial.

It is important to observe that the SF expansion for t_l accounts adequately for the degeneracy of the excitation threshold. This is apparent since the two-body poles in t_l appear at $\gamma_{\lambda l}(E)=1$ [see Eq. (4.5)]. From Eq. (4.9), we see that this corresponds to the two-body bound-state energies

$$E=-Z^2\mu/2\lambda^2 \quad . \tag{4.11}$$

At $\gamma_{\lambda l}(E)=1$, the SF become the HF function [see Eq. (4.15)] within a factor. Consequently, the SF expansion for t_l, unlike for the three-body collision wave function, is adequate to account for the strong coupling arising from the degeneracy in l for each principal quantum state of the two-body bound subsystems.

B. HF Representation

A single-sum term-by-term separable series representation for $t_l(k,k';E)$ can also be obtained in terms of eigenfunctions of the Schrödinger equation. In momentum representation, the Schrödinger equation for potential $V_l(k,k')$ is

$$(k^2-2\mu\epsilon_n)\psi_{nl}(nk)=-\frac{2\mu}{\pi}\int_0^\infty dk'k'^2\,V_l(k,k')\psi_{nl}(nk')\,, \tag{4.12}$$

where ϵ_n is the eigenvalue associated with the eigenfunction $\psi_{nl}(nk)$. ψ_{nl} satisfies the orthonormality relation

$$\int_0^\infty \psi_{nl}^*(nk)\psi_{n'l}(n'k)k^2dk=\delta_{nn'}\,. \tag{4.13}$$

For a Coulomb potential [Eq. (4.8)], we have for discrete states

$$\epsilon_n=-Z^2\mu/2n^2 \quad \text{and} \tag{4.14}$$

$$\psi_{nl}(nk)=\left(\frac{2^{4l+5}n(n-l-1)!}{\pi(n+l)!}\right)^{1/2} l!\,(-2\mu\epsilon_n)^{(2l+5)/4}\,\frac{k^l}{(k^2-2\mu\epsilon_n)^{l+2}}\,C_{n-l-1}^{l+1}\left(\frac{k^2+2\mu\epsilon_n}{k^2-2\mu\epsilon_n}\right). \tag{4.15}$$

The discrete functions together with continuum functions form a complete orthonormal set.

Utilizing this property, the off-shell two-body amplitude $t_l(k,k';E)$ can be expanded in the form

$$t_l(k,k',E)=\sum_n{}' C_{nl}(k,E)\psi_{nl}(nk')\,, \tag{4.16}$$

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. Substitution of Eq. (4.16) into Eq. (4.1) yields, after forming matrix elements with ψ_{nl} functions, the equation

$$C_{nl}(k',E)=\int_0^\infty dk\,k^2V_l(k,k')\psi_{nl}^*(nk)-\frac{2\mu}{\pi}\sum_{n'}{}' C_{n'l}(k',E)\int_0^\infty dk''\frac{k''^2}{k''^2-2\mu E}\psi_{n'l}(n'k'')$$
$$\times\int_0^\infty dk\,k^2V_l(k,k'')\psi_{nl}^*(nk)\,. \tag{4.17}$$

When Eq. (4.12) is utilized, we then obtain

$$C_{nl}(k',E)=-\frac{\pi}{2\mu}(k'^2-2\mu\epsilon_n)\psi_{nl}^*(nk')+\sum_{n'}{}' C_{n'l}(k',E)$$
$$\times\int_0^\infty dk''\,\frac{k''^2}{k''^2-2\mu E}\psi_{n'l}(n'k'')(k''^2-2\mu\epsilon_n)\psi_{nl}^*(nk'')\,. \tag{4.18}$$

By writing $(k''^2 - 2\mu\epsilon_n)$ as $(k''^2 - 2\mu E) + 2\mu(E - \epsilon_n)$ in Eq. (4.18), we obtain the sum rule for the expansion coefficients

$$\sum_{n'}' C_{n'l}(k', E) \int_0^\infty dk'' \frac{k''^2}{k''^2 - 2\mu E} \psi_{nl}^*(nk'') \psi_{n'l}(n'k'') = \frac{\pi}{4\mu^2} \left(\frac{k'^2 - 2\mu\epsilon_n}{E - \epsilon_n} \right) \psi_{nl}^*(nk') . \tag{4.19}$$

By using Eqs. (4.12) and (4.13), $V_l(k, k')$ may be expressed in terms of ψ_{nl} as series

$$V_l(k, k') = -\frac{\pi}{2\mu} \sum_n' (k^2 - 2\mu\epsilon_n) \psi_{nl}^*(nk) \psi_{nl}(nk') \tag{4.20a}$$

$$= -\frac{\pi}{2\mu} \sum_{n'}' (k'^2 - 2\mu\epsilon_n) \psi_{nl}^*(nk) \psi_{nl}(nk') . \tag{4.20b}$$

When the series expressions for $t_l(k, k'; E)$ as given by Eq. (4.16) and for $V_l(k, k')$, as given by Eq. (4.20a), are substituted into the second term at the right-hand side of Eq. (4.1), we obtain, with the help of the sum rule for C_{nl}, the separable representation for $t_l(k, k'; E)$

$$t_l(k, k'; E) = V_l(k, k') - \frac{\pi}{4\mu^2} \sum_n' \frac{(k^2 - 2\mu\epsilon_n)(k'^2 - 2\mu\epsilon_n)}{E - \epsilon_n} \psi_{nl}^*(nk) \psi_{nl}(nk'), \tag{4.21}$$

where $V_l(k, k')$ may take either the separable expression given by Eqs. (4.20) or by a symmetrized expression

$$V_l(k, k') = -\frac{\pi}{4\mu} \sum_{n'}' [(k^2 - 2\mu\epsilon_n) + (k'^2 - 2\mu\epsilon_n)] \psi_{nl}^*(nk) \psi_{nl}(nk') . \tag{4.20c}$$

V. CONVERGENCE PROPERTIES OF SEPARABLE SERIES

Numerical investigation of the convergence properties of the two separable series for the off-shell amplitude [Eqs. (4.5), (4.6), (4.21), (4.20)] are carried out for the case with Coulomb potential. The s-wave results for $Z = -1$ Coulomb interaction are shown in Figs. 1–3 for three sets of values for the arguments k, k', and E. It is seen that the off-shell amplitude as a function of the number of terms (included in the series) behaves differently for the two series representations. For the HF series t_l appears to be a smooth function of the number of terms. For the SF series, t_l is an oscillating function of the number of terms.

For the purpose of illustrating the details, we plot in Figs. 1–3, in addition to t_0, $V_0(kk')$ and $[t_0(k, k'; E) - V_0(k, k')]$ as a function of the number of terms. By comparison with the exact values for $V_0(k, k')$, it is observed that the SF expansion for V_0 [Eq. (4.6)] oscillates about the exact V_0 value and slowly converges to the exact value. On the other hand, the HF expansion for V_0 [Eq. (4.20a)] converges uniformly and rapidly to a limit which is displaced from the exact value. The displacements which depend sensitively upon the arguments k and k', arise from contribution coming from the continuum states. For $(t_0 - V_0)$ [i.e., the VGt part of Eq. (4.1)] both series converge rapidly and uniformly (except for the first few terms) but not exactly to the same limit. The difference in the two limits is, however, very small and for most cases is less than 1%.

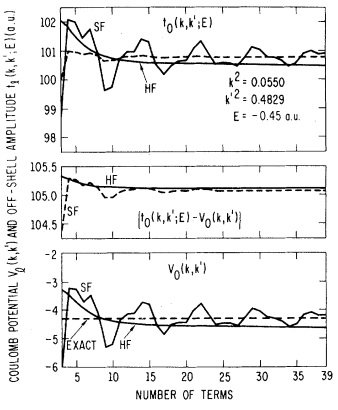

FIG. 1. Comparison of the convergence behavior of the SF and the HF expansions for the s-wave Coulomb potential ($Z = -1$) and off-shell amplitudes for a fixed set of arguments k, k', and E as given by Eqs. (4.5) and (4.6) and by Eqs. (4.21) and (4.20c), respectively. The dashed curve for $t_0(k, k', E)$ is obtained from Eq. (4.5) with the exact $V_0(k, k')$ [Eq. (4.8)].

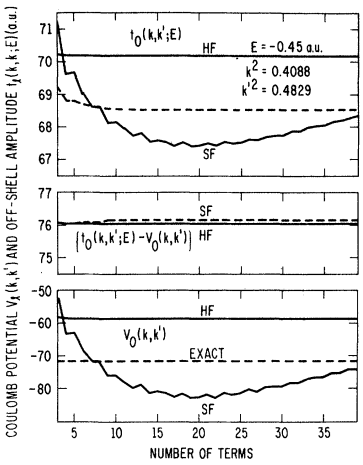

FIG. 2. Comparison of the convergence behavior of the SF and the HF expansions for the s-wave Coulomb potential ($Z=-1$) and off-shell amplitudes for a fixed set of arguments k, k', and E as given by Eqs. (4.5) and (4.6) and by Eqs. (4.21) and (4.20c), respectively. The dashed curve for $t_0(k, k', E)$ is obtained from Eq. (4.5) with the exact $V_0(k, k')$ [Eq. (4.8)].

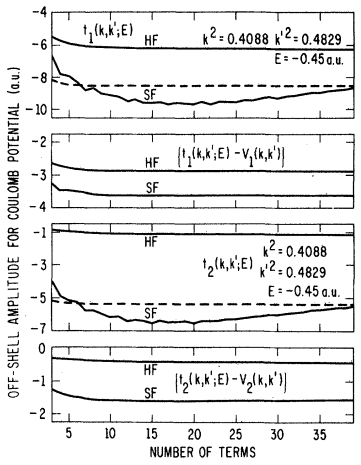

FIG. 4. Comparison of the convergence behavior of the SF and the HF expansions for the p-wave and d-wave off-shell amplitudes for the $Z=-1$ Coulomb interactions as given by Eqs. (4.5) and (4.6) and by Eqs. (4.21) and (4.20c), respectively. The dashed curve for $t_1(k, k'; E)$ and $t_2(k, k'; E)$ is obtained from Eq. (4.5) with the exact $V_0(k, k')$ [Eq. (4.8)].

The convergence behavior of the two series for the p-wave and d-wave amplitudes are essentially the same as for the s-wave amplitudes. The continuum contribution now appears to be slightly larger. In Fig. 4, illustrative results for $Z=-1$ Coulomb interaction for each partial wave are shown for a set of values for the arguments k, k', and E.

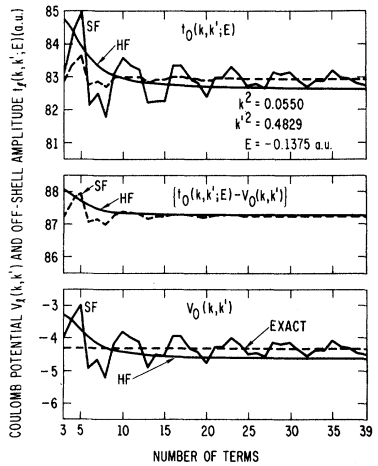

FIG. 3. Comparison of the convergence behavior of the SF and the HF expansions for the s-wave Coulomb potential ($Z=-1$) and off-shell amplitudes for a fixed set of arguments k, k', and E as given by Eqs. (4.5) and (4.6) and by Eqs. (4.21) and (4.20c), respectively. The dashed curve for $t_0(k, k', E)$ is obtained from Eq. (4.5) with the exact $V_0(k, k')$ [Eq. (4.8)].

From these results, it becomes clear that the source of difficulty in both series for t_l comes primarily from the $V_l(k, k')$ part of the series. This is not unexpected since $V_l(k, k')$ is essentially a logarithmic function (actually the Legendre functions of the second kind). The series for $V_l(k, k')$ in both the SF and HF converges essentially as n^{-1}, characteristic of the logarithmic divergence when k equals k'. This behavior is more apparent when the argument k approaches k' as shown in Fig. 2.

The SF expansion for V_l depends arbitrarily on E. It does not seem possible to determine an optimal value for E so that the series would converge with minimum oscillations. The convergence of the SF expansion can be improved by introducing screening constant for the Coulomb potential as shown in the Appendix. The significance and its effect on the three-body solution for such a screened two-body potential is, however, not clear and requires further studies.

There are several alternative expressions [Eqs. (4.20a)–(4.20c)] for the HF expansion for $V_l(k, k')$. A comparison of the three equivalent (in principle) expansions for $Z=-1$ Coulomb potential is given in Fig. 5 for the $l=0$ case. It is seen that the three expansions converge uniformly but to different limits which depend sensitively upon their arguments. For the unsymmetrized series, Eqs. (4.20a) and (4.20b), the convergence is better if the smaller of the two arguments is taken to be the weighting factor $(k^2-2\mu\epsilon_n)$.

Utilizing the completeness properties, the

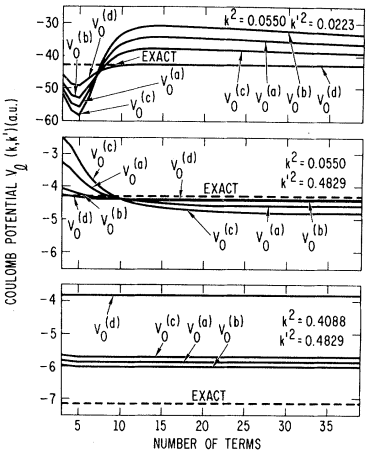

FIG. 5. Comparison of the convergence behavior of the various HF expansions for $V_0(k,k')$ with $Z=-1$ at three sets of arguments: $V_0^{(a)}$[Eq. (4.20c)], $V_0^{(b)}$[Eq. (4.20a)], $V_0^{(c)}$[Eq. (4.20b)], and $V_0^{(d)}$[Eq. (5.1)].

series for $V_l(k,k')$ may be rewritten

$$V_l(k,k')=\pi\left(\sum_n{}' \epsilon_n \psi^*_{nl}(nk)\psi_{nl}(nk') - (2\mu)^{-1}\delta(k-k')\right) \tag{5.1}$$

Though the δ function, $\delta(k-k')$, is not separable in k and k', it is of interest to examine whether the error introduced by truncating the closure relation

$$\sum_n{}' \psi_{nl}(nk)\psi^*_{nl}(nk') = k^{-2}\delta(k-k') \tag{5.2}$$

in the truncated series for $V_l(k,k')$ is large. The result is also shown in Fig. 5. It is seen when the arguments k and k' are far apart, so that Vl is away from the logarithmic singularity, the series for V_l [Eq. (5.1)] converges rapidly to a value very close to the exact value. From the comparison in Fig. 5, it is seen that continuum-state contributions to the closure relation is of importance. As the argument k and k' approach each other, so that V_l moves closer to the logarithmic singularity the series given by Eq. (5.1) converges badly.

It is obvious that all the expansions for $V_l(k,k')$ fail badly when the two arguments become equal to each other, since the expansions must now reproduce the logarithmic singularity. This failure may not be as serious as it appears for the intended applications for solving the Faddeev equations below the three-body break-up threshold. This is because the kernel in the coupled integral equations [compare Eqs. (3.7) and (3.15)] depends on quantities in which $V_l(k,k')$ has been integrated once over one of its arguments. Since the singularity at $k=k'$ is only logarithmatic, the integration removes this singularity and the kernel therefore no longer contains the singularity.

For a similar reason that the kernel depends on quantities in which $t_l(k,k',E)$ has been integrated once the oscillations in the SF series are not as discouraging as it appears to be. After integrating over the three-body phase space, the oscillations are smoothed out considerably. There are, however, residual oscillations. The effect of these residual oscillations is critical as is apparent from the work of Ball, Chen, and Wang.[14] They have observed that the Faddeev equations converge in an oscillatory manner with respect to the number of terms to be kept in the SF series for the off-shell amplitudes. These oscillations can, nevertheless, be confined if sufficient terms are included in the SF series.

The HF series for the off-shell amplitudes converges uniformly for most of its arguments, k and k' at fixed values of E. For small values of k and k' some oscillations at small values of n have been found in the V_l part of the series. Though the HF series is not, in principle, limited to the negative values of E, it has, however, the uncontrolled error from the continuum states. In the case where the Coulomb potential is repulsive, the entire contribution comes from the continuum states. Because the continuum Couloub states are difficult to deal with numerically, this then limits the practical usefulness of the HF series for repulsive Coulomb interactions and for the case with $E>0$.

The convergence behavior of the SF series for repulsive Coulomb interactions, on the other hand, appears to be the same as for the attractive interaction. In Fig. 6, the convergence behavior for SF series is shown for two sets of values for the arguments.

It appears that a mixed-mode representation for the three off-shell amplitudes for the alternative pair of particles may be satisfactory for the Faddeev equations. In the mixed-mode representation, the HF series is adopted for pairs of particles with attractive interaction and for pairs of particles with repulsive interaction the SF series is adopted. This would be a particularly suitable representation for cases with large negative E where the continuum contribution in the HF series is small.

An investigation of the continuum contribution is carried out for the $Z=-1$ Coulomb interaction at negative energies. (The zero energy for the three-body system is set at the three-body breakup threshold.) Some representative results are presented in Tables I and II for several sets of values for the arguments k, k', and E. In Table I the converged values for V_0, with $Z=-1$ calculated from Eqs. (4.20c) and (5.1), are compared with the exact values for various values for k and k'. It is seen

TABLE I. Continuum contributions[a] in the HF expansion for the Coulomb potential $V_0(k,k')$.

k^2 / k'^2	0.05502			0.40876			2.07077		
	HF[b]	Exact	$\lvert\Delta V\rvert$/exact[c]	HF[b]	Exact	$\lvert\Delta V\rvert$/exact[c]	HF[b]	Exact	$\lvert\Delta V\rvert$/exact[c]
0.02233	−36.4496	−42.9752	0.1518	−5.0080	−4.9850	0.0046	−0.3049	−0.9693	0.6854
	−42.9017		0.0017	−5.0771		0.0185	−1.0082		0.0401
0.05502	−65.1070	∞	...	−5.0997	−5.1320	0.0063	−1.6713	−0.9745	0.7150
	−44.0152		...	−5.2166		0.0165	−0.9995		0.0256
0.11111	−23.6686	−22.3713	0.0580	−5.7190	−5.4263	0.0539	−0.1497	−0.9837	0.8479
	−22.7890		0.0187	−5.4975		0.0131	−1.0598		0.0774
0.20185	−8.9104	−10.9925	0.1894	−6.5963	−6.0760	0.0856	−1.5487	−0.9992	0.5500
	−11.6402		0.0589	−5.3594		0.1179	−1.0986		0.0995
0.34492	−5.6513	−6.1401	0.0796	−6.4471	−8.4156	0.2339	−2.2305	−1.0255	1.1750
	−6.2738		0.0218	−4.5831		0.4554	−0.9708		0.0534
0.56910	−4.2068	−3.6347	0.1574	−5.4676	−5.1718	0.0572	−2.0213	−1.0725	0.8846
	−3.7406		0.0291	−3.4538		0.3322	−0.7398		0.3103
0.92311	−3.1053	−2.2113	0.4696	−4.1759	−2.6129	0.5982	−1.5015	−1.1667	0.2870
	−2.3840		0.0781	−2.3099		0.1160	−0.4958		0.5751
1.49383	−2.1858	−1.3557	0.6123	−2.9347	−1.4860	0.9749	−0.9926	−1.4257	0.3038
	−1.4661		0.0814	−1.3694		0.0785	−0.2936		0.7941
2.44642	−1.4452	−0.8237	0.7544	−1.9191	−0.8683	1.2103	−0.6025	−1.4122	0.5733
	−0.8065		0.0210	−0.7136		0.1782	−0.1527		0.8919
4.12213	−0.8911	−0.4874	0.8283	−1.1721	−0.5023	1.3337	−0.3403	−0.6056	0.4381
	−0.3894		0.2011	−0.3216		0.3596	−0.0687		1.1425
7.31001	−0.5079	−0.2743	0.8517	−0.6647	−0.2789	1.3832	−0.1790	−0.3050	0.4130
	−0.1493		0.4558	−0.1218		0.5633	−0.0260		0.9147
14.15193	−0.2615	−0.1415	0.8479	−0.3417	−0.1427	1.3940	−0.0862	−0.1489	0.4208
	−0.0458		0.6761	−0.0366		0.7439	−0.0467		0.6867

[a]Values are given in a.u.

[b]Upper and lower values are the converged values calculated from the HF expansions, Eqs. (4.20c) and (5.1), without including continuum states, respectively.

[c]$\lvert\Delta V\rvert$ denotes the absolute differences between the values listed in the columns under "HF" and "Exact" headings.

TABLE II. Continuun contributions[a] in the HF expansion for $[t_0(k,k';E) - V_0(k,k')]$.

k^2 / k'^2	0.05502 HF[b]	0.05502 SF[c]	0.05502 $\lvert\Delta Vt\rvert$/SF[d]	0.40876 HF[b]	0.40876 SF[c]	0.40876 $\lvert\Delta Vt\rvert$/SF[d]	2.07079 HF[b]	2.07079 SF[c]	2.07079 $\lvert\Delta Vt\rvert$/SF[d]	14.15193 HF[b]	14.15193 SF[c]	14.15193 $\lvert\Delta Vt\rvert$/SF[d]
					$E=-0.5500$ a.u.							
0.02233	-1.61736×10^{-2}	-1.62051×10^{-2}	0.00194	−108.7568	−108.7965	0.00036	−49.0289	−49.1721	0.00291	−9.94473	−10.03039	0.00854
0.05502	-1.56097×10^{-2}	-1.56549×10^{-2}	0.00288	−105.7702	−105.8214	0.00048	−47.7669	−47.8491	0.00171	−9.68776	−9.76172	0.00757
0.11111	-1.41967×10^{-2}	-1.41947×10^{-2}	0.00014	−101.0610	−101.0694	0.00008	−45.5182	−45.7395	0.00484	−9.23148	−9.33284	0.01085
0.20185	-1.27028×10^{-2}	-1.27152×10^{-2}	0.00097	−94.1667	−94.2342	0.00071	−42.8249	−42.7020	0.00287	−8.68179	−8.71554	0.00387
0.34492	-1.11300×10^{-2}	-1.11369×10^{-2}	0.00061	−84.6784	−85.1257	0.00525	−38.9375	−38.6708	0.00689	−7.89050	−7.89611	0.00070
0.56910	−0.943126	−0.943302	0.00018	−72.8579	−72.9080	0.00068	−33.7370	−33.7155	0.00063	−6.83491	−6.88901	0.00786
0.92311	−0.765021	−0.765126	0.00013	−59.5595	−59.2503	0.00521	−27.6737	−28.0798	0.01446	−5.60584	−5.74405	0.02406
1.49380	−0.588508	−0.588997	0.00082	−45.9645	−45.6624	0.00661	−21.3858	−22.1677	0.03527	−4.33189	−4.54344	0.04656
2.44642	−0.425568	−0.426536	0.00227	−33.2667	−33.0902	0.00533	−15.4834	−16.3395	0.05237	−3.13626	−3.38446	0.07333
4.12213	−0.286384	−0.287563	0.00412	−22.3827	−22.3185	0.00287	−10.4171	−11.0481	0.05711	−2.11055	−2.35390	0.10359
7.31001	−0.176585	−0.177644	0.00599	−13.7948	−13.7914	0.00025	−6.4192	−6.8363	0.06102	−1.30025	−1.50821	0.13788
14.15193	-9.68776×10^{-2}	-9.76172×10^{-2}	0.00757	−7.5649	−7.5799	0.00196	−3.5196	−3.7601	0.06396	−0.71293	−0.86681	0.17751
					$E=-0.1125$ a.u.							
0.02233	546.8501	545.8597	0.00181	−78.0045	−78.0603	0.00071	−80.7357	−81.0835	0.00429	−15.9752	−16.1106	0.00840
0.05502	356.6955	354.0503	0.00747	−44.6090	−46.6825	0.00157	−49.8585	−49.9220	0.00127	−9.8569	−9.9367	0.00803
0.11111	191.9335	192.2598	0.00169	−16.0510	−15.9690	0.00513	−18.7803	−19.4310	0.03348	−3.6998	−3.8950	0.05010
0.20185	56.1117	55.7274	0.00689	−6.3065	6.1398	0.02715	1.5983	2.4293	0.34209	0.33959	0.43582	0.22080
0.34492	−29.5790	−29.7449	0.00557	18.7355	17.4171	0.07569	12.3241	13.4052	0.08064	2.4653	2.6102	0.05549
0.56910	−66.4783	−66.4350	0.00065	22.7379	22.7141	0.00105	16.0302	16.0036	0.00166	3.1979	3.1244	0.02354
0.92311	−71.1448	−71.0675	0.00108	21.3042	22.3178	0.04541	15.3406	14.0707	0.09025	3.0580	2.7408	0.11573
1.49380	−60.1848	−60.1879	0.00005	17.2988	18.2988	0.05465	12.5497	10.5873	0.18535	2.5010	1.0474	0.22155
2.44642	−44.5718	−44.6641	0.00206	12.6849	13.3716	0.05135	9.2199	7.3050	0.26212	1.8373	1.3645	0.34644
4.12213	−29.8740	−30.0040	0.00433	8.5156	8.9078	0.04403	6.1869	4.8333	0.28005	1.2329	0.81952	0.50440
7.31001	−18.1921	−18.3099	0.00643	5.2121	5.4097	0.03653	3.7824	2.9245	0.29337	0.75377	0.43607	0.72855
14.15193	−9.8569	−9.9367	0.00803	2.8386	2.92767	0.04639	2.0576	1.5799	0.30231	0.41005	0.19608	1.09134
					$E=-0.0300$ a.u.							
0.02233	110.4786	109.6306	0.00773	21.8279	21.5886	0.01108	246.7351	243.2637	0.01427	43.1353	43.0873	0.00111
0.05502	4.2842	4.2803	0.00091	0.86705	0.79905	0.08510	64.9047	56.6761	0.14518	6.1430	5.9892	0.02568
0.11111	−46.8296	−48.2176	0.02878	−9.2227	−9.5650	0.03578	5.1234	6.4110	0.20083	−12.7193	−12.4270	0.02352
0.20185	−24.9264	−22.3578	0.11488	−4.8979	−4.4597	0.09826	2.0198	1.2954	0.55920	−2.6837	−3.1566	0.14980
0.34492	3.5941	5.8260	0.38309	0.73195	1.0998	0.33443	5.3500	5.0499	0.05941	9.3922	7.0959	0.32361
0.56910	17.7550	17.3157	0.02537	3.5254	3.3701	0.04606	6.8995	7.0038	0.01488	14.6955	14.8231	0.00860
0.92311	20.3592	17.8519	0.14044	4.0362	3.4753	0.16138	6.4890	6.6761	0.02802	14.6561	16.3998	0.10632
1.49380	17.4645	14.1663	0.23281	3.4610	2.7447	0.26095	5.2296	5.3244	0.01781	12.1064	13.8323	0.12477
2.44642	12.9688	9.9979	0.29715	2.5698	1.8838	0.36419	3.8236	3.7918	0.00838	8.9116	10.1366	0.12085
4.12213	8.6980	6.6392	0.31010	1.7236	1.1642	0.48053	2.5736	2.4787	0.03827	5.9829	6.7334	0.11145
7.31001	5.2997	4.0092	0.32188	1.0502	0.63884	0.64393	1.5835	1.4886	0.06380	3.6592	4.0732	0.10164
14.15193	2.8733	2.1638	0.32793	0.56941	0.30916	0.84185	0.86705	0.79905	0.08510	1.9914	2.1977	0.09387

[a] Values are given in a.u.

[b] The values are the converged values calculated from the HF expansion [Eq. (4.21)] without including continuum states.

[c] The values are the converged values calculated from the SF expansion [Eq. (4.5)].

[d] $\lvert\Delta Vt\rvert$ denotes the absolute differences between the values listed in the columns under "HF" and "SF" headings.

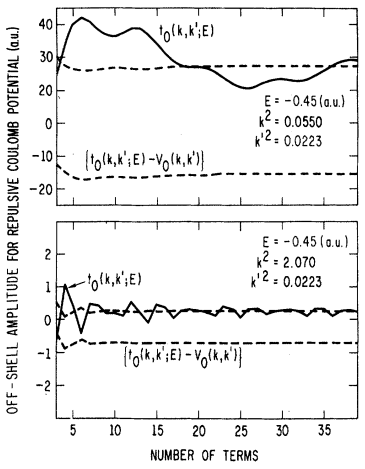

FIG. 6. Convergence behavior of the SF expansion for the s-wave off-shell amplitude [Eqs. (4.5) and (4.6)] for repulsive ($Z=1$) Coulomb interactions.

that the continuum contributions are significant for most of the arguments.

To estimate the continuum contribution in the HF series for $t_0(k,k',E)-V_0(k,k')$, we consider the converged values obtained from the SF series [Eq. (4.5)] to be a good approximation to the exact value for t_0-V_0. A comparison of the two series for t_0-V_0 is given in Table II for various values for k and k' at three E values. Utilizing these results, an estimate of the continuum contribution is made. It is seen that, in general, the continuum contributions are very small.

From this study, it is clear that the source of convergence difficulty in both separable series representation comes mostly from the V_l part of t_l. The series for V_l converges, except for certain cases in the HF expansion, in an oscillatory manner. The continuum contribution in the HF series for $t_l(k,k',E)$ at $E<0$ comes also largely from the V_l part of the series. This then suggests that numerically it would be advantageous if the V_l part of t_l may be treated separately in the Faddeev equations.

APPENDIX: SCREENING IN $t_l(k,k',E)$

The convergence of the separable SF expansion for the off-shell amplitude $t_l(k,k',E)$ may be improved by introducing into the expansion a convergence parameter. By replacing γ_λ in Eqs. (4.5) and (4.6) by $(1+Z')^\lambda\gamma_\lambda$ we have[28]

$$\tilde{t}_l(k,k',E)=\sum_\lambda[1-(1+Z')^\lambda\gamma_{\lambda l}]^{-1}\phi_{\lambda l}(k,E)\phi_{\lambda l}(k',E)\ , \tag{A1}$$

where Z' is a constant. If $Z'=0$ we have $\tilde{t}_l=t_l$. It can be shown that the constant Z' so introduced has the physical significance of being a screening constant.

To demonstrate this we examine the part of Eq. (A1) corresponding to the potential part of the series, [see Eq. (4.6)]

$$\tilde{V}_l(k,k')=-\sum_\lambda[(1+Z')^\lambda\gamma_{\lambda l}]^{-1}\phi_{\lambda l}(k,E)\phi_{\lambda l}(k',E)\ . \tag{A2}$$

We show (for the $l=0$ case) that the series at the right-hand side of Eq. (A2) may be summed up to give a screened potential.

For $l=0$, we have
$$\phi_{\lambda 0}(k,E)=(8/\mu)^{1/2}[(-2\mu E)^{3/4}/(k^2-2\mu E)]\sin\lambda\varphi_k/\sin\varphi_k \tag{A3}$$

with
$$\cos\varphi_k=(k^2+2\mu E)/(k^2-2\mu E)\ . \tag{A4}$$

Then
$$\tilde{V}_0(k,k')=+\frac{2Z}{kk'}\sum_{\lambda=1}^{\infty}\frac{\sin\lambda\varphi_k\sin\lambda\varphi_{k'}}{\lambda(1+Z')^\lambda}=\frac{Z}{2kk'}\sum_{\lambda=1}^{\infty}\frac{1}{\lambda}\left[\left(\frac{e^{i(\varphi_k-\varphi_{k'})}}{1+Z'}\right)^\lambda+\left(\frac{e^{-i(\varphi_k-\varphi_{k'})}}{1+Z'}\right)^\lambda\right.$$
$$\left.-\left(\frac{e^{i(\varphi_k+\varphi_{k'})}}{1+Z'}\right)^\lambda-\left(\frac{e^{-i(\varphi_k+\varphi_{k'})}}{1+Z'}\right)^\lambda\right]=\frac{Z}{2kk'}\ln\left[\left(1-\frac{e^{i(\varphi_k+\varphi_{k'})}}{1+Z'}\right)\left(1-\frac{e^{-i(\varphi_k+\varphi_{k'})}}{1+Z'}\right)\right]$$
$$\times\left[\left(1-\frac{e^{i(\varphi_k-\varphi_{k'})}}{1+Z'}\right)\left(1-\frac{e^{-i(\varphi_k-\varphi_{k'})}}{1+Z'}\right)\right]^{-1}$$

$$= \frac{Z}{kk'} Q_0 \left[\frac{k^2+k'^2}{2kk'} \left(1 - \frac{Z'^2(k^2-2\mu E)(k'^2-2\mu E)}{8\mu E(1+Z')(k^2+k'^2)} \right) \right]. \quad \text{(A5)}$$

This then demonstrates that the constant Z' introduced in Eq. (A2) as well as in Eq. (A1) has the physical significance of being a screening constant. The interesting feature of the screening lies in the fact that it is energy-dependent.

---

*Research supported by the Advanced Research Projects Agency of the Department of Defense and was monitored by the U.S. Army Research Office, Durham under Contract No. DA-31-124-ARO-D-257.

†Present address: Department of Physics, University of California, Riverside, California.

[1]N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Oxford University Press, London, 1965), 3rd ed.

[2]M. Rotenberg, Ann. Phys. (N. Y.) 19, 262 (1962).

[3]P. G. Burke and H. M. Schey, Phys. Rev. 126, 149 (1962).

[4]R. Marriott, Proc. Phys. Soc. (London) 72, 121 (1958).

[5]K. Omidvar, Phys. Rev. 133, A970 (1964).

[6]E. Holoien (private communication).

[7]D. F. Gallaher and L. Wilets, Phys. Rev. 169, 139 (1968).

[8]A. J. Taylor and P. G. Burke, Proc. Phys. Soc. (London) 92, 336 (1967).

[9]R. J. Damburg and S. Geltman, Phys. Rev. Letters 20, 485 (1968).

[10]H. Feshbach, Ann. Phys. (N. Y.) 5, 357 (1958); 19, 287 (1962).

[11]J. C. Y. Chen, Phys. Rev. 152, 1454 (1966).

[12]M. F. Fels and M. Mittleman, Phys. Rev. 163, 129 (1968).

[13]L. D. Faddeev, Mathematical Aspects of the Three-Body Problem in the Quantum Scattering Theory (The Israel Program for Scientific Translations, Jerusalem, 1965).

[14]J. S. Ball, J. C. Y. Chen, and D. Y. Wong, Phys. Rev. 173, 202 (1968).

[15]For a preliminary account of this expansion, see J. C. Y. Chen and T. Ishihara, Proc. Phys. Soc. (London) [J. Phys. B 2, 12 (1969)].

[16]I. C. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. 53, 654 (1957).

[17]F. S. Levin, Phys. Rev. 142, 33 (1966).

[18]For a review, see P. G. Burke in Advances in Atomic and Molecular Physics, edited by D. R. Bates and I. Estermann (Academic Press Inc., New York, 1968), Vol. 4.

[19]S. J. Ormonde, J. McEwen, and J. William McGowan Phys. Rev. Letters 22, 1165 (1969).

[20]G. E. Chamberlain, S. J. Smith, and D. W. O. Heddle, Phys. Rev. Letters 12, 647 (1964).

[21]H. Kleinpoppen and E. Kraiss, Phys. Rev. Letters 20, 361 (1968).

[22]J. F. Williams and J. Wm. McGowen, Phys. Rev. Letters 21, 719 (1968).

[23]M. Gailitis and R. J. Damburg, Proc. Phys. Soc. (London) 82, 192 (1963).

[24]C. Lovelace, Phys. Rev. 135, B1225 (1964).

[25]A. Ahmadzadeh and J. A. Tjon, Phys. Rev. 139, B1085 (1965).

[26]T. Osborn and H. P. Noyes, Phys. Rev. Letters 17, 215 (1966).

[27]R. Balian and E. Brézin, Nuovo Cimento (to be published).

[28]One of us (J. C. Y. C.) is grateful to Professor J. S. Ball for discussions of the screening problem.