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[1]See, for example, H. S. W. Massey, *Electronic and Ionic Impact Phenomena*, 2nd ed. (Oxford U. P., London, 1969) Vol. II; L. O. Brockway, *Physical Methods of Organic Chemistry*, 2nd ed. (Interscience, New York, 1949), Chap. XIX, pp. 1109–1140. For accurate form factors for the H_2 molecule, see R. F. Stewart, E. R. Davidson, and W. T. Simpson, J. Chem. Phys. 42, 3175 (1965). For recent work on interference effects in electron diffraction from diatomic molecules, see S. P. Khare and B. L. Moiseiwitsch, Proc. Phys. Soc. (London) 85, 821 (1965). For earlier work on this subject see W. E. Frye, Phys. Rev. 60, 586 (1941); F. C. Hoyt and W. E. Frye, *ibid.* 58, 784 (1940); C. H. Shaw and T. M. Snyder, *ibid.* 58, 600 (1940); J. B. Fisk, *ibid.* 51, 25 (1937); 49, 167 (1936). For similar interference effects in the photo-ionization of diatomic molecules, see H. D. Cohen and U. Fano, Phys. Rev. 150, 30 (1966).

[2]In this connection one may note H. S. W. Massey, *Electronic and Ionic Impact Phenomena*, 2nd ed. (Oxford U. P., London, 1969) Vol. II, Chap. 10. There, in Fig. 10.14 on p. 687 is plotted the ratio of the elastic scattering from H_2 to the sum of the elastic scattering from two isolated H atoms, calculated by Born's approximation, for three different models: (a) the independent atom model (which is what we are using in this paper), (b) using Wang's wave function for H_2 and (c)using Weinbaum's wave function for H_2. The latter two models allow for valence distortion. It may be noticed in that figure, that there is no difference in the results predicted by the three models for momentum transfers above that at which the first interference minimum occurs.

[3]W. K. H. Panofsky, *Springer Tracts in Modern Physics*, (Springer-Verlag, Berlin, 1965), Vol. 39, p. 138. H. Olsen, *ibid.* (Springer-Verlag, Berlin, 1968), Vol. 44, p. 195. These articles contain other references.

[4]W. Heitler, *The Quantum Theory of Radiation*, 3rd ed. (Oxford U. P., London, 1954) p. 242.

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[8]*National Bureau of Standards Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (U. S. G. P. O., Washington, D. C. 1964), p. 229, Eq. (5.1.22).

[9]Values of R were obtained from E. U. Condon and H. Odishaw, *Handbook of Physics*, 2nd ed. (McGraw-Hill, New York, 1967), Chap. 7, p. 113.

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Faddeev Equations for Atomic Problems. III. Convergence of the Separable-Expansion Method for Coulomb Interactions *

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The convergence of the separable-expansion method for solving the Faddeev equations is investigated for systems with pure Coulomb interactions between particles in each pair. Two alternative separable expansions for the off-shell two-body amplitudes are utilized. It is observed that the expansion method is capable of predicting qualitatively all the characteristic features such as the three-body bound-state and resonance poles, the scattering length, and the energy dependence of the phase shift in atomic systems such as the (e, H) system. Although some convergence behavior is observed, this method in the present form does not provide the desired accuracy when reasonable numbers of terms are included in the expansion for the attractive $(e\text{-}p)$ scattering amplitudes. This behavior is interpreted as due to the failure of the two alternative expansions for the off-shell two-body amplitudes to converge monatonically.

I. INTRODUCTION

A systematic method for solving the Faddeev equations for atomic problems has recently been proposed and investigated in Paper I of this series.[1] Two alternative term-by-term separable-series representations for the two-body off-shell amplitudes were utilized in Paper II to reduce the Faddeev equations to a set of coupled single-variable integral equations.[2] Since these equations are algebraic results, they are exact and independent of the strength and range of the interaction. In practice it is always necessary to truncate the series; this then leads to the problem of convergence with

respect to the inclusion of the remaining terms which may be regarded as perturbations.[1] The convergence behavior of these reduced equations depends obviously upon the details of the convergence behavior of the separable-series representations for each two-body off-shell amplitude.

For cases where the kernels of the two-body Lippmann-Schwinger equations are compact for each of the pair interactions, the two-body off-shell amplitude may always be accurately approximated by a finite number of separable terms,[3] and the procedure for solving the Faddeev equations described in Papers I and II should work well. For Coulomb potentials, the two-body kernel is no longer compact; the problem of convergence for these separable-series representations becomes serious.

It has been observed[4,5] that these term-by-term separable-series representations for the two-body off-shell amplitude of an unscreened Coulomb potential behave as n^{-1}, indicating a logarithmic divergence, where n is the principal quantum number of the eigenfunctions in terms of which the series representations are expressed. However, the two-body off-shell amplitudes which appear in the Faddeev equations have one of their arguments integrated once. This should result in a better convergent set of equations. We have conjectured in Paper I that these resultant equations should converge reasonably rapidly. To test our conjecture, the expansion method in the Sturmian-function representation was applied to the (e, H) scattering system. Very encouraging results were obtained for the bound and resonant H^- states and for the phase shift with a few terms in the leading partial waves. As additional terms were included, the results did not converge uniformly towards the verified known results but oscillated about them, although the amplitude of oscillation appeared to decrease as the number of terms increased. This then led to a detailed examination of the separable-series representation for the off-shell two-body amplitudes.[5]

Two such term-by-term separable-series representations for off-shell two-body amplitudes, namely the Sturmian- and the Coulomb-function series representations, were investigated for the unscreened Coulomb interaction.[4,5] Significant differences were found in the convergence behavior for these two series representations. It was observed that the oscillatory behavior found in the Sturmian-function series could be controlled only after a prohibitive number of terms were included. The Coulomb-function series converged with a reasonable number of terms to a limit which was shifted from the exact value. The shift which comes from the neglected continuum states was usually small although its contribution to the three-body scattering processes was not clear. In view of these, a mixed-mode representation was proposed in Paper II. In this representation, the Coulomb-function (CF) representation was adopted for pairs where the interaction potential is attractive. For pairs where the interaction potential is repulsive and the continuum contribution is dominating, the Sturmian-function (SF) representation was adopted.

The purpose of the present paper is to investigate the convergence of the Faddeev equations in this mixed-mode series representation.[6] In this mixed-mode representation, it is possible to investigate the convergence of the SF series for the repulsive interactions with a fixed number of terms in the CF series for the attractive interactions. For the purpose of comparison with the result of Paper I, we will again take the (e, H) system for our investigation. It may well be mentioned that for systems with short-range pair interactions, we expect rapid convergence for the expansion method.

II. RESUME OF EXPANSION METHOD

In this section, we outline briefly the separable-expansion method for solving the Faddeev equations and correct an error[7] which appears in the previous works in the angular momentum reduction. For further details, the reader is referred to Papers I and II of this series.

The separation of the angular momentum states in the Faddeev equations[8] can be carried out using the relative angular momentum l between two particles, which is combined with the angular momentum L of the third particle to give the total angular momentum J in the over-all c. m. system. We have from Eqs. (II 2. 10)–(II 2. 15) the partial-wave Faddeev equations

$$\Psi_\alpha^{(i)}(p, q, s) = \Phi_\alpha^{(i)}(p, q, s) - \tfrac{1}{4} \sum_{\alpha_j} \sum_{j \neq i} \int_0^\infty dp_j^2 \int_0^\infty dq_j^2 \, \mathcal{K}_j^{(i)}(pq\alpha / p_j q_j \alpha_j) \frac{p_j q_j}{p_j^2 + q_j^2 - s} \Psi_{\alpha_j}^{(j)}(p_j, q_j, s), \quad i = 1, 2, 3 \tag{2.1}$$

with

$$\mathcal{K}_j^{(i)}(pq\alpha \,|\, p_j q_j \alpha_j) = \int_{-1} d(\cos\theta)_{\vec{p}_i \vec{q}_j} A_{\alpha\alpha_j}(\theta_{\vec{p}_i \vec{p}_j}, \theta_{\vec{p}_j \vec{q}_i}, \theta_{\vec{p}_j \vec{q}_j}) \delta(q^2 - q_i^2) t_l^{(i)}(p, p_i; s - q^2), \tag{2.2}$$

$$A_{\alpha\alpha'}(\theta_{\vec{\mathfrak{p}}_i\vec{\mathfrak{p}}_j},\ \theta_{\vec{\mathfrak{p}}_j\vec{\mathfrak{q}}_i},\ \theta_{\vec{\mathfrak{p}}_j\vec{\mathfrak{q}}_j}) = (-)^{L+L'-l-l'}\ (16\pi^{1/2}/q)\ (2l'+1)^{1/2}\,\delta_{J,J'}\delta_{MM'} \sum_{m_l m_L m_{L'}} \begin{pmatrix} l & L & J & l' & L' & J' \\ m_l & m_L & -M & m_l' & m_L' & -M' \end{pmatrix}$$
$$\times Y^*_{lm_l}\{\theta_{\vec{\mathfrak{p}}_i\vec{\mathfrak{p}}_j},\ [1+(ij)]\tfrac{1}{2}\pi\}\ Y^*_{Lm_L}(\theta_{\vec{\mathfrak{p}}_j\vec{\mathfrak{q}}_i},\ \pi)\ Y_{L'm_{L'}}(\theta_{\vec{\mathfrak{p}}_j\vec{\mathfrak{q}}_j},\ 0), \tag{2.3}$$

where $\alpha \equiv (JMlL)$, $p_i^2 = p_j^2 + q_j^2 - q^2$, and $\theta_{\vec{\mathfrak{p}}_i\vec{\mathfrak{p}}_j}$, for example, is the angle between momentum variable $\vec{\mathfrak{p}}_i$ and $\vec{\mathfrak{p}}_j$.

We call attention to the fact that in the previous works[1,2,9,10] the azimuthal angles which appear in the spherical harmonics are incorrectly taken to be zero.[7] In the expression for $A_{\alpha\alpha'}$ given by Eq. (2.3) the correct values for the azimuthal angles are given. These can be seen as follows. Since the angular decoupling is invariant under simultaneous rotation of the basis vectors, we may take p_j along the z axis. The azimuthal angles (in the spherical harmonics) which can either be equal or differ by π may be chosen to be either zero or π. From the cross product of the basis vectors we have

$$\vec{\mathfrak{p}}_i\times\vec{\mathfrak{p}}_j = [-\alpha_{ij}\vec{\mathfrak{p}}_j - (ij)\,\beta_{ij}\vec{\mathfrak{q}}_j]\times\vec{\mathfrak{p}}_j = -(ij)\,\beta_{ij}\vec{\mathfrak{p}}_j\times\vec{\mathfrak{q}}_j, \tag{2.4}$$

$$\vec{\mathfrak{p}}_j\times\vec{\mathfrak{q}}_i = \vec{\mathfrak{p}}_j\times[(ij)\,\beta_{ij}\vec{\mathfrak{p}}_j - \alpha_{ij}\vec{\mathfrak{q}}_j] = -\alpha_{ij}\vec{\mathfrak{p}}_j\times\vec{\mathfrak{q}}_j, \tag{2.5}$$

where (ij) denotes that $(12)=(23)=(31)=1$ and $(21)=(32)=(13)=-1$ and where α_{ij} and β_{ij} are defined in terms of the particle masses m_i:

$$\alpha_{ij} \equiv \{m_i m_j/[(m_i+m_k)(m_j+m_k)]\}^{1/2}, \quad \beta_{ij} \equiv (1-\alpha_{ij}^2)^{1/2}. \tag{2.6}$$

It is then clear that if we choose the azimuthal angle to be zero for $\vec{\mathfrak{q}}_j$ (remember that $\vec{\mathfrak{p}}_j$ is taken along the z axis), we have for $\vec{\mathfrak{q}}_i$ the azimuthal angle π and for $\vec{\mathfrak{p}}_i$ the azimuthal angle $\frac{1}{2}[1+(ij)]\pi$. It should be noted that the previous error in the azimuthal angle does not affect the numerical results which are obtained for the $J=0$ case.

Returning now to Eq. (2.1) we consider, for simplicity, only states corresponding to zero total angular momentum. For this $J=0$ case, $\alpha=(00ll)\equiv l$ and Eq. (2.1) becomes[1]

$$\Psi_l^{(i)}(p,q,s) = \Phi_l^{(i)}(p,q,s) + \sum_{j\neq i}\sum_{l'=0} \int_0^\infty dq_j^2 \int_{L_{ij}}^{U_{ij}} dp_j^2\, B_{ll'}^{(i,j)}(q,p_j,q_j;s)\, t_l^{(i)}(p,p_i;s-q^2)\,\Psi_{l'}^{(j)}(p_j,q_j,s), \tag{2.7}$$

with

$$B_{ll'}^{(i,j)}(q,p_j,q_j;s) \equiv \frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{1/2}}{4\pi\,\alpha_{ij}\beta_{ij}\,q(p_j^2+q_i^2-s)}\ P_l(\omega_i)\,P_{l'}(\overline{\omega}_j), \tag{2.8}$$

$$\omega_i \equiv \cos\theta_{\vec{\mathfrak{p}}_i\vec{\mathfrak{q}}_i} = (ij)\,[\alpha_{ij}^2(q_i^2-q^2) + \beta_{ij}^2(q^2-p_j^2)]/2\alpha_{ij}\beta_{ij}qp_i, \tag{2.9}$$

$$\overline{\omega}_j \equiv \cos\theta_{\vec{\mathfrak{p}}_j\vec{\mathfrak{q}}_j} = (ij)\ (\beta_{ij}^2 p_j^2 + \alpha_{ij}^2 q_j^2 - q^2)/2\alpha_{ij}\beta_{ij}p_j q_j, \tag{2.10}$$

where the limits of integration are given by the equations

$$U_{ij} \equiv (\alpha_{ij}q_j+q)^2/\beta_{ij}^2, \quad L_{ij} \equiv (\alpha_{ij}q_j-q)^2/\beta_{ij}^2. \tag{2.11}$$

The scattering amplitude between particles j and k with angular momentum l, $t_l^{(i)}(p,p_i;s-q^2)$, which appears in the kernels of Eqs. (2.1) and (2.4), is the solution of the Lippmann-Schwinger equations

$$t_l^{(i)}(p,p';E) = V_l^{(i)}(p,p') - (1/\pi)\int_0^\infty dp''\,[p''^2/(p''^2-E)]\ V_l^{(i)}(p,p'')\,t_l^{(i)}(p'',p';E), \tag{2.12}$$

where $V_l^{(i)}(p,p')$ is the partial-wave two-body interaction potential. The two-body scattering amplitude is normalized on the energy shell according to the equation

$$t_l^{(i)}(p,p;p^2) = -e^{i\delta_l^{(i)}}(\sin\delta_l^{(i)})/p. \tag{2.13}$$

Here p^2 is the two-body c.m. energy. We remark that, for Coulomb potential scattering, the on-shell expansion given by Eq. (2.13) cannot be obtained from the off-shell amplitude $t_l(p,p';E)$ of Eq. (2.12) in a straightforward manner. This is because the plane-wave states are used in obtaining Eq. (2.12) [or $t_l(p,p';E)$]. The on-shell expansion can be obtained if the correct asymptotic Coulomb states are used. However, in our intended applications, the two-body on-shell amplitudes are not required as long as we stay below the three-body break-up threshold as we have already remarked in Paper I.

In the mixed-mode representation, the off-shell two-body amplitudes are represented, for attractive interaction, by the series[4]

$$t_l^{(i)}(p, p'; E) = \frac{\pi}{2} \sum_n{}' \frac{(p^2 - \epsilon_n^{(i)})(p'^2 - E)}{\epsilon_n^{(i)} - E} \psi_{nl}^{(i)*}(np) \psi_{nl}^{(i)}(np') \tag{2.14}$$

and, for repulsive interaction, by the series

$$t_l^{(i)}(p, p'; E) = \sum_\lambda \frac{1}{1 - \gamma_{\lambda l}^{(i)}(E)} \phi_{\lambda l}^{(i)}(p, E) \phi_{\lambda l}^{(i)}(p', E) . \tag{2.15}$$

The CF (i.e., the $\psi_{nl}^{(i)}$'s) and SF (i.e., the $\phi_{\lambda l}^{(i)}$'s) are, respectively, of the forms

$$\psi_{nl}^{(i)}(np) = \left(\frac{2^{4l+5} n(n-l-1)!}{\pi(n+l)!}\right)^{1/2} l!(-\epsilon_n)^{(2l+5)/4} \frac{p^l}{(p^2 - \epsilon_n^{(i)})^{l+2}} C_{n-l-1}^{l+1}\left(\frac{p^2 + \epsilon_n^{(i)}}{p^2 - \epsilon_n^{(i)}}\right) , \tag{2.16}$$

$$\phi_{\lambda l}^{(i)}(p, E) = \left(\frac{2^{4l+3}\lambda(\lambda-l-1)!}{\Gamma(\lambda+l+1)}\right)^{1/2} l!(-E)^{(2l+3)/4} \frac{p^l}{(p^2 - E)^{l+1}} C_{\lambda-l-1}^{l+1}\left(\frac{p^2 + E}{p^2 - E}\right) , \tag{2.17}$$

where C_{n-l-1}^{l+1} and $C_{\lambda-l-1}^{l+1}$ are the Gegenbauer polynomials. These functions satisfy the orthonormality properties

$$\int_0^\infty \psi_{nl}^*(np)\, \psi_{n'l}(n'p)\, p^2\, dp = \delta_{nn'} , \tag{2.18}$$

$$(1/\pi) \int_0^\infty \phi_{\lambda l}(p, E)\, \phi_{\lambda' l}(p, E)\, [p/(p^2 - E)]\, dp^2 = \delta_{\lambda\lambda'} . \tag{2.19}$$

Their corresponding eigenvalues $\epsilon_n^{(i)}$ and $\gamma_{\lambda l}^{(i)}(E)$ are given, respectively, by

$$\epsilon_n^{(i)} = -Z_i^2 \mu_i / 2n^2 , \quad \gamma_{\lambda l}^{(i)}(E) = -\lambda(-2E/\mu_i)^{1/2}/Z_i , \tag{2.20}$$

where μ_i is the reduced mass of ith pair and Z_i is the product of the charges of the constituent particles in the ith pair.

When these series representations given by Eqs. (2.14) and (2.15) for the off-shell two-body amplitudes are utilized in Eq. (2.7), we obtain the set of single-variable Faddeev equations in the mixed-mode representation:

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

$$+ \sum_{\lambda' l'} \int_0^\infty dq_3^2\, \mathcal{K}_{nl,\lambda' l'}^{(i,3)}(q, q_3; s)\, \chi_{\lambda' l'}^{(3)}(q_3, s), \quad i = 1, 2 \tag{2.21a}$$

$$\chi_{\lambda l}^{(3)}(q, s) = \eta_{\lambda l}^{(3)}(q, s) + \sum_{n' l'} \sum_{j\neq 3} \int_0^\infty dq_j^2\, \mathcal{K}_{\lambda l,n'l'}^{(3,j)}(q, q_j; s)\, \chi_{n'l'}^{(j)}(q_j, s) , \tag{2.21b}$$

with

$$\mathcal{K}_{nl,n'l'}^{(i,j)}(q, q_j; s) = -\frac{\pi}{2} \int_{L_{ij}}^{U_{ij}} dp_j^2\, B_{ll'}^{(i,j)}(q, p_j, q_j; s)\, \frac{(p_j^2 + q_j^2 - s)(p_j^2 - \epsilon_{n'}^{(j)})}{s - \epsilon_{n'}^{(j)} - q_j^2}\, \psi_{nl}^{(i)}(np_i)\, \psi_{n'l'}^{(j)}(n'p_j) , \tag{2.22a}$$

$$\mathcal{K}_{nl,\lambda' l'}^{(i,3)}(q, q_j; s) = \int_{L_{i3}}^{U_{i3}} dp_3^2\, B_{ll'}^{(i,3)}(q, p_3, q_3; s)\, \frac{p_3^2 + q_3^2 - s}{1 - \gamma_{\lambda' l'}^{(3)}(s - q_3^2)}\, \psi_{nl}^{(i)}(np_i)\, \phi_{\lambda' l'}^{(3)}(p_3, s - q_3^2) , \tag{2.22b}$$

$$\mathcal{K}_{\lambda l,n'l'}^{(3,j)}(q, q_j; s) = \frac{\pi}{2} \int_{L_{3j}}^{U_{3j}} dp_j^2\, B_{ll'}^{(3,j)}(q, p_j, q_j; s)\, \frac{p_j^2 - \epsilon_{n'}^{(j)}}{s - \epsilon_{n'}^{(j)} - q_j^2}\, \phi_{\lambda l}^{(3)}(p_3, s - q_3^2)\, \psi_{n'l'}^{(j)}(n'p_j) , \tag{2.22c}$$

$$\eta_{nl}^{(i)}(q, s) = -\sum_{l', j\neq i} \int_0^\infty dp_j^2 \int_{L_{ij}}^{U_{ij}} dp_j^2\, B_{ll'}^{(i,j)}(q, p_j, q_j; s)(p_j^2 + q_j^2 - s)\, \psi_{nl}^{(i)}(np_i)\, \Phi_{l'}^{(j)}(p_j, q_j; s), \quad i = 1, 2 \tag{2.23a}$$

$$\eta_{\lambda l}^{(3)}(q,s)=\sum_{l',j\neq 3}\int_0^\infty dq_j^2\int_{L_{3j}}^{U_{3j}} dp_j^2\, B_{ll'}^{(3,j)}(q,p_j,q_j;s)\,\phi_{\lambda l}^{(3)}(p_3,s-q_3^2)\,\Phi_{l'}^{(j)}(p_j,q_j,s)\,, \tag{2.23b}$$

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 potential.

The χ functions which satisfy the above equations are related to the off-shell three-body amplitudes:

$$\Psi_l^{(i)}(p,q,s)=\Phi_l^{(i)}(p,q,s)+\frac{\pi}{2}\sum_n \frac{p^2-\epsilon_n^{(i)}}{s-\epsilon_n^{(i)}-q^2}\,\psi_{nl}^{(i)}(np)\,\chi_{nl}^{(i)}(q,s),\quad i=1,2 \tag{2.24a}$$

$$\Psi_l^{(j)}(p,q,s)=\Phi_l^{(j)}(p,q,s)+\sum_\lambda \frac{1}{\gamma_\lambda^{(j)}(s-q^2)-1}\,\phi_{\lambda l}^{(j)}(p,s-q^2)\,\chi_{\lambda l}^{(j)}(q,s)\,,\quad j=3. \tag{2.24b}$$

Once these χ functions are determined, the three-body scattering amplitudes can be easily calculated by taking appropriate energy limits to the energy shell.[2]

III. INVESTIGATION OF THE CONVERGENCE

In this section, we investigate the convergence of the set of single-variable Faddeev equations in the mixed-mode representation as given by Eqs. (2.21). As a test case, we consider again the (e, H) system. Equations (2.21) may be solved for $\chi(s)$ by digitizing the continuous variables q and q_j and inverting the matrix $(\underline{I}-\underline{\mathcal{K}})$:

$$\underline{\chi}(s)=[\underline{I}-\underline{\mathcal{K}}(s)]^{-1}\underline{\eta}(s)\,. \tag{3.1}$$

To calculate the bound states and resonances, we need to determine the pole in the inverse operator $[\underline{I}-\underline{\mathcal{K}}(s)]^{-1}$. Since bound states are located at the three-body energy region lying below the elastic threshold, the matrix $(\underline{I}-\underline{\mathcal{K}})$ contains no branch point and is real. The bound-state pole may be easily located by locating the energy s at which the determinant of the matrix [i.e., $\det(\underline{I}-\underline{\mathcal{K}})$] is zero.

A bound-state pole associated with the $^1SH^-$ ground state is obtained by taking only the $1s$ term in the CF series for the attractive pair interactions. The $1s$-configuration result is shown in Fig. 1. The interesting feature of this bound-state result is the convergence behavior: the number of terms used in the SF series for the repulsive e-e interaction. It is seen that the three-body bound-state pole, i.e., the zero of $\det(\underline{I}-\underline{\mathcal{K}})$, moves towards the accurate Pekeris result for the ground H^- state as more terms in the SF series are included. Because these SF terms represent repulsive interactions it is not surprising that the bound-state pole should shift towards the right. The surprising feature is the manner in which the magnitude of the shift decreases with increasing SF terms. This suggests a convergence behavior. Such a convergence behavior (with respect to the SF series for the repulsive e-e interaction) with fixed configuration for the attractive interaction appears also in the results for the H^- resonances.

The lowest resonance, in the singlet $J=0$ (e, H) scattering, appears in the elastic-scattering region where the corresponding matrix $(\underline{I}-\underline{\mathcal{K}})$ becomes complex and contains a branch point associated with the ground state of hydrogen. As expected, by taking only the $1s$ term in the CF series for the attractive pair interactions, it is not possible to reproduce the resonances with the inclusion of any number of terms in the SF series for the repulsive $(e$-$e)$ interaction. The resonance is obtained by the inclusion of the $2s$ term in the CF series for the attractive interactions. In Fig. 2, we have plotted both the real and imaginary parts of the determinant of the matrix $\underline{I}-\underline{\mathcal{K}}$ as a function of the three-body energy s calculated with a $1s$-

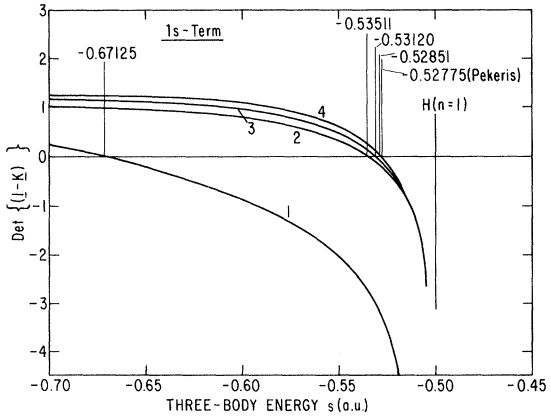

FIG. 1. H^- bound-state calculation; the zero in the function $\det(\underline{I}-\underline{\mathcal{K}})$ gives the position of the pole in the three-body T matrix. In this calculation, the e-p amplitude is approximated by $1s$ hydrogenic function only, and 1, 2, 3, 4 indicates the number of the SF included in the s-wave e-e amplitude.

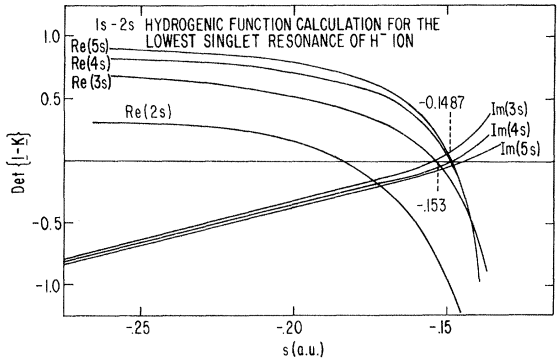

FIG. 2. e-H lowest ^1S resonance-state calculation; (ns) indicates $1s$, $2s, \ldots,$ ns partial waves are included in the e-e amplitude. Re and Im denote the real part and the imaginary part of $\det(\underline{I}-\underline{\mathcal{K}})$, respectively. The zeros of $\mathrm{Re}(\underline{I}-\underline{\mathcal{K}})$ are the positions of the resonances.

$2s$ configuration for the attractive interactions. We observe that the resonance pole located at the zero of the real part of $\det(\underline{I}-\underline{\mathcal{K}})$ shifts, as expected, towards the left as the number of SF in the repulsive interaction increases. The magnitude of the shift again decreases rapidly with the increase in the number of SF functions. It is seen in Fig. 2 that the $1s$-$2s$ result appears to converge to a limit at -0.1487 a.u. lying close to the known position of the resonance at -0.14865 a.u. The present $1s$-$2s$ result is actually better than the corresponding $1s$-$2s$ close-coupling result.[11] The corresponding $1s$-$2s$-$2p$ close-coupling result is -0.147 a.u.[12]

Since the χ's are related to the three-body amplitudes according to Eqs. (2.24), it is not difficult to see from Eq. (3.1) that the scattering amplitude $\mathcal{T}$ may be written as

$$\mathcal{T} = [\underline{\mathcal{C}}(s)/\det(\underline{I}-\underline{\mathcal{K}})]\underline{\eta}\,, \tag{3.2}$$

where $\mathcal{C}(s)$ is usually a complex matrix coming from the matrix $(\underline{I}-\underline{\mathcal{K}})^{-1}$.

In the elastic scattering energy region, there is only one branch point in the matrix $(\underline{I}-\underline{\mathcal{K}})$, and the inhomogeneous term $\underline{\eta}$ is real. By utilizing the indistinguishability of electrons, the three sets of coupled single-variable Faddeev equations given by Eqs. (3.21) may be reduced to a single set and to two sets of coupled equations for both singlet and triplet (e, H) scattering [see Eqs. (II 4.17) and (II 4.21)]. When these reduced equations are adopted for the calculation, it is not difficult to see that the branch point associated with the H ground state appears only in elements of one of the columns of the matrix $(\underline{I}-\underline{\mathcal{K}})$. Consequently, only one column of the matrix $(\underline{I}-\underline{\mathcal{K}})$ is complex. In this case, the matrix $\mathcal{C}$ in Eq. (3.2) becomes real.

At the resonance energy s_0, the determinant $\det(\underline{I}-\underline{\mathcal{K}})$ which is complex, can be expanded as

$$f(s) \equiv \det(\underline{I}-\underline{\mathcal{K}}) = (s-s_0)\,\mathrm{Re}[f'(s_0)] + i\,\mathrm{Im}[f(s)]\,, \tag{3.3}$$

with

$$\mathrm{Re}[f'(s_0)] \equiv \frac{\partial}{\partial s}\,\mathrm{Re}[\underline{I}-\underline{\mathcal{K}}(s)]\,\big|_{s=s_0}\,, \tag{3.4}$$

where we have made use of $\mathrm{Re}[f(s_0)]=0$. Utilizing the expansion for $\det(\underline{I}-\underline{\mathcal{K}})$, we obtain from Eq. (3.2)

$$|\mathcal{T}_r|^2 \cong \frac{|\underline{C}(s)\underline{\eta}(s)|^2/[\mathrm{Re}f'(s_0)]^2}{(s-s_0)^2+\frac{1}{4}\Gamma^2(s)}\,, \tag{3.5}$$

with

$$\Gamma(s) = 2\,\mathrm{Im}[f(s)]/\mathrm{Re}[f'(s_0)]\,, \tag{3.6}$$

where $\Gamma(s)$ at $s=s_0$ is the usual half-width of the resonance. This permits us to calculate the resonance width Γ from the imaginary part of $\det(\underline{I}-\underline{\mathcal{K}})$ and the slope of the real part of $\det(\underline{I}-\underline{\mathcal{K}})$. It should be noted that this derivation for $\Gamma(s)$ assumes that $\mathrm{Im}[f(s)]$ is a slowly varying function of s in the neighborhood of the resonance energy.

Returning now to our calculation, we observe that the rate of convergence with respect to terms in the SF series for the e-e interaction appears to become slower when the $2p$ term is included in the CF series for the attractive e-p interactions. The result for the $1s$-$2s$-$2p$ configuration calculation is displayed in Fig. 3. It is seen that more repulsive terms are needed to compensate for the additional attraction introduced by the inclusion of the $2p$ term. This is a discouraging result since the

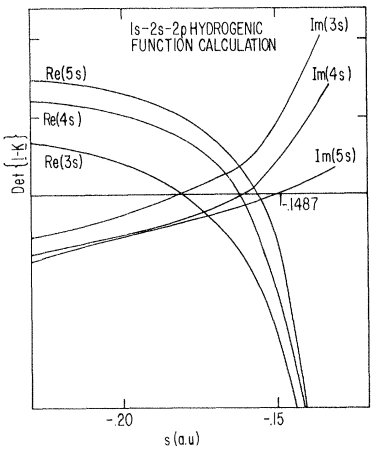

FIG. 3. e-H lowest ^1S resonance-state calculation; (ns) indicates $1s$, $2s\ldots$, ns partial waves are included in the e-e amplitude. Re and Im denote the real and imaginary part of $\det(\underline{I}-\underline{\mathcal{K}})$, respectively. The zeros of $\mathrm{Re}(\underline{I}-\underline{\mathcal{K}})$ are the positions of the resonances.

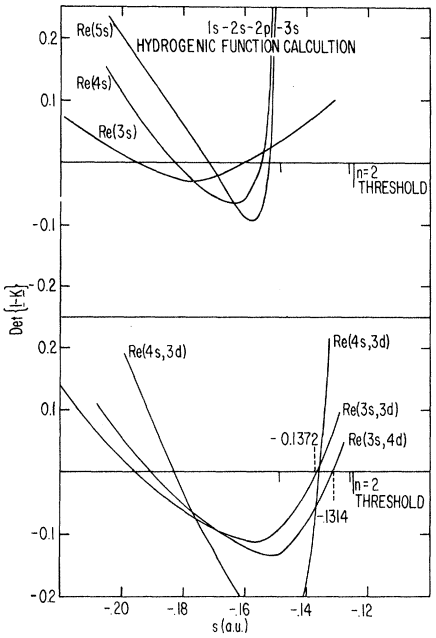

FIG. 4. e-H ^1S resonance-states calculation; (ns) indicates 1s, 2s, ..., ns and ($n'd$) indicates 3d, 4d, ..., $n'd$ partial waves are included in the e-e amplitude. The zeros in the Re($\underline{I} - \underline{\mathcal{K}}$) are the positions of the resonances.

number of terms needed to obtain accurate results increases rapidly. In addition, the inclusion of the 2p term in the CF series does not provide us with the description of the higher member resonances in the singlet $J = 0$ (e, H) scattering system as shown in Fig. 3.

Higher members of the resonances in the elastic channel can be obtained by including further terms in the CF series for the attractive e-p interactions. The results for the 1s-2s-2p-3s and the 1s-2s-2p-3s-3p configuration calculations are displayed in Figs. 4 and 5, respectively. It is seen from Fig. 4 that two resonances are obtained with the 1s-2s-2p-3s configuration calculation. The addition of the 3p term provides the description of three resonances as shown in Fig. 5. These results, however, are very discouraging because whenever a new resonance appears, the entire sequence of the resonances is shifted to the left. A large number of terms in the SF series for the repulsive e-e interaction is needed to shift back the displaced resonances. This behavior may be interpreted as due to the failure of the expansion method to converge. Further investigations with more terms included will not alter this conclusion, unless a prohibitive number of terms are included. In order to take more terms into the calculation, a method which does not digitize the continuous variable for solving Eqs. (2.21) is available. Such a method is discussed in Sec. IV.

We remark here that not all zeros of the real part of the determinant det($\underline{I} - \underline{\mathcal{K}}$) are associated with resonance poles of the system. A resonance pole is associated not only with a zero in Re[$f(s)$], but also with a zero in Im[$f(s)$] and in addition with the sign and the slope of the imaginary and real parts of det($\underline{I} - \underline{\mathcal{K}}$), respectively. A zero in Re[$f(s)$] at $s = s_0$ is to be associated with a resonance pole in the matrix $[\underline{I} - \underline{\mathcal{K}}(s)]^{-1}$ only when the sign of Im[$f(s)$] agrees with the sign of the slope of Re[$f(s)$] at $s = s_0$. The first zero of Re[$f(s)$] in Fig. 6 does not satisfy these requirements and therefore is not associated with a resonance. This zero physically reflects the return of the bound-state pole associated with the ground ^1S H^- state.

IV. DOUBLE-EXPANSION METHOD

The set of coupled single-variable Faddeev equations both in the mixed-mode representation [Eqs. (2.21)] and in the SF representation [Eq. (II 2.28)] can also be solved by expanding the χ functions in terms of a suitable set of basis functions. Such an expansion would reduce the coupled integral equations into a set of coupled linear algebraic equations which may be solved by standard methods.

Before proceeding with the expansion of the χ functions, we remark that the use of the separable-series representation for the off-shell two-body amplitude for variable reduction in the Faddeev equations [such as, for example, Eq. (2.7) in the $J = 0$ case] is equivalent to the method of expanding the off-shell three-body amplitudes as follows:

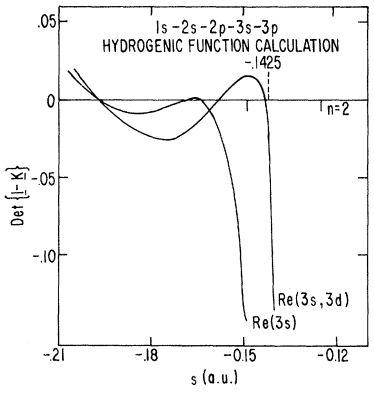

FIG. 5. e-H ^1S resonance-states calculation; (ns) indicates 1s, 2s, ..., ns and ($n'd$) indicates 3d, 4d, ..., $n'd$ partial waves are included in the e-e amplitude. The zeros in the Re($\underline{I} - \underline{\mathcal{K}}$) are the positions of the resonances.

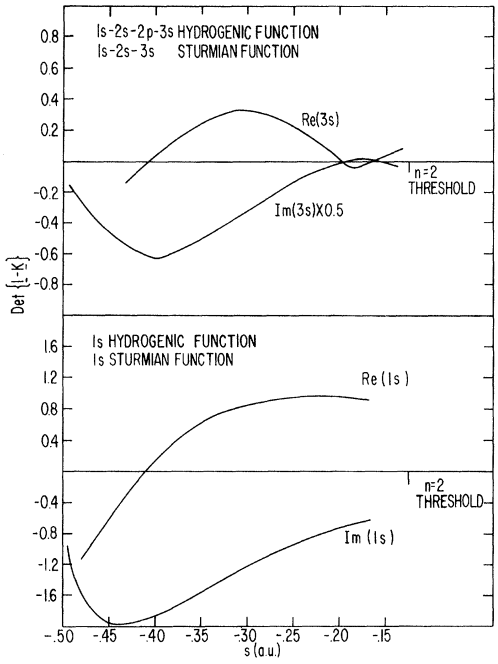

FIG. 6. Energy dependence of $\det(I-\underline{\mathcal{K}})$ in the range of elastic threshold to the first excitation threshold. The 1s term alone in the e-p amplitude does not give rise to resonances.

$$\Psi_l^{(i)}(p,q,s)-\Phi_l^{(i)}(p,q,s)=\sum_\lambda \frac{1}{\gamma_\lambda^{(i)}(s-q^2)-1} \times \phi_{\lambda l}^{(i)}(p,s-q^2)\chi_{\lambda l}^{(i)}(q,s)\ . \quad (4.1)$$

This is evident from Eq. (2.24). To illustrate this, we will be working in the SF representation only. By substituting $\Psi_l^{(i)}(p,q,s)$ from Eq. (4.1) into Eq. (2.7) and then projecting the resultant equations onto the two-body $\phi_{\lambda l}$ state, we obtain

$$\chi_{\lambda l}^{(i)}(q,s)=\eta_{\lambda l}^{(i)}(q,s)+\sum_{\lambda' l'}\sum_{j\neq i}\int_0^\infty dq_j^2\ \mathcal{K}_{\lambda l,\lambda' l'}^{(i,j)} \times(q,q_j;s)\chi_{\lambda' l'}^{(j)}(q_j,s),\ i=1,2,3 \quad (4.2)$$

where

$$\mathcal{K}_{\lambda l,\lambda' l'}^{(i,j)}(q,q_j;s)=-\int_{L_{ij}}^{U_{ij}}\frac{dp_j^2}{1-\gamma_{\lambda'}^{(j)}(s-q_j^2)} \times B_{ll'}^{(i,j)}(q,p_j,q_j;s) \times\phi_{\lambda l}^{(i)}(p_i,s-q^2)\,\phi_{\lambda' l'}^{(j)}(p_j,s-q_j^2)\ , \quad (4.3)$$

$$\eta_{\lambda l}^{(i)}(q,s)=\sum_{j\neq i}\sum_{l'}\int_0^\infty dq_j^2\int_{L_{ij}}^{U_{ij}}dp_j^2\,B_{ll'}^{(i,j)}(q,p_j,q_j;s) \times\phi_{\lambda l'}^{(j)}(p_i,s-q^2)\ \Phi_{l'}^{j}\ (p_j,q_j,s). \quad (4.4)$$

In deriving Eq. (4.2) we have utilized the orthonormality properties of the SF as given by Eq. (2.19) and the relation

$$\frac{1}{\pi}\int_0^\infty \phi_{\lambda l}^{(i)}(p,s-q^2)\,t_l^{(i)}(p,p_i,s-q^2)\,\frac{p\,dp^2}{p^2+q^2-s} =\frac{1}{1-\gamma_{\lambda l}^{(i)}(s-q^2)}\ \phi_{\lambda l}^{(i)}(p_i,s-q^2)\ , \quad (4.5)$$

which can be derived from the Lippmann-Schwinger equations [Eq. (2.12)]. Equation (4.2) which is the set of single-variable Faddeev equations in the SF representation is identical to Eq. (II 2.28) derived using the separable SF series representation of the off-shell two-body amplitudes. This then demonstrates that the two expansion approaches involving $t_l^{(i)}(p,p',s-q^2)$ and $\Psi(p,q,s)$ are equivalent.

The method of expanding $\Psi_l(p,q,s)$ outlined above has some resemblance to the method developed by Jasperese and Friedman.[13] The important difference lies in our choice of E in the SF $\phi_{\lambda l}^{(i)}(p,E)$. The constant E which is related to the two-body interaction strength is left to be an arbitrary parameter in the Jasperese-Friedman treatment. It is clear from Paper II that E should be $s-q^2$ so that the final physical state may be specified when the three-body amplitude is put back on the energy shell. In the present treatment we expand, instead of $\Psi_l(p,q,s)$, the function $\Psi_l(p,q,s)-\Phi_l(p,q,s)$. This permits us to remove the δ function in the inhomogeneous term corresponding to the physical initial state. The final-state poles are also factored out in the expansion adopted in Eq. (4.1). Because of this difference, our approach is not restricted to bound-state problems and is free from arbitrariness in the assignment of two-body interaction strengths.

When the χ functions in Eq. (4.2) are again expanded in a set of basis functions (such as the SF), we have

$$\chi_{\lambda l}^{(i)}(q,s)=\textstyle\sum_\mu c_{\lambda\mu l}^{(i)}(s)\ \phi_{\mu l}^{(i)}(q,s)\ . \quad (4.6)$$

Equation (4.2) may then be reduced to a set of algebraic equations

$$c_{\lambda\mu l}^{(i)}(s)=v_{\lambda\mu l}^{(i)}(s)+\sum\sum_{j\neq i}c_{\lambda'\mu' l'}^{(j)}(s)\,u_{\lambda\mu l,\lambda'\mu' l'}^{(i,j)}(s), \quad (4.7)$$

where

$$v^{(i)}_{\lambda\mu l}(s)=\int_0^\infty \frac{dq^2 q}{q^2-s}\ \phi^{(i)}_{\mu l}(q,s)\,\eta^{(i)}_{\lambda l}(q,s)\ , \qquad (4.8)$$

$$u^{(i,j)}_{\lambda\mu l,\lambda'\mu' l'}(s)=\int_0^\infty \frac{dq^2 q}{q^2-s}\int_0^\infty dq_j^2\ \phi^{(i)}_{\mu l}(q,s) \times \mathcal{K}^{(i,j)}_{\lambda l,\lambda' l'}(q,q_j;s)\,\phi^{(j)}_{\mu' l'}(q_j,s)\ . \qquad (4.9)$$

The algebraic equations for the expansion coefficients, the c's, which are related to the off-shell three-body amplitudes through the relations

$$\Psi^{(i)}_l(p,q,s)=\Phi^{(i)}_l(p,q,s)+\sum_{\lambda\mu}\frac{c^{(i)}_{\lambda\mu l}(s)}{\gamma^{(i)}_\lambda(s-q^2)-1} \times \phi^{(i)}_{\lambda l}(p,s-q^2)\,\phi^{(i)}_{\mu l}(q,s)\ ,$$

may be solved by the standard method. The convergence of the expansion for $\chi_{\lambda l}$ [given by Eq. (4.6)] is found to be in general rapid. A sample result which demonstrates the rate of convergence for the χ-function expansion [see Eq. (4.6)] is shown in Fig. 7. It is seen that only a few terms in the expansion are sufficient to bring the expansion result into agreement with the result obtained by digitizing the continuous variable. This then provides a possible method for further investigation of the convergence problem raised in Sec. III. We remark that the convergence of the χ-function expansion provides only an effective method for solving the coupled single-variable Faddeev equations which are obtained from utilizing the separable expansions [Eqs. (2.14) and (2.15)] for the off-shell two-body amplitude; it bears no relation to the convergence of these separable expansions for the off-shell two-body amplitude raised in Sec. III. The χ-function expansions, however, permit more terms to be included in the investigation of the convergence of the separable expansion.

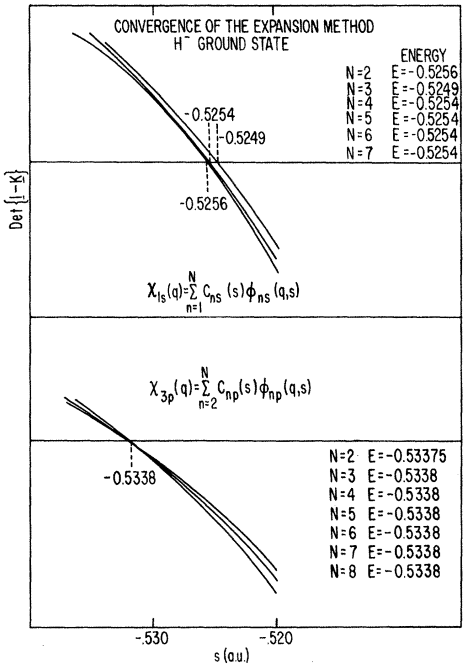

FIG. 7. Double-expansion method in terms of the SF for calculation of the H^- bound state.

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