Scattering theory of close-coupling equations

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The scattering theory implied by the close-coupling equations is studied using a Lippmann-Schwinger formalism. The new results derived can be summarized as follows: An alternative form of the equations that ensures there are no spurious solutions in the scattering region can be constructed, and moreover there is an infinite number of such forms. The Neumann- (perturbation-) series expansion diverges in general for most energies for both the old and new forms. The Born limit nevertheless holds and can be recovered by appropriate rearrangement of the Neumann series. The original integral formulation may give convergent scattering amplitudes despite the lack of uniqueness of the solutions. The conditions under which this happens are examined.

I. INTRODUCTION

There is a vast literature that testifies to the success of the close-coupling equations applied to electron-atom and electron-ion scattering. A review of the equations and their methods of solution in coordinate space has been given by Burke and Seaton;[1] further extensions and refinements have been discussed by Poet[2] and van de Ree.[3] An alternative approach to their solution was presented by McCarthy and Stelbovics,[4] who employed a Lippman-Schwinger formulation for the T matrix and solved it in momentum space. A feature of the close-coupling equations for electron-atom scattering, in the symmetrized form, is that they have nonunique solutions in the scattering region that can cause numerical instabilities. Norcross[5] demonstrated that these instabilities could be removed by imposing further orthogonality constraints, in addition to the ordinary scattering boundary conditions. In the Lippmann-Schwinger formulation, one should also anticipate numerical instabilities because the Fredholm determinant vanishes, on account of the spurious solutions, for all scattering energies. Interestingly though, McCarthy and Stelbovics reported no such evidence of instability in their numerical work and therefore found no need to impose orthogonality constraints. The solutions they obtained were in good agreement with the other methods. It suggests that some, as yet unspecified mechanism, is responsible for the stability. This is further reinforced by our recent observation that there exists an alternative form of the close-coupling equations[6] whose Fredholm determinant does not vanish and thus leads to a stable numerical solution of the Lippmann-Schwinger equation. In the results presented there, both forms of equation yielded identical on-shell amplitudes.

The purpose of this paper is to examine the scattering theory of the close-coupling equations motivated by the above considerations. We will assume that the eigenfunctions for the target are known exactly, so restricting ourselves to the special case of hydrogenic targets. It differs from that encountered in normal potential scattering through the existence of the nonunique solutions. Also, the effective potential is energy dependent and nonlocal and has the feature that the energy dependence is linear in energy. It will be shown that the energy dependence, contained in the separable part of the nonlocality, is responsible for the behavior reported here. The existence of different forms of close-coupling equations will be demonstrated to be due to the relationship between this separable part of the potential and its representation in terms of the nonphysical solutions. In addition, an explanation for the stability of the standard close-coupling equations will be given using the representation of the potential noted above. It will be shown further that there is a surprising corollary to this study of the Lippmann-Schwinger form, namely that the Neumann-series expansion of the close-coupling equations often diverges no matter how great the energy for the scattering is. This is in contrast to the situation in potential scattering where the free Green's function ensures the higher-order terms in the series become unimportant at sufficiently high energies. The lack of convergence is due to the cancellation of the free Green's-function energy dependence with the energy-dependent terms in the effective potential. This result does not rule out the validity of the Born approximation at high energy but does, in contrast to potential scattering theory, demonstrate that questions relating to convergence to the Born limit cannot be exhaustively answered by a consideration of the Neumann series alone. In fact, the special separable nature of the energy-dependent term can be used to advantage to sum to infinite order, the diagrams which are responsible for the anomalous behavior. It is shown that on the energy shell the contribution of these terms to the scattering amplitudes tends to zero at high energies and that the remaining terms also die off with the exception of the Born term. Thus, as has been amply confirmed by numerical computation, the Born limit is valid for electron-hydrogen scattering but not for the reasons one might have assumed.

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II. LIPPMANN-SCHWINGER EQUATIONS

We take an explicitly symmetrized expansion for the electron-hydrogen three-body wave function

$$\psi^{\pm N}(1,2)=\tfrac{1}{2}(1\pm P_{12})\sum_{i=1}^{N}\phi_i(1)f_i^{\pm N}(2)\ , \tag{1}$$

where the + (−) superscripts refer to singlet (triplet) scattering, the superscript N indicates the dependence of the solution on the basis-set size, and P_{12} is the space exchange operator. In the limit $N\to\infty$, $\Psi^N\to\Psi$. The limiting sum is to be interpreted in the general sense of summing over the denumerably infinite discrete excited states of the target and an integral over the scattering continuum of the target. It will be assumed that the sum over discrete states and integral over continuum states can be approximated by the denumerable sum in the limit as $N\to\infty$. However, for definiteness we will consider only the states taken from the discrete spectrum, and so normalizable in the L^2 sense. The f^N are the solutions of the close-coupling equations.

$$(-H_0+E-\varepsilon_j)f_j^{\pm}=\sum_{k=1}^{N}V_{jk}^{\pm}f_k^{\pm}\ , \tag{2}$$

where we set

$$V_{jk}^{\pm}=U_{jk}^{\pm}+W_{jk}^{\pm} \tag{3}$$

with

$$U_{jk}^{\pm}=\int d\mathbf{r}_1\int d\mathbf{r}_2|\mathbf{r}_1\rangle\phi_i^*(\mathbf{r}_2)\times\left[\left[-\frac{1}{r_1}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\right]\phi_j(\mathbf{r}_2)\langle\mathbf{r}_1|\pm\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_j(\mathbf{r}_1)\langle\mathbf{r}_2|\right] \tag{4}$$

and

$$W_{jk}^{\pm}=\pm|\phi_k\rangle(\varepsilon_j+\varepsilon_k-E)\langle\phi_j|\ . \tag{5}$$

The ϕ_j and ε_j are the target atom eigenfunctions and energies. We shall usually suppress the explicit dependence on N in our notation for the scattering function and its associated T matrix. The total energy of the system connecting the initial and final states $i\to f$ satisfies

$$E=\varepsilon_i+\tfrac{1}{2}k_i^2=\varepsilon_f+\tfrac{1}{2}k_f^2\ . \tag{6}$$

The above system does not have a unique solution upon applying the standard scattering boundary conditions, for if $F_i^{\pm N}$ is the particular solution we seek, then it can be shown by direct substitution in Eq. (2) that the general solution is

$$f_i^{\pm}=F_i^{\pm}+\sum_{\alpha=1}^{N^{\pm}}\lambda_\alpha^{\pm}\Phi_i^{\pm\alpha}\ , \tag{7}$$

where the $\lambda_\alpha^{\pm}$ are arbitrary constants and

$$N^{\pm}=-\tfrac{1}{2}N(-N\pm1)\ . \tag{8}$$

The $\Phi^{\pm\alpha}$ form a total of $N^+ + N^- = N^2$ independent degenerate solutions for which a convenient basis is defined by choosing

$$\begin{aligned}\Phi_i^{\pm\alpha}&=\frac{1}{\sqrt{2}}\sum_{j=1}^{N}B_{ij}^{\pm\alpha}\phi_j,\quad \alpha\notin\alpha_d\ ,\\ \Phi_i^{-\alpha}&=\sum_{j=1}^{N}B_{ij}^{-\alpha}\phi_j,\quad \alpha\in\alpha_d\ ,\\ \alpha_d&=\{\alpha|\alpha=\alpha(i,i),i=1,2,\ldots,N\}\ .\end{aligned} \tag{9}$$

The $\alpha=\alpha(i,j)$ form a canonical ordering of the two channel indices for singlet and triplet scattering as defined below. The α_d exist only for the triple channel

$$\begin{aligned}\alpha(i,j)&=\tfrac{1}{2}(i-1)(i-2)+j,\quad i>j\ ,\\ \alpha(i,i)&=N^+ +i\ .\end{aligned} \tag{10}$$

The B arrays associated with this ordering are defined as follows:

$$\begin{aligned}B_{ij}^{+\alpha}&=1\ \text{ if } \alpha=\alpha(i,j),\ i>j\\ &=-1\ \text{ if } \alpha=\alpha(j,i),\ j>i\\ &=0\ \text{ otherwise}\end{aligned} \tag{11a}$$

$$\begin{aligned}B_{ij}^{-\alpha}&=1\ \text{ if } \alpha=\alpha(i,j),\ i\geq j\\ &=1\ \text{ if } \alpha=\alpha(j,i),\ j>i\\ &=0\ \text{ otherwise}\ .\end{aligned} \tag{11b}$$

The $\Phi_i^{\pm\alpha}$ constructed by the above method form an orthonormal basis for subspaces of dimension $N^{\pm}$ which are orthogonal to each other,

$$\begin{aligned}\langle\Phi^{\pm\alpha}|\Phi^{\pm\beta}\rangle&=\delta_{\alpha\beta},\quad \alpha,\beta=1,2,\ldots,N^{\pm}\\ \langle\Phi^{+\alpha}|\Phi^{-\beta}\rangle&=\langle\Phi^{-\alpha}|\Phi^{+\beta}\rangle=0\ .\end{aligned} \tag{12}$$

Here in an obvious notation we have set

$$\langle\Phi^{\pm\alpha}|\equiv(\langle\Phi_1^{\pm\alpha}|,\langle\Phi_2^{\pm\alpha}|,\ldots,\langle\Phi_N^{\pm\alpha}|)\ .$$

Further, we adopt a similar convention for $f^{\pm}$, $F^{\pm}$, and the operators over two channel indices and write G_0 for the diagonal free Green's-function array

$$G_0(E+i0)_{ij}=\delta_{ij}(E+i0-\varepsilon_i-H_0)^{-1}\ . \tag{13}$$

Then the Lippmann-Schwinger equation can be expressed as

$$|f^{\pm}(i,\mathbf{k}_i)\rangle=|i,\mathbf{k}_i\rangle+G_0V^{\pm}|f^{\pm}(i,\mathbf{k}_i)\rangle\ , \tag{14}$$

where the inhomogeneous term corresponds to a plane wave in entrance channel i with momentum $\mathbf{k}_i$. This representation has the solution (7) where, in addition to a particular solution of the inhomogeneous equation, there are N^2 solutions $\Phi^{\pm\alpha}$ of the homogeneous equation

$$G_0V^{\pm}|\Phi^{\pm\alpha}\rangle=|\Phi^{\pm\alpha}\rangle,\quad \alpha=1,2,\ldots,N^{\pm}\ . \tag{15}$$

The integral equation for the scattering functions can also be converted to the T-matrix form by defining

$$|f^{\pm}(i,\mathbf{k}_i)\rangle=[1+G_0(E)t^{\pm}(E)]|i,\mathbf{k}_i\rangle\ . \tag{16}$$

In what follows we adopt the convention that all on-shell momenta are labeled by $\mathbf{k}$ and off-shell ones by $\mathbf{p}$. The on-shell momenta are defined in Eq. (6). The T matrix then satisfies the operator equation

$$t^{\pm}=V^{\pm}+V^{\pm}G_0t^{\pm}\ . \tag{17}$$

[In keeping with our usage of $f^{\pm}$ and $F^{\pm}$, $t^{\pm}$ denotes the T-matrix operator of the general equation (14), while $T^{\pm}$ corresponds to that of the particular solution $F^{\pm}$.] This T matrix also has a general solution which comprises a particular solution of the inhomogeneous equation and $N^{\pm}$ solutions to the homogeneous part. It can be expressed as

$$t^{\pm}=T^{\pm}+\sum_{\alpha=1}^{N^{\pm}}\lambda_{\alpha}^{\pm}G_0^{-1}|\Phi^{\pm\alpha}\rangle\sum_{i=1}^{N}\int d\mathbf{p}_i\langle i\mathbf{p}_i|\ . \tag{18}$$

The on-shell amplitudes are given by $\langle f,\mathbf{k}_f|t^{\pm}|i,\mathbf{k}_i\rangle\equiv\langle\mathbf{k}_f|t_{fi}^{\pm}|\mathbf{k}_i\rangle$. In order to solve the T matrix equation numerically for the on-shell amplitudes one has to close it and this necessitates solving it for the half-on-shell amplitudes

$$\langle f,\mathbf{p}_f|t^{\pm}|i,\mathbf{k}_i\rangle=\langle\mathbf{p}_f|T_{fi}^{\pm}|\mathbf{k}_i\rangle+\tfrac{1}{2}(k_f^2-p_f^2)\times\sum_{\alpha=1}^{N^{\pm}}\lambda_{\alpha}^{\pm}\langle\mathbf{p}_f|\Phi_f^{\pm\alpha}\rangle\ . \tag{19}$$

We note that on-shell the homogeneous terms do not contribute. This provides a key to the observed stability of the amplitudes calculated by McCarthy and Stelbovics[4] using the T-matrix equation but imposing no extra constraints. The stability will be analyzed further in Sec. V.

III. ALTERNATIVE EQUATIONS

As mentioned in the introduction, the nonuniqueness of the solutions can be removed by the addition of extra constraints. In this section we will show there is a natural way to impose the constraints. It results in the formation of a different close-coupling potential which leads to a set of equations with a unique solution. There are many "different" forms for the potential which lead to the same unique solution.

If we observe that the scattering functions obey the symmetry

$$\psi^{\pm}(1,2)=\tfrac{1}{2}\sum_{i,j=1}^{\infty}\phi_i(1)\phi_j(2)(\langle\phi_i|f_j^{\pm}\rangle\pm\langle\phi_j|f_i^{\pm}\rangle)\ , \tag{20}$$

then without loss of generality we can choose the particular solution from the manifold possible in Eq. (7) to be the one for which

$$\langle\phi_i|F_j^{\pm}\rangle=\pm\langle\phi_j|F_i^{\pm}\rangle\ . \tag{21}$$

To see this one can argue as follows. The $\Phi^{\pm\alpha}$ when folded with the ϕ_i have the opposite symmetry to that of (21) as can be seen using Eqs. (9)–(11). Therefore, if we select a particular solution which does not possess the symmetry, we can always construct one with the required property by adding an appropriate combination of the $\Phi^{\pm\alpha}$. Thus, with the imposition of the condition (21), a completely equivalent set of close-coupling equations may be derived using the expansion

$$\psi^{\pm}(1,2)=\sum_{i,j=1}^{\infty}\phi_i(1)\phi_j(2)\langle\phi_i|F_j^{\pm}\rangle=\sum_{i=1}^{\infty}\phi_i(1)F_i^{\pm}(2)\ . \tag{22}$$

We will now show how to apply the new conditions to the integral forms we have developed. First, it is convenient to restructure the $W^{\pm}$ potential in terms of the basis states (9). For compactness we set

$$d_{ij}=(\varepsilon_i+\varepsilon_j-E)\ . \tag{23}$$

Then one can deduce the following representation:

$$\begin{aligned}W^{\pm}&=\pm\sum_{\alpha=1}^{N^{+}}|\Phi^{+\alpha}\rangle(-d^{+\alpha})\langle\Phi^{+\alpha}|\\&\quad\pm\sum_{\alpha=1}^{N^{-}}|\Phi^{-\alpha}\rangle d^{-\alpha}\langle\Phi^{-\alpha}|\\&=\pm|\Phi^{+}\rangle(-D^{+})\langle\Phi^{+}|\pm|\Phi^{-}\rangle D^{-}\langle\Phi^{-}|\ .\end{aligned} \tag{24}$$

The d^{α}'s are the matrix elements of the lower triangle of d above listed in the canonical ordering (10),

$$d^{+\alpha}=\{d_{ij}|\alpha=\alpha(i,j),i>j\}\quad\text{for }\alpha=1,\ldots,N^{+} \tag{25a}$$

$$d^{-\alpha}=d^{+\alpha}\quad\text{for }\alpha=1,\ldots,N^{+} \tag{25b}$$

$$d^{-\alpha}=\{d_{ii}|\alpha=\alpha(i,i),i=1,2,\ldots,N\}\quad\text{for }\alpha=N^{+}+1,\ldots,N^{-}\ . \tag{25c}$$

Here we have written

$$\langle\Phi^{\pm}|\equiv(\langle\Phi^{\pm 1}|,\langle\Phi^{\pm 2}|,\ldots,\langle\Phi^{\pm N^{\pm}}|) \tag{26}$$

and set

$$D_{\alpha\beta}^{\pm}=\delta_{\alpha\beta}d^{\pm\alpha},\quad\alpha,\beta=1,2,\ldots,N^{\pm}\ . \tag{27}$$

Now from the definitions (9)–(11) we see

$$\langle\Phi^{\pm\alpha}|F^{\pm}\rangle=\sum_{i=1}^{N}\langle\Phi_i^{\pm\alpha}|F_i^{\pm}\rangle=\sum_{i,j=1}^{N}B_{ij}^{\pm\alpha}\langle\phi_j|F_i^{\pm}\rangle=0\ . \tag{28}$$

Thus, upon inserting this condition into the integral equations (14) and (17), and making use of the expansion (24), we find

$$|F^{\pm}(i,\mathbf{k}_i)\rangle=|i,\mathbf{k}_i\rangle+G_0(U^{\pm}+|\Phi^{\mp}\rangle D^{\mp}\langle\Phi^{\mp}|)|F^{\pm}(i,\mathbf{k}_i)\rangle\ , \tag{29}$$

$$T^{\pm}=(U^{\pm}+|\Phi^{\mp}\rangle D^{\mp}\langle\Phi^{\mp}|)(1+G_0T^{\pm})\ . \tag{30}$$

The homogeneous forms of Eqs. (29) and (30) will not, in general, have any solution since the effective potential is different from that of the original form (3)–(5). Thus, since the equations constitute a Fredholm system of the second kind, they have a unique solution. Therefore this

form is suitable for numerical analysis.

We may extend the result just developed by noting that the Eqs. (29) and (30) for F and T are only one form of a more general class. To see its nature, suppose we have solved (29). Then by construction the (unique) solution satisfies the orthogonality property (28). We now form a manifold of potentials V_{gen} such that

$$V^{\pm}_{\text{gen}} = U^{\pm} + |\Phi^{\mp}\rangle D^{\mp} \langle \Phi^{\mp}| + |\Gamma^{\pm}\rangle\langle \Phi^{\pm}| \ . \tag{31}$$

$\Gamma^{\pm}$ is a row of $N^{\pm}$ columns as per (26), where each column is an arbitrary element of the Hilbert space of L^2 functions over the channel indices. Now if we take our solution and replace the potential by the general form (31), then on account of (28) $F^{\pm}$ is also a solution of the equation

$$|F^{\pm}(i,\mathbf{k}_i)\rangle = |i,\mathbf{k}_i\rangle + G_0 V^{\pm}_{\text{gen}} |F^{\pm}(i,\mathbf{k}_i)\rangle \ . \tag{32}$$

The system (32) is the most general representation of the close-coupling equations. We consider some specific choices for $\Gamma^{\pm}$. The first one is

$$|\Gamma^{\pm}_{\text{cc}}\rangle = -|\Phi^{\pm}\rangle D^{\pm} \ , \tag{33}$$

which is the choice that retrieves the old form of the close-coupling equations. A second choice is that which leads to the close-coupling equations reported by Stelbovics and Bransden.[6] They discovered a form whose separable part is diagonal in channel space,

$$[V^{\pm}_{\text{SB}}]_{ij} = U^{\pm}_{ij} + \delta_{ij} \sum_{i=1}^{N} |\phi_i\rangle \gamma_i^{\pm} (\varepsilon_i + \varepsilon_i - E) \langle \phi_i| \ ,$$
$$\gamma_i^{+} = 1, \ \gamma_i^{-} = 1 - \delta_{ji} \ . \tag{34}$$

This corresponds to the setting of $\Gamma^{\pm}$ to

$$|\Gamma^{+}_{\text{SB}}\rangle = |\Phi^{+}\rangle D^{+} \ ,$$
$$|\Gamma^{-}_{\text{SB}}\rangle = |\Phi^{-}\rangle D^{+} \oplus O \ . \tag{35}$$

O represents the $N \times N$ zero matrix. Examples showing the application of these equations to $1s$-$2s$-$2p$ close coupling for electron-hydrogen scattering and demonstrating their equivalence were presented in their letter. Finally, as a third choice we note that one can even set the separable energy-dependent term to be not only diagonal in channel space but also identical for both singlet and triplet scattering by defining

$$|\Gamma^{\pm}_{\text{eq}}\rangle = |\Phi^{\pm}\rangle D^{\pm} \ . \tag{36}$$

IV. NEUMANN-SERIES DIVERGENCE AND THE BORN LIMIT

It is generally regarded that the solutions of the close-coupling equations provide a good description of intermediate energy scattering and approach asymptotically the Born limit at high energies. In this section we show that this can be proved from the new form of the close-coupling equation, but surprisingly the proof is quite intricate. To see why this is so we note that the standard potential-scattering proof is iterate the Lippmann-Schwinger equation in the form

$$T^{\pm} = V^{\pm} + K^{\pm} V^{\pm} + \cdots \ , \tag{37}$$

where

$$K^{\pm} = V^{\pm} G_0 \ . \tag{38}$$

The series will diverge in the strong operator norm sense, that is, $\|T^{\pm} - T^{\pm}{}_n\| \to \infty$ as $n \to \infty$ where $T^{\pm}{}_n$ refers to the nth partial sum if the operator norm of the kernel defined by

$$\|K^{\pm}\| = \sup_x \frac{\|K^{\pm}|x\rangle\|}{\||x\rangle\|}, \quad \text{with } \||x\rangle\| = \sqrt{\langle x|x\rangle}$$

is greater than or equal to unity. One way to study the norm is to determine the eigenvalue spectrum of the kernel

$$K^{\pm}|r_s^{\pm}\rangle = r_s^{\pm}|r_s^{\pm}\rangle, \quad s = 1,2,\ldots \ . \tag{39}$$

It is useful to work with a compact kernel since compactness ensures that the eigenvectors form a complete denumerable set with accumulation point zero for the eigenvalues in the Hilbert space of L^2 functions. The kernel $K^{\pm}$ can, under suitable transformations, be put into a compact form. Details of the procedures used are, for example, discussed by Meetz[7] and Scadron, Weinberg, and Wright.[8] General properties of the eigenvalues have been discussed by Weinberg.[9] Using the fact that the potential in the kernel is Hermitian one can prove that the eigenvectors satisfy the modified orthogonality property

$$\langle r_s^{\pm}|G_0|r_t^{\pm}\rangle = \delta_{st} \ . \tag{40}$$

If we order the eigenvalues in order of decreasing magnitude then it is easy to see that

$$\|K^{\pm}\| = |r_1^{\pm}| \ . \tag{41}$$

For the original form of close-coupling equations it follows from Eq. (15) that the set of Hilbert space vectors

$$\{G_0^{-1}|\Phi^{\pm\alpha}\rangle | \alpha = 1,2,\ldots,N^{\pm}\} \subset \{|r_s^{\pm}\rangle s = 1,2,\ldots\} \ . \tag{42}$$

Therefore there are $N^{+} + N^{-} = N^2$ degenerate eigenvectors with eigenvalue 1. Thus $\|K^{\pm}\| \geq 1$ and the T-matrix equation will diverge in the operator norm sense independently of the energy. This is in contrast to the situation in potential scattering theory and is a consequence of the nature of the energy dependence of the $W^{\pm}$ potential. Convergence in the operator norm is a stronger condition than we require because it involves on- and off-the-energy-shell T-matrix elements. Since we are interested in studying the Born limit, one really only requires the on-shell matrix elements of (37). The convergence of the on-shell series partial sums can be investigated by taking the half-on-shell T-matrix equation

$$T^{\pm}|i,\mathbf{k}_i\rangle = V^{\pm}|i,\mathbf{k}_i\rangle + K^{\pm} T^{\pm}|i,\mathbf{k}_i\rangle \tag{43}$$

and considering the sequence of partial sums of the form

$$T_n^{\pm}|i,\mathbf{k}_i\rangle = V^{\pm}|i,\mathbf{k}_i\rangle + K^{\pm} V^{\pm}|\mathbf{i},\mathbf{k}_i\rangle$$
$$+ \cdots + (K^{\pm})^n V^{\pm}|i,\mathbf{k}_i\rangle \ ,$$

where the convergence is convergence in the function norm regarding $T^{\pm}|i,\mathbf{k}_i\rangle$ as an element of the Hilbert space of L^2 functions. (Any on-shell term can be regarded as an inner product of terms in the half-on-shell partial sums.) It is a weaker convergence criterion than convergence in the operator norm requiring only the half-on-shell amplitudes. In this case determining whether the kernel norm is less than 1 is sufficient but not necessary. This consideration comes into play for the old form of the close-coupling equations. To see how, consider the expansion in terms of the complete set of eigenvectors of the kernel of the inhomogeneous term of (43),

$$V^{\pm}|i,\mathbf{k}_i\rangle=\sum_{s=1}^{\infty} c_s^{\pm}(i,\mathbf{k}_i)|r_s^{\pm}\rangle \ . \tag{44}$$

Then the last term in each partial sum can be expressed as

$$(K^{\pm})^n V^{\pm}|i,\mathbf{k}_i\rangle=\sum_{s=1}^{\infty} c_s^{\pm}(i,\mathbf{k}_i)(r_s^{\pm})^n|r_s^{\pm}\rangle \ .$$

If any eigenvalues in this expansion have a magnitude greater than or equal to unity they will dominate the partial sums for large n unless the corresponding Fourier coefficient vanishes. For the eigenvalues of unity, which the close coupling equations possess, this is exactly what happens. Using the orthogonality (40) we have

$$c_s^{\pm}(i,\mathbf{k})=\langle r_s^{\pm}|G_0V^{\pm}|i,\mathbf{k}_i\rangle \ . \tag{45}$$

The eigenvectors (42) of the eigenvalues of unity may thus be used to write

$$c_s^{\pm}(i,\mathbf{k}_i)\propto\langle\Phi^{\pm\alpha}|V^{\pm}|i,\mathbf{k}_i\rangle=\langle i,\mathbf{k}_i|G_0^{-1}|\Phi^{\pm\alpha}\rangle=0 \ ,$$
$$i=1,2,\ldots,N,\ \alpha=1,2,\ldots,N^{\pm} \ . \tag{46}$$

Thus the convergence of the Neuman series is independent of the eigenvalues of unity. The convergence is governed by the remaining eigenvalues and finding which, if any, have magnitude greater than or equal to 1. This can, in general, only be determined by numerical calculation; we give examples in the next section for e-H scattering which show that there is at least one other eigenvalue with magnitude greater than unity for most scattering energies.

We now present an argument to show the Neumann series may diverge in the limit $E\to\infty$. Our proof consists of demonstrating that the kernel will have several eigenvalues which tend to -1 at high energies. Consider the eigenvalue equation (15). Then as

$$E\to\infty,\quad \|G_0U^{\pm}\|\to 0 \ ,$$

so

$$|\Phi^{\pm\alpha}\rangle=G_0V^{\pm}|\Phi^{\pm\alpha}\rangle\underset{E\to\infty}{\approx}G_0W^{\pm}|\Phi^{\pm\alpha}\rangle \ . \tag{47}$$

Thus the $G_0^{-1}\Phi^{\pm\alpha}$ are approximate eigenvectors of $W^{\pm}G_0$ with eigenvalue 1 and there are $N^{\pm}$ of them; but we also have $W^{+}=-W^{-}$ from Eq. (5) so, in addition, there will be N^{+} approximate eigenvectors $\Phi^{+\alpha}$ for the triplet $(-)$ channel with eigenvalues which approach -1 and $E\to\infty$. Similarly, there will be N^{-} approximate eigenvectors $\Phi^{-\alpha}$ for the singlet $(+)$ channel with such eigenvalues. Since $W^{\pm}$ dominates the potential at high energies, we can conclude that there will be at least one eigenvalue which approaches -1 for all close-coupling models save that for $N=1$, in which case the triplet channel has no such eigenvalue.

By the argument given we cannot distinguish whether the -1 value is approached from outside or from within the unit circle. If the latter occurred, then the Neumann series would converge for finite energies in the asymptotic region but at an increasingly slow rate; in all our examples studied numerically it seems that these special eigenvalues approach the unit circle from outside.

Suppose we turn to a consideration of the most general new form (31) and (32) of the close-coupling equations and construct its Neumann series. Again, the high-energy Neumann-series behavior revolves around the eigenvalues of the separable part of the potential. It is clear from the structure of the general form (31) that $\|W_{\text{gen}}^{\pm}G_0\|\geq 1$ as $E\to\infty$, using the argument above, and that at least some eigenvalues approach -1. The various choices available for the general form determine how many such eigenvalues there are. (At most there can be N^2 of them in each channel since this is the maximum rank of $W^{\pm}$.) For the form derived from the choice (35), which we use to illustrate the theory, it is not difficult to show the singlet scattering has N^2 eigenvalues with limit point -1, while the triplet scattering supports N^2-N such eigenvalues.

Despite the failure of the Neumann series to converge, one must still consider the possibility that the Born limit holds because convergence of the Neumann series is only a sufficient condition. We therefore turn to an alternative method to determine its validity, based on a two-potential formalism and define a T matrix for the well-behaved part $U^{\pm}$ of the potentials $V^{\pm}$,

$$T_u^{\pm}=U^{\pm}(1+G_0T_u^{\pm}) \ . \tag{48}$$

Then making use of the separable nature of the remaining contributions to the potential in Eq. (29) one obtains after some algebra the relationship

$$T^{\pm}=T_u^{\pm}+(1+T_u^{\pm}G_0)|\Phi^{\mp}\rangle D^{\mp}$$
$$\times(1-\langle\Phi^{\mp}|G_0+G_0T_u^{\pm}G_0|\Phi^{\mp}\rangle D^{\mp})^{-1}$$
$$\times\langle\Phi^{\mp}|(1+G_0T_u^{\pm}) \ . \tag{49}$$

If we examine the asymptotic form for second term at high energies we find

$$T^{\pm}=T_u^{\pm}+|\Phi^{\mp}\rangle\tfrac{1}{2}E\langle\Phi^{\mp}|+O(1) \ ,$$

hence

$$\|T^{\pm}-T_u^{\pm}\|=O(E),\quad \text{as } E\to\infty \ .$$

Thus, in the strong operator norm sense, $T^{\pm}$ does not converge to $T_u^{\pm}$. Since $\|T_u^{\pm}-U^{\pm}\|\to 0$ as $E\to\infty$, it is seen that $T^{\pm}$ cannot converge to $U^{\pm}$ in the strong sense. But if we consider the convergence of the half-on-shell T matrix regarded as an element of the Hilbert space of L^2 functions

$$\|T^{\pm}|i,\mathbf{k}_i\rangle - T_u^{\pm}|i,\mathbf{k}_i\rangle\| = \hat{O}(E)(\langle i,\mathbf{k}_i|\Phi^{\mp}\rangle\langle\Phi^{\mp}|i,\mathbf{k}_i\rangle)^{1/2} .$$

Then because the Φ's comprise a linear combination of orbitals whose momentum-space form is L^2 if they represent discrete states, as the on-shell momentum increases it follows that they die off. For example, if the term contributing to elastic scattering in the ground state is examined, it behaves asymptotically as $O(E^{-2})$, and this is sufficiently rapid to ensure that the norm above tends to zero as $E\to\infty$. As $\|T_u^{\pm}-U^{\pm}\|\to 0$ when $E\to\infty$, it follows that $\|T^{\pm}|i,\mathbf{k}_i\rangle - U^{\pm}|i,\mathbf{k}_i\rangle\|\to 0$. Thus since convergence of the half-on-shell amplitudes to the Born term has been demonstrated, it certainly holds for the special case of the fully on-shell amplitude. (Actually, the plus-minus superscript in the potential U is redundant because the electron-electron exhange term dies off rapidly at high energies.) Implicit in our discussion have been the assumptions that the number of coupled channels is fixed and that continuum channels are not considered.

V. STABILITY QUESTIONS

It was mentioned already that reliable answers for the on-shell amplitudes could be obtained numerically by solving the standard (nonunique) close-coupling equations (16) in the T-matrix version. Our observation (18) that the on-shell amplitudes are unique indicates the reason why it is possible. Nevertheless, in the process of solving the equation numerically one is inverting the operator $1-K^{\pm}$ whose Fredholm denominator is singular; potentially this must lead to some type of instability in the numerical solution. Therefore further analysis is desirable to justify the solutions obtained by McCarthy and Stelbovics.[4]

Our beginning point is to note that the numerical solution involves two distinct sources of approximation; the integral over the kernel is replaced by a suitable quadrature rule and the potential matrix elements themselves are computed to a limited accuracy because their calculation involves a quadrature also.[4] On account of these approximations, the operator that is to be inverted is close to being singular. The effect of the approximation in the potential may be simulated by applying a perturbation to the potential. The effect of the error due to the quadrature of the integral equation is more difficult to include, but since it is our intention to study the solutions in the neighborhood of the singularity, perturbing the potential alone is sufficient to achieve this end. If δ is the perturbing parameter, then

$$V^{\pm}\to(1+\delta)V^{\pm} ,$$
$$D^{\pm}\to D_{\delta}^{\pm}=(1+\delta)D^{\pm} ,$$
$$T_u^{\pm}\to T_{u\delta}^{\pm}=(1+\delta)T_u^{\pm}+O(\delta^2) .$$

Now employing the two-potential formalism, one derives after some algebra that

$$t_{\delta}^{\pm}=T^{\pm}+(1+T_{u\delta}^{\pm}G_0)\{|\Phi^{+}\rangle(-D_{\delta}^{+})[1-\langle\Phi^{+}|G_0+G_0T_{u\delta}^{\pm}G_0|\Phi^{+}\rangle(-D_{\delta}^{+})]^{-1}\langle\Phi^{+}| + |\Phi^{-}\rangle(\pm D_{\delta}^{-})[1-\langle\Phi^{-}|G_0+G_0T_{u\delta}^{\pm}G_0|\Phi^{-}\rangle(\pm D_{\delta}^{-})]^{-1}\langle\Phi^{-}|\}(1+G_0T_{u\delta}^{\pm}) . \quad (50)$$

This form can be simplified by noting the identities

$$(1+T_u^{\pm}G_0)|\Phi^{\pm}\rangle D^{\pm}=-(G_0)^{-1}|\Phi^{\pm}\rangle ,$$
$$\langle\Phi^{\pm}|G_0+G_0T_u^{\pm}G_0|\Phi^{\pm}\rangle D^{\pm}=-1 . \quad (51)$$

They are just a restatement of the eigenvalue equation (15) using the T matrix defined in (48). Their insertion gives the result

$$t_{\delta}^{\pm}=T^{\pm}+(G_0)^{-1}|\Phi^{\pm}\rangle[-\delta^{-1}(2+\langle\Phi^{\pm}|G_0|\Phi^{\pm}\rangle D^{\pm})^{-1} + O(1)]\langle\Phi^{\pm}|(G_0)^{-1} + (G_0)^{-1}|\Phi^{\pm}\rangle O(1)+O(1)\langle\Phi^{\pm}|(G_0)^{-1} . \quad (52)$$

Here $T^{\pm}$ is the T matrix of Eq. (30). The $O(1)$ symbol represents elements which when developed in a power series in δ have their leading term independent of δ. When the on-shell matrix elements of $t^{\pm}$ are formed, it is clear that all terms possessing $(G_0)^{-1}$ vanish and the old and new amplitudes are identical. It is also clear that off the energy shell they diverge because of the term with the inverse power of δ. As the perturbation is reduced (in effect simulating the calculation of the potentials to higher precision), this divergence will become more pronounced. It is important to note that the expression for $t^{\pm}$ we used above was developed analytically. In an actual numerical inversion it is valid to the extent that a quadrature rule approximates the kernel integral. This has the effect of introducing an error term due to the quadrature approximation to the $(G_0)^{-1}$ operators. Similarly, δ in the δ^{-1} term is replaced by a sum of potential and integral error terms. The reason we mention this is that the T-matrix equations solved by McCarthy and Stelbovics are solved in the half-on-shell mode, which is sufficient to close the integral equations, and it would at first glance appear that the δ^{-1} term should vanish when one of the channel momenta is put on-shell. In practice, as one decreases δ, a situation is eventually reached where the integral equation quadrature error dominates and further reduction of δ does not alter the result. An example is given in the next section.

VI. EXAMPLES AND DISCUSSION

In order to illustrate various aspects of the theory given we consider some examples for the electron-hydrogen system. Since our intention is to make them as illuminating as possible, we will confine ourselves to the

simplest possible cases, namely, 1s and 1s-2s close coupling. There are no practical difficulties in including higher-l states. The use of s states has the added advantage that all the degenerate solutions are confined to the $J=0$ partial wave.

We begin by showing in Fig. 1 the eigenvalue trajectories as a function of energy E from $-\infty$ to $+\infty$ for the singlet (+) kernel of the old equations (14). There are an infinite number of eigenvalues so we show only those few which have a bearing on the convergence of the Neumann series in each case. We consider 1s-2s close coupling for which $N^+=1$, so the kernel has one eigenvalue identically unity. In addition, there are $N^-=3$ eigenvalues which tend to the limit -1 as $|E|\to\infty$. Their number is such that the total when added to the eigenvalues with unit values is $N^2=4$, as discussed earlier. The remaining eigenvalues all approach zero as $|E|\to\infty$ and are the type found in ordinary potential scattering.[9] Thus there are three points of accumulation $+1$, -1, and 0 for the eigenvalue trajectories. The four trajectories shown are labeled in order of decreasing magnitude at the elastic scattering threshold. Below this threshold all the eigenvalues are real; above the threshold they describe arcs in the complex plane. The ones shown have positive imaginary parts, but there are also eigenvalues which describe trajectories in the lower half complex plane. As can be seen from Fig. 1, the eigenvalues have a complicated energy variation and as a result their ordering in terms of absolute magnitude changes with energy. η_1^+ is the lone eigenvalue trajectory which lies outside the unit circle at the scattering threshold having passed through unity at the binding energy of the H^- ion. It has described a major part of its trajectory by the time the ionization threshold is reached, subsequently approaching the value -1 as $E\to\infty$ from outside the unit circle. η_2^+ is the only eigenvalue of unity since $N^+=1$. It of course does not describe a trajectory. The η_3^+ begins inside the unit circle, but approaches it rapidly near the threshold for inelastic scattering to the 2s channel and is responsible for a resonance feature noted by Smith, McEachran, and Fraser[10] in this model. There is a marked effect on this eigenvalue due to the opening of the 2s channel as there is also for η_4^+. It appears characteristic of the e-H system that some eigenvalues have pronounced variations near a particular threshold. At energies above about 20 eV their behavior with energy is more predictable and they approach -1 in a very uniform and featureless manner. All other eigenvalues (an infinite number of them) describe arcs within the unit circle, beginning at zero for large negative energies returning to zero as $E\to\infty$.

Because there is no unique choice for the new form of close-coupling equations, we will restrict ourselves to showing the behavior of the kernel for the particular choice (35). The eigenvalues which pass outside the unit circle are plotted in Fig. 2. Again we label the trajectories according to their magnitude at the scattering threshold (the ordering is different to that of Fig. 1; for example, the resonance feature is contained in different trajectories). As before, the eigenvalues become complex in the scattering region and initially appear to have a small change in their imaginary part compared to their real part; they then move rapidly into the complex plane. η_1^+ appears to be unaffected by the presence of the threshold altogether (it is the trajectory which contains the H^- ion). The eigenvalue η_4^+ gives rise to the reso-

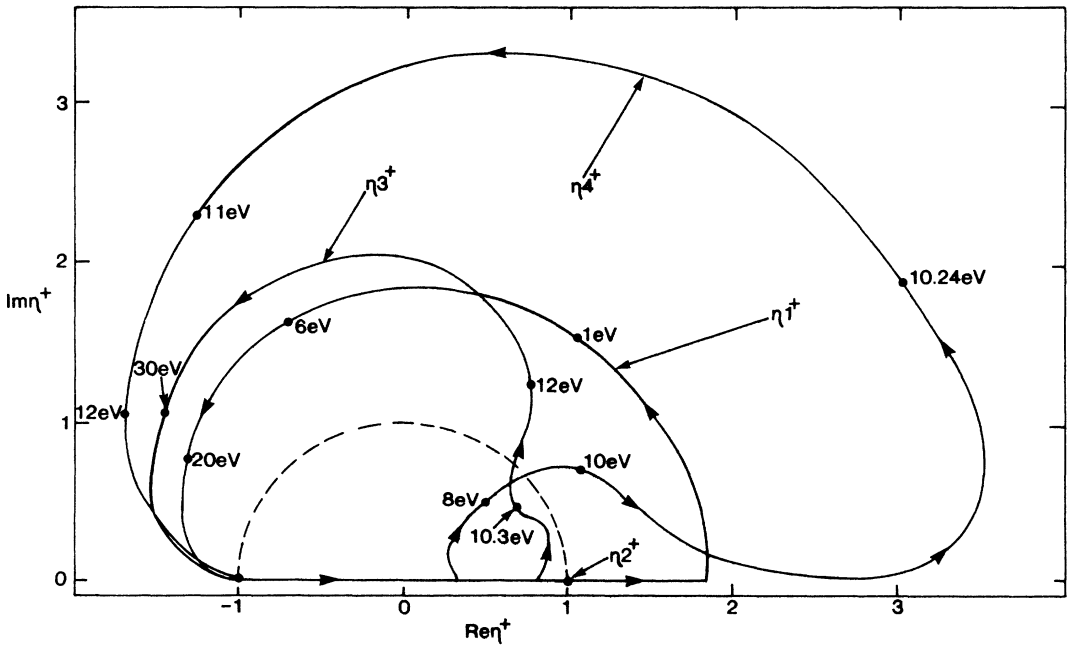

FIG. 1. Leading eigenvalue trajectories for the $J=0$ partial wave of the e-H system are shown for singlet scattering using the kernel of the old close-coupling equations. For scattering energies there is at least one eigenvalue outside the unit circle; hence the Neumann series diverges.

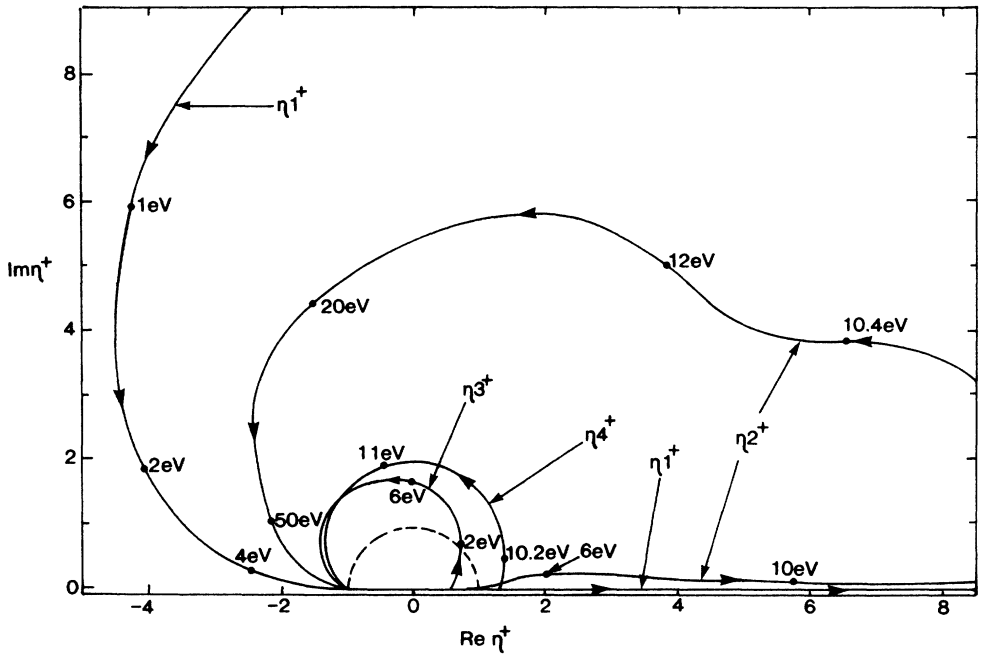

FIG. 2. Leading eigenvalue trajectories for the $J=0$ partial wave of the e-H system are shown for singlet scattering using the new close-coupling equations and making the choice (35). Similar to the Fig. 1 case at all scattering energies, there is at least one eigenvalue outside the unit circle. The magnitudes of the trajectories are quite different for energies in the neighborhood of the 2s threshold.

nance feature described by the η_3^+ in the old equations. Its position and width are the same despite the difference in the trajectory shapes. Meetz[7] has shown how to find the position and width of a resonance from the real and imaginary parts of the eigenvalue. An example of such an application has been given for 1s-2s-2p close coupling using this method.[6] The magnitude of the eigenvalues varies considerably. η_1^+ attains a maximum magnitude of about 13 below 1 eV. At energies above 2 a.u. the eigenvalues have all completed the major part of their trajectories and approach the limiting value of -1 from outside the unit circle. As noted in the theory discussion this form of the kernel leads to $N^2=4$ singlet eigenvalues tending to -1. We have not shown the eigenvalue trajectories for triplet scattering because their characteristics are very similar to those discussed for the singlet scattering and in all cases confirm the theory predictions of Sec. IV.

Comparing the two figures we see that there is at least one eigenvalue which lies outside the unit circle for all scattering energies. Thus it may be concluded the Neumann series for the singlet $J=0$ partial wave scattering diverges always. In this respect the close-coupling theory equations fall outside the domain of standard scattering theory.

Next we turn to some examples to demonstrate our conclusions about the convergence of the Neumann series. In Table I we consider the results for 1s close coupling. In the singlet channel the theory predicts a single eigenvalue should approach -1 as $E\to\infty$. At 100 eV it can be seen that $r_{\max}^+$ is approaching this limit from outside the unit circle. Thus, as for the two channel case just discussed, the Neumann series must diverge at high energies for singlet scattering. This is confirmed by the sequence of Neumann-series partial sums shown in the table. It appears that the series is converging for the first few terms in the sequence, but thereafter it slowly diverges by oscillating about the correct model value. This behavior is due entirely to the value of $r_{\max}^+$ since from a consideration of the Fourier-series expansion of Eq. (44) it can be seen that in the limit of large n

$$r_{\max}^{\pm}\approx\frac{(T_n^{\pm}-T_{n-1}^{\pm})}{(T_{n-1}^{\pm}-T_{n-2}^{\pm})}\ .$$

The triplet channel is interesting because there is one eigenvalue of unity which, according to the analysis, should have no bearing on the convergence of the Neumann series. Also there should be no eigenvalue that approaches -1. This is confirmed in the Table I results. We see that there is a rapid convergence of the Neuman series and its rate of convergence is that expected from the quoted $r_{\max}^-$ value.

In the second part of Table I we show a 1s-2s example at 6 eV. There, as we have seen from the eigenvalue trajectories, the singlet amplitude should have a divergent Neumann series which is confirmed by the table. On the other hand, the Neumann series for the triplet scattering is converging albeit slowly. This can be understood from the theory which predicts that there should be $N^+(=1)$ eigenvalues which accumulate at -1. At the scattering threshold all the eigenvalues lie within the unit circle because there is no bound state for the triplet channel; as the energy increases one of the eigenvalues passes

through the unit circle near the $2s$ threshold and thereafter describes a trajectory which approaches -1 from outside the unit circle. For the energy of 6 eV this eigenvalue lies just inside the unit circle. There are also three eigenvalues of unity which play no role in the Neumann-series convergence so the triplet amplitude has a slowly convergent Neumann series as indicated in Table I.

We investigate the nature of the Neumann-series divergence further by means of the example of Table II. There, the triplet amplitudes for elastic and inelastic scattering are given for the higher energy of 250 eV. The Neumann series diverges as required, but it is clear that the sequence of partial sums is approaching the exact model values for the first few terms, subsequently diverging in a slowly oscillatory manner. The elastic scattering amplitude is reproduced to better than 1% accuracy for $n=5$. This is similar to the behavior we observed in the $1s$ example of single elastic scattering of Table I but the convergence is more pronounced at the higher energy. The explanation for this behavior is to realize that the Neumann sequence, while diverging, is an example of an asymptotic series. That is, the correct values are approached until, for large enough n, the series begins to diverge, and in the examples illustrating this effect, the correct values are approached more closely with increasing energy. To understand this behavior more formally we return to the Fourier expansion (44) from which it follows that for large enough n, the partial sums will be dominated by the eigenvector (and its Fourier coefficient) corresponding to the eigenvalue of maximum magnitude $r^-_{\max} \to -1_+$. Now it was demonstrated in the discussion of Sec. V that the eigenvector with this eigenvalue is approximated (with increasing accuracy as energy increases) by one of the eigenvectors in the set (42). However, we also showed in Eq. (46) that c_r^-, the Fourier coefficients associated with these eigenvectors vanished. Thus, for the eigenvector $|r^-_{\max}\rangle$, we can infer that c_r^- is small compared to other coefficients in the expansion and further that it becomes smaller still as the energy is increased. For large enough n the Neumann series will diverge because of the terms of the form $c_r^-(r^-_{\max})^n$ which occur in the expansion of the higher-order terms in each partial sum. For small values of n this term may be small compared to the coefficients of the remaining eigenvec-

TABLE I. The on-shell T matrix is shown in two cases for singlet and triplet scattering in the e-H system for $J=0$ using the old close-coupling equations. The amplitudes are as defined in Ref. 4. The Neumann series for various n are also given. The convergence or divergence, as the case may be, is determined by the eigenvalues listed as $r^{\pm}_{\max}$. See the text for a full discussion. $x[y]=x\times 10^y$.

	$T^+_{1s\text{-}1s}$		$T^-_{1s\text{-}1s}$	
	Real	Imaginary	Real	Imaginary
		$1s$ close coupling $E_{\text{inc}}=100$ eV		
Exact	−0.5134[−1]	−0.3024[−1]	−0.5708[−1]	−0.4498[−1]
T_n n				
0	−0.6025[−1]		−0.6998[−1]	
1	−0.5218[−1]	−0.3092[−1]	−0.7985[−1]	−0.4146[−1]
2	−0.6340[−1]	−0.2264[−1]	−0.6295[−1]	−0.5344[−1]
3	−0.4320[−1]	−0.4285[−1]	−0.5493[−1]	−0.4886[−1]
4	−0.6024[−1]	−0.1621[−1]	−0.5520[−1]	−0.4489[−1]
5	−0.4208[−1]	−0.4879[−1]	−0.5676[−1]	−0.4426[−1]
10	−0.4830[−1]	−0.2064[−1]	−0.5707[−1]	−0.4497[−1]
15	−0.1200[−1]	−0.1362[−1]	−0.5708[−1]	−0.4498[−1]
20	−0.2262[−1]	−0.1141[−1]	−0.5708[−1]	−0.4498[−1]
	$r^+_{\max}$		$r^-_{\max}$ (excluding 1)	
	−1.193	0.1235	0.1855	0.3786
		$1s$-$2s$ close coupling $E_{\text{inc}}=6$ eV		
Exact	−0.2394	-0.2516	0.1070	−0.4541
T_n n				
1	−0.2341	−1.291	0.5011	−0.1904
2	−1.0471	0.5227	0.5415	−0.4413
5	−1.059[+1]	0.7958	0.1079	−0.7888
10	−1.684[+2]	−1.145[+2]	−0.2491[−1]	−0.2647
50			0.1175	−0.4451
100			0.1076	−0.4537
	$r^+_{\max}$		$r^-_{\max}$ (excluding 1)	
	−0.723	1.64	0.814	−0.453

TABLE II. The on-shell T matrix and Neumann series partial sums are shown for triplet scattering for $J=0$ in the 1s-2s close-coupling model for e-H scattering using the old close-coupling equations. The example illustrates the way the Neumann series sums form an asymptotic series. The partial sums converge for the first few terms then slowly diverge oscillating about the exact values. The divergence rate is determined by the eigenvalue $r_{\max}^{-}$. $x[y]=x\times10^{y}$.

	$T_{1s\text{-}1s}^{-}$		$T_{2s\text{-}1s}^{-}$	
	Real	Imaginary	Real	Imaginary
	1s-2s close coupling $E_{\text{inc}}=250$ eV			
Exact	−0.3076[−1]	−0.1675[−1]	0.1081[−2]	0.4007[−2]
T_n n				
0	−0.3523[−1]		0.4477[−2]	
1	−0.3690[−1]	−0.1698[−1]	0.4079[−2]	0.5737[−2]
2	−0.3123[−1]	−0.1851[−1]	0.0847[−2]	0.5435[−2]
3	−0.3020[−1]	−0.1711[−1]	0.0049[−2]	0.4463[−2]
4	−0.3072[−1]	−0.1648[−1]	0.1017[−2]	0.3120[−2]
5	−0.3076[−1]	−0.1686[−1]	0.1155[−2]	0.4349[−2]
6	−0.3085[−1]	−0.1660[−1]	0.1282[−2]	0.3545[−2]
7	−0.3069[−1]	−0.1695[−1]	0.0906[−2]	0.4682[−2]
8	−0.3083[−1]	−0.1654[−1]	0.1142[−2]	0.3304[−2]
9	−0.3070[−1]	−0.1699[−1]	0.0944[−2]	0.4754[−2]
10	−0.3084[−1]	−0.1649[−1]	0.1180[−2]	0.3134[−2]
	$r_{\max}^{-}$		$r_{\max}^{-}$	
	−1.116	0.024	−1.116	0.024

tors. In the case of 1s-2s close coupling the remaining eigenvectors have eigenvalues which lie within the unit circle so coefficients resulting from these terms die off quickly with n and hence the Neumann series will appear to converge until such n is reached for which $c_r^{-}(r_{\max}^{-})^n \approx c_t^{-}(r_t^{-})^n$, where r_t^{-} is the eigenvalue for the minimum n. The coefficients for each channel are different and therefore it is not surprising that the elastic amplitude converges better in the asymptotic sense than the inelastic 1s-2s amplitude. For large n the divergence

TABLE III. A test of the stability of the old form of close-coupling equations T_{cc}^{-} for triplet channel elastic scattering in the e-H system. δ is a perturbing parameter to the potential as discussed in the text. The half-on-shell T-matrix elements are shown for $J=0$ for various off-shell momenta. The last column is the on-shell element; note that it is fairly stable under variations in δ. The half-off-shell behavior is also shown for the new forms T_{SB}^{-} defined by Eq. (35), and T_{eq}^{-} by Eq. (36). $x[y]=x\times10^{y}$.

	1s close coupling $E_{\text{inc}}=54.42$ eV			
	Real part of half-on-shell T matrix $\langle \mathbf{p}_1 \vert T_{1s\text{-}1s}^{-} \vert \mathbf{k}_1 \rangle$ ($k_1=2$ a.u.)			
p_1	0.4824[−2]	0.5883	1.042	2.000
T_{cc}^{-}	−0.2276[+1]	−0.1189[+1]	0.4516	−0.7928[−1]
T_{SB}^{-}	−0.8230[−1]	−0.8305[−1]	−0.8396[−1]	−0.7928[−1]
T_{eq}^{-}	−0.8229[−1]	−0.8305[−1]	−0.8396[−1]	−0.7928[−1]
T_{δ}^{-} δ				
10^{-2}	0.5297	0.2257	0.1891[−1]	−0.7913[−1]
10^{-3}	0.5592	0.2404	0.2359[−1]	−0.7927[−1]
10^{-4}	0.8812	0.4027	0.7753[−1]	−0.7928[−1]
10^{-5}	−0.2471[+2]	−0.1250[+2]	−0.4212[+1]	−0.7929[−1]
	Imaginary part of half-on-shell T matrix $\langle \mathbf{p}_1 \vert T_{1s\text{-}1s}^{-} \vert \mathbf{k}_1 \rangle$ ($k_1=2$ a.u.)			
T_{cc}^{-}	−0.2482[+1]	−0.1296[+1]	−0.4924	−0.8641[−1]
T_{SB}^{-}	−0.8970[−1]	−0.9052[−1]	−0.9151[−1]	−0.8642[−1]
T_{eq}^{-}	−0.8969[−1]	−0.9052[−1]	−0.9151[−1]	−0.8642[−1]
T_{δ}^{-} δ				
10^{-2}	0.5890	0.2509	0.2102[−1]	−0.8798[−1]
10^{-3}	0.6107	0.2626	0.2576[−1]	−0.8657[−1]
10^{-4}	0.9606	0.4390	0.8451[−1]	−0.8644[−1]
10^{-5}	−0.2969[+2]	−0.1361[+2]	−0.4587[+1]	−0.8636[−1]

rate of both amplitudes is governed by r^{-}_{max}.

An interesting point which we do not attempt to answer here can be stated as follows: Given the flexibility in choosing inequivalent equations which have the same on-shell amplitudes, is it possible to find an optimum representation where $r^{\pm}_{max}$ has its minimum value, this ensuring the most rapid convergence (or least rapid divergence) for the Neumann series?

We turn, finally, to an illustration of the stability of the on-shell amplitudes generated by the old (nonunique solution) close-coupling equations. Since the question of stability arises for all cases of close coupling we take the simplest, which is 1*s* close coupling in the triplet channel, whose Lippmann-Schwinger form has one solution to the homogeneous equation. The results are summarized in Table III where we have tabulated the solution of the half-off-the-energy-shell T-matrix amplitudes. The off-shell p values are a subset of those generated by a typical Gaussian quadrature mesh in our method of solution. All the results given in Table III are calculated using the same mesh. It can be seen that as the perturbation δ to the potential is reduced the behavior of the off-shell T matrix varies in accord with the analysis of Sec. V. For comparison we also show the off-shell behavior of the new equations and note how steady and smooth their variation is off the energy shell. It must be emphasized that the off-shell behavior of the old form of the equations is strongly dependent on the quadrature mesh as well, so that if, for example, we attempt to incorporate a larger quadrature mesh, the off-shell behavior will be different again. Thus, although the on-shell amplitude is relatively stable, the off-shell elements do not converge.

In conclusion, we reiterate that the underlying assumptions of our analysis in this work have been (a) the limitation to problems where the target-state wave functions are known, that is, we exclude pseudostates and (b) the continuum states of the target have been omitted in our discussion of convergence so that we could make use of the L^2 nature of the discrete states for some of the convergence questions. Further work in this area should be directed towards investigating how the theory should be modified, and indeed if it can be, to remove these restrictions. As a final comment we note that all the examples considered have employed only *s* target states and as a result the nonuniqueness phenomenon is confined to the $J=0$ partial wave of the *e*-H system. In order to ensure the expansion over target states is nearly complete, one must include states of higher orbital angular momentum, which in turn causes the nonuniqueness of the close-coupling equations to be present in a large number of partial waves and in the limit of a complete set present in every partial wave.

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