Computational Study of Channel Coupling Arrays:
Low Energy e^- -H Scattering Parameters in the 1S Approximation

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Abstract

Low energy electron-hydrogen scattering parameters have been calculated using the new set of coupled equations for the transition operators for different arrangement channels derived recently. A key feature of this approach to multi-channel scattering is the use of the channel coupling array, W , whose elements link the various channels together and thus determine which arrangements are explicitly coupled in the equations. In this work, the dependence of the low energy scattering parameters on the elements W_{IJ} is studied numerically within an approximation retaining only the $n=1$, hydrogen ground state in the expansion of the channel Green's operator. Because of the channel coupling, this is not the same approximation as the familiar static or static exchange approximation of more conventional calculations. The best results for singlet and triplet parameters taken together occur for the channel permuting array values $W_{11} = W_{22} = 0$, $W_{21} = W_{12} = 1$; these are the values that guarantee a connected integral equation for the matrix of transition operators. In particular, we find singlet and triplet scattering length values (in a.u.) of 6.230 and 2.077, which compare well with the variational results of Schwartz, 5.96 and 1.77.

1. Introduction

We have recently reported theoretical and computational studies of new sets of coupled integral equations for various rearrangement channel T operators describing $e^- - H$ scattering.^{1,2,3} These equations, unlike other sets in the literature,⁴ lead to a simple damping relation between the T operators and $K(\text{reaction})$ operators derived in the usual manner.¹ For a system such as electron plus H-atom where Pauli principle exchange effects must be taken into account, we have shown that the properly symmetrized operators $T^\pm$ and $K^\pm$ are also related by a damping equation. The importance of working with operators which satisfy a damping relation, especially in approximate calculations, has been underscored by the previously reported calculations² and their theoretical interpretation.³

The key feature of this new approach is the use of the channel coupling array⁵ W , which links all the rearrangement channels together. It can be used for systems of arbitrary size,^{6,7} i.e., n -body systems having available N rearrangement channels, and not merely the present case of $n = 2$, $N = 2$. Apart from a normalization condition, the elements W_{ij} may take on apparently arbitrary values. However, the arbitrariness is eliminated by requiring the W_{ij} to be chosen so as to avoid one of the major problems encountered in many-body scattering theory: the occurrence of the disconnected diagram.⁸ We have shown⁹ that there are $(N-1)!$ choices of the W 's, denoted channel permuting arrays, which guarantee that the $(N-1)^{\text{st}}$ iterate of the kernel of the integral equation for the T operators is connected; hence, use of any of these channel permuting arrays eliminates the divergence difficulties associated with disconnected diagrams.

As has been noted elsewhere,⁷ if only bound states are retained in expanding the channel Green's operators, the connectedness problem is greatly simplified. Such an approximation was in fact made in the $e-H$ calculations

reported earlier² where numerical results were obtained using two different sets of coupled equations: one which did lead to a damping relation, and one which did not. Only the channel permuting array was used in these latter calculations. In this article, we examine numerically the dependence of the e^-H scattering lengths and low energy ($E = .01$ Rydberg) phase shifts on the choice of channel coupling array elements W_{ij} . No disconnected diagram divergences arise for choices of W other than the channel permuting array because, as in Ref. 2, the channel Green's operator, G , is approximated by retaining only the $1s$ hydrogenic ground state in the expansion of G_1 . The e^-H system has become a natural testing ground for many theories, and we use it here for the usual reasons that both the interactions and target wave functions are known exactly (in the non-realistic limit) and also because a wide variety of numerical results are available with which our's may be compared.¹⁰⁻¹³ In particular, we are able to study the effect of varying the values of the W_{ij} . As we discuss in detail in Section III, the most reliable results are obtained using the channel permuting array^{6,7,9} values $W_{11} = 0$, $W_{21} = 1$. This is no surprise, since these are the values which rigorously guarantee connected, iterated kernels for the exact integral equations.

In Section II, we briefly review the coupled equations and the properties of W . In Section III, we present the numerical results for the singlet and triplet scattering lengths, $a_{\pm}$, and phase shifts, $\eta_{\pm}$, as a function of W and discuss their implications. Finally, in Section IV, we make some general comments regarding the coupled channel T operator approach in light of these computational studies.

II. Integral Equations for the Channel T Operators

The coupled equations for the operators T_{jk} describing the transition from a state in channel k to a state in channel j have been derived and discussed elsewhere,¹⁻³ and we simply reproduce the result of that derivation here:

$$T_{jk} = V_j W_{jk} + V_j \sum_i W_{ji} G_i^+ T_{ik} \quad (1)$$

In matrix notation, this reads

$$\underline{T} = \underline{V} + \underline{V} \underline{G}^+ \underline{T} \quad (2)$$

where

$$(\underline{V})_{jk} = V_j W_{jk} \quad (3)$$

$$(\underline{G}^+)_{ij} = \delta_{ij} G_i^+ \quad (4)$$

and

$$G_j^+ = (E - H_j + i\epsilon)^{-1} \quad (5)$$

We use the symbols V_j to denote the interaction in channel j , W_{jk} to denote the elements of the channel coupling array, and H_j to indicate the j^{th} channel Hamiltonian. This latter quantity describes the internal states of the subsystems forming the channel and also their relative motion. The Hamiltonian for the entire system, including all interactions, is denoted H , so that

$$V_j = H - H_j \quad (6)$$

We note that in Eq. (1), the row index i of W_{ji} is free to be specified. However, in the two-channel problem to be considered here (e^- -H scattering below the ionization threshold), the 2×2 nature of W actually fixes i to be equal to j . Hence, in this case, $(\underline{V})_{jk} = V_j W_{jk}$. The numerical values assigned to the W_{jk} determine the strength with which the two channels are

coupled to each other, these values are arbitrary except that the w_{jk} are required to obey

$$\sum_j w_{jk} = 1 = \sum_j w_{kj} \quad , \quad \text{all } k \quad . \quad (7)$$

The sum on j in Eq. (7) runs over all channels, as does the corresponding sum on i in Eq. (1).

In addition to the channel Green's operators G_i^+ , there is the full Green's operator G^+ for the system defined by

$$G^+ = (E - H + i\epsilon)^{-1} \quad . \quad (8)$$

This operator gives rise to outgoing waves in each (open) channel i , as is made explicit by use of the Lippmann-Schwinger equation

$$G^+ = G_i^+ + G_i^+ V_i G^+ \quad . \quad (9)$$

Such an equation may be written using the channel Green's operator for any of the channels i . The use of the channel coupling array enables us to replace Eq. (9) by an expression in which G^+ is formally partitioned over all the channel G_i^+ at once:

$$G^+ = \sum_i w_{i1} (G_i^+ + G_i^+ V_i G^+) \quad . \quad (10)$$

Equation (10) is derived by multiplying both sides of Eq. (9) by w_{i1} , summing on i and using Eq. (7). As shown elsewhere, substitution of Eq. (10) into the definition

$$T_{jk} = V_j + V_j G^+ V_k \quad (11)$$

gives a coupled set of equations for the T_{jk} . Using the relation¹⁴

$$G_i^+ (V_i - V_k) |k\rangle = (1 - \delta_{ik}) |k\rangle = \bar{\delta}_{ik} |k\rangle \quad (12)$$

where $|k\rangle$ is an on the energy shell state of arrangement k we may define a new set of operators³ T_{jk} which has the same on shell matrix elements as

the set given by Eq. (11). The set so derived is that presented in Eq. (1). We emphasize that because of our use of Eq. (12) in defining Eq. (1), it is a particular off shell extension of Eq. (11), and seems to be the only version which is related in a simple way to channel reactance operators K_{jk} even when truncated expansions of the Green's functions G_i^+ and G_i^P , the principal value Green's function, are used.^{1,3,7}

There are several points which we wish to stress. First, we note that individual W_{ij} are not restricted in magnitude or sign. In order to obtain Eq. (10) from Eq. (9), it is only necessary that the W_{ij} sum to unity, i.e., that they obey Eq. (7). Thus, we should be prepared to examine choices of W_{ij} which are greater than unity (and some of course concurrently negative). Second, while the constraint Eq. (7) is so weak as to place almost no restriction on the choice of the W_{ij} that may enter a calculation, the requirement that the kernel of the exact integral equation be connected after iteration places quite stringent limitations on the W_{ij} . Indeed, as we shall see later, the best values for singlet and triplet scattering lengths and phase shifts together occur for the choice of channel permuting W , as noted above, and this choice is the one that guarantees connected, iterated kernels for the exact equation.⁷⁻⁹ Third, it is plausible that by varying the values of W_{ij} (which we may do freely because we approximate the G_i^+ by keeping only a bound hydrogenic state, thus eliminating any possible occurrence of the divergences due to disconnected diagrams), we are effectively varying the form of the basis set used to expand the G_i^+ . This remark is based on the fact that a variation in W alters the strength with which the channels are coupled to each other. But to describe bound states of one channel in terms of the states of a second, we need to include the three-body continuum. Therefore, when the amount of coupling is changed, the size of the basis set in a channel is effectively changed. In our case, this means that keeping only the 1s state in channel 1, but varying the W_{ij} actually varies the states of channel 2

needed to describe the 1s state. We are assuming that for any W the correct scattering result may be obtained by using increasingly large basis sets. Of course, for choices of W which lead to exact equations with disconnected diagrams, this is not necessarily the case. Determining the effects of such variations in the W_{ij} is one of the main considerations of the present study.

For a two-channel system, such as e^- -H below the ionization threshold, the coupled equations derived from Eq. (1) are:^{1,2}

$$T_{11} = V_1 W_{11} + V_1 W_{11} G_1^+ T_{11} + V_1 W_{12} G_2^+ T_{21}$$

and

$$T_{21} = V_2 W_{21} + V_2 W_{21} G_1^+ T_{11} + V_2 W_{22} G_2^+ T_{21} \quad (13)$$

For the e^- -H system under study here, the channel interaction V_i has the functional form

$$V_i = -\frac{e^2}{r_i} + \frac{e^2}{r_{12}} \quad (14)$$

where r_i is the distance from electron i to the proton and $r_{12} = |\vec{r}_1 - \vec{r}_2|$. We take the mass of the proton to be infinite.

In the non-relativistic limit, the total spin is a good quantum number, and it is convenient to work with the symmetrized amplitudes

$$\mathcal{T}^\pm = T_{11} \pm P_{12} T_{21} \quad (15)$$

where P_{12} is the two-particle transposition operator and the $+$ ($-$) sign refers to the case of singlet (triplet) spin. From the pair Eq. (13), it is straightforward to show³ that $\mathcal{T}^\pm$ obeys

$$\mathcal{T}^\pm = (V_1 W_{11} \pm P_{12} V_2 W_{21}) [1 + G_1^+ \mathcal{T}^\pm] \quad (16)$$

where G_1^+ is defined by Eq. (5).

The singlet (+) and triplet (-) amplitudes $T^\pm$ are obtained from $\mathcal{T}^\pm$ by

$$T^\pm = \langle \Phi_{k^1, \alpha^1}(1) | \mathcal{T}^\pm | \Phi_{k, \alpha}(1) \rangle \quad (17)$$

where $|\Phi_{k, \alpha}(1)\rangle$ is an eigenstate of H_1 in which electron 1 is in a plane

wave state of momentum k and electron 2 is in a hydrogenic state whose quantum numbers are collectively denoted by α . Clearly, $T^{\pm}$ is a sum of direct and exchange amplitudes, T_d and T_{ex} :

$$T^{\pm} = T_d \pm T_{ex} \quad (18)$$

where

$$T_d = \langle \phi_{k',\alpha}(1) | T_{11} | \phi_{k,\alpha}(1) \rangle \quad (19)$$

and

$$T_{ex} = \langle \phi_{k',\alpha}(1) | P_{12} T_{21} | \phi_{k,\alpha}(1) \rangle . \quad (20)$$

In consequence of this, the present approach must be viewed as basically different from approaches where antisymmetrization plays a fundamental role in the derivation of the equations. That is, as discussed in a previous study,¹⁵ there are two basic approaches to treating identical particle collisions. The first of these (and by far the most common) is based on the use of antisymmetric states at the outset, leading to a single amplitude containing direct and exchange effects. No explicit separation of the direct and exchange amplitudes is made in deriving the equations leading to this amplitude. Methods leading to such an approach include projection operators,¹⁶ second quantization¹⁷ and explicit antisymmetrization of wavefunctions.^{10,18} In the second approach the rearrangement nature of the exchange process is explicitly taken into account and labelled amplitudes for direct and exchange processes play a central role in the equations (here the direct amplitude is our T_{11} and the exchange amplitude is our T_{21}). Methods based on this philosophy include the present coupled T operator approach and the inhomogeneous equations approach.¹⁹

The procedures used to solve Eq. (16) have been extensively discussed elsewhere,^{2,5} and we shall not discuss them here. We merely comment that a truncated eigenfunction expansion for G_1^+ and $T^{\pm} | \phi_{k,\alpha}(1) \rangle$ is introduced, and from that point on, no further approximations are employed. The resulting integral equations are solved numerically by a non-iterative procedure.^{2,20}

Finally, we note that the condition given by Eq. (7) shows that only one of the pair W_{1i} , W_{2i} is independent. Thus, we present all results by specifying only W_{1i} and note that W_{2i} is always given by $1-W_{1i}$.

III. Scattering Lengths and Phase Shifts for Various W

We have employed Eq. (16) for calculations of the singlet and triplet scattering lengths and phase shifts for a range of values of W_{11} . In all the calculations, we have employed the minimal basis set of the 1s hydrogenic state. For the e-H system, in the limit of low energies, only the S-wave needs to be considered since the P and higher partial waves make no contribution to the cross section.²⁰ Furthermore, there is a well-known singlet bound state for H^- so that the singlet phase shift tends to π in the limit of zero energy.²¹ This must, of course, be taken into account when computing scattering lengths. There is no similar triplet state so that its phase shift tends to zero in the limit of zero energy. (We discuss this further in Section IV.)

In order to ensure that our computer programs were working properly, it was convenient to use several special values of W_{11} as test cases. Thus, when $W_{11} = 1$ and $W_{21} = 0$, we expect to obtain simply the Hartree results for both ℓ_+ and ℓ_- ; that is for this choice of W_{11} our equations are simply

$$\tau^{\pm} = v_1 + v_1 G^+ \tau^{\pm} \quad (21)$$

which clearly contains no exchange effects. The results for $\ell_{\pm}$ are found to agree with this well known result (i.e., $\ell_{\pm} = -9.44$). Next we used the value $W_{11} = 0$ and verified that phase shift results of our earlier studies² were likewise properly reproduced. Finally, two versions of the programs were independently written and tested in order to ensure that reliable results were obtained.

In Figure 1 we present the variation of the singlet scattering length ℓ_+ as a function of W_{11} . It is to be noted that the range of W_{11} studied includes both W_{11} which are greater than 1 and also less than 0. Of course,

for $W_{11} > 1$, we have $W_{21} < 0$, while for $W_{11} < 0$, we have $W_{21} > 1$ in order that our fundamental constraint on W_{21} be satisfied. We notice first of all a striking similarity in the qualitative dependence of l_+ on W_{11} and that of the scattering length for a potential $V(r)$ given by²²

$$V(r) = \alpha V_0(r) \quad . \quad (22)$$

Here, we assume $V_0(r) > 0$ so that the sign of $V(r)$ depends on α . For positive values of α , the scattering length, $l = \lim_{k \rightarrow 0} [k \cot \eta]^{-1}$, will be positive.

When α goes from positive to negative, the scattering length will also change sign (and of course, $l = 0$ when $\alpha = 0$). This corresponds to a "Ramsauer effect." As α becomes more negative, eventually at a value of α equal to α_b , a bound state will appear at zero energy and the scattering length displays a singularity, diverging to $-\infty$ as $\alpha \rightarrow \alpha_b$ from above and to $+\infty$ as $\alpha \rightarrow \alpha_b$ from below. As α continues to decrease, l again eventually becomes negative (giving rise again to an $l = 0$ Ramsauer point). Continuing to decrease α can then lead to a second bound state at zero energy again giving rise to the same singular behavior in l as before, and so on.

Consideration of Fig. 1 shows that W_{11} plays a role in the singlet scattering similar to α discussed above. However, the point A at which one characterizes the "effective interaction" as changing from repulsion to attraction is not at $W_{11} = 0$ but rather $W_{11} \cong 1.18$. At this value of W_{11} , for the minimal basis set, one has an "effective interaction" that leads to a Ramsauer effect (it is important to emphasize that we do not conclude that e^-H has true Ramsauer scattering but rather that for $W_{11} \cong 1.18$, the coupling between channels plus a minimal expansion basis gives such approximate results). Just as in our example (Eq. (22) above), decreasing W_{11} causes the effective interaction to become more and more attractive until, at $W_{11} \cong 0.905$, a bound state with zero energy results. This may perhaps be the

H^- singlet bound state well known from earlier studies; the fact, for $W_{11} \approx 0.905$, that its energy is zero would indicate that for this particular inter-channel coupling, the minimal basis set (1s hydrogenic state and S-waves) can just bind the electron. Continuing to decrease W_{11} causes the ℓ_+ to become positive and it then decreases with decreasing W_{11} . It is interesting to note that, unlike the illustrative example Eq.(22), the dependence of ℓ_+ on W_{11} in Fig. 1 for $W_{11} \lesssim 0$ suggests a leveling off rather than the appearance of yet more bound states as W_{11} is decreased further. This suggests that W_{11} is not the only factor influencing the degree of attractiveness of the effective potential and suggests further that larger basis sets combined with variable W_{11} may eventually lead to results independent of W_{11} . Pursuing this point, we notice in Fig. 1 the value $W_{11} = 1$. This corresponds, as remarked earlier, to the ordinary Hartree non-exchange result and it is clear that for this choice of W_{11} , it is essential to include the ionization continuum of the bound electron in order to obtain the correct amplitude. This serves to emphasize the inter-relation of W_{11} and the expansion basis. Of course, this assumes that for any W_{11} , a basis set size can be found that will lead to the correct

results. However, it is obvious that as W_{11} gets closer to 1, the role of the continuum part of the basis set becomes more and more significant. It also has proved relatively easy to devise an analytical fit to these singlet scattering length results over the W_{11} range $-0.3 \leq W_{11} < 0.8$. Using this expression, one finds that the approximate value of W_{11} at which ℓ_+ equals the "static-exchange" or Hartree-Fock^{21,10} 1s-S-wave value is 0.51. Also shown on the ordinate of Fig. 1 is the value of ℓ_+ obtained by Schwartz.¹³

In Fig. 2 we present a similar plot for the triplet scattering length ℓ_- as a function of W_{11} . It is immediately clear on comparing Figs. 1 and

2 that the singlet and triplet scattering lengths depend on W_{11} in quite different fashion (even though each has a Ramsauer point and a W_{11} leading to a bound state at zero energy). Indeed, Fig. 2 more closely resembles a plot of scattering length as a function of atomic number Z for an electron colliding with a Thomas-Fermi atom.²² That is, the repulsion decreases and attraction increases with increasing W_{11} (in contradistinction to the singlet case). However, once this basic difference is noted, the discussion of Fig. 2 follows that of Fig. 1 except that now, one has a repulsive "effective potential" for W_{11} less than $W_{11}^A \cong 0.86$ (the value of W_{11} giving rise to Ramsauer behavior). Of course, both Figs. 1 and 2 have $\ell_+ = \ell_- = -9.44$ when $W_{11} = 1$ since they both lead to the same Hartree approximation. As W_{11} increases, one eventually sees a bound state appearing at zero energy (for $W_{11} \cong 1.04$) and ℓ_- displays the familiar singular behavior. Further increase in W_{11} causes an increased effective attraction and ℓ_- decreases. Again, it appears that there is a limit to the amount of attractiveness and as W_{11} becomes large (or small) ℓ_- appears to be leveling off. Indeed, for $W_{11} < 0.86$, ℓ_- changes rather slowly and of course, in the most "physical" region ($W_{11} \cong 0$), we note that there is no triplet bound state of H^- , but there is a singlet bound state. We would expect that increasing the basis set for a large positive W_{11} , the bound singlet state should appear and the bound triplet state should vanish if the equations converge at all with a disconnected iterated kernel. For reference convenience, we again have denoted the value of ℓ_- obtained by Schwartz.¹³ As for the singlet, an analytical fit of the triplet scattering length was easily made and it gives the approximate value $W_{11} = -0.6$ for ℓ_- to equal the Hartree-Fock 1s-S-wave result.

In Figures 3 and 4 we present the dependence of the singlet and triplet phase shifts (η_+ and η_- , respectively) as functions of W_{11} . Before discussing details of these, we first make the general observation that one expects to obtain positive phase shifts when the potential is attractive and negative phase shifts when it is repulsive. Furthermore, by Levinson's theorem we expect to have η_+ tend to π while η_- should tend to 0 as the

energy tends to zero. Finally, all results shown have been computed at a relative kinetic energy of 0.01 Ryd.

In Fig. 3 for η_+ , we first notice that the phase shift is positive throughout the range $-0.3 \leq W_{11} < 1.1$ and in general decreases as W_{11} increases. This behavior is easily understood by noting that in Fig. 1, the Ramsauer point A occurs at $W_{11} \cong 1.18$. This implies that for the entire region of interest, we are in the range of W_{11} that implies an attractive potential, thereby giving rise to positive phase shifts. Furthermore, we notice that η_+ is seen to vary most rapidly with W_{11} in the region where l_+ is changing most rapidly. Since²³ $k \cot \eta_+ \approx 1/l_+$ for k small, this result is not too surprising. Finally, we also display the values of W_{11} at which η_+ agrees with the Hartree and Hartree-Fock results, and also indicate the value of η_+ obtained by Schwartz.¹³

For the triplet case shown in Fig. 4, one sees a quite different behavior. From Fig. 2, the point A denoting the change of the triplet effective potential from repulsive to attractive falls within the range of W_{11} considered. We therefore must expect a change of sign in η_- as a function of W_{11} . Since for $W_{11} \lesssim 0.86$, the effective potential is repulsive, in this range η_- will be negative while for $W_{11} \gtrsim 0.86$ it should become positive. This is indeed the observed behavior seen in Fig. 4. Again we indicate the Hartree, Hartree-Fock and Schwartz values of η_- for reference. As a final comment, we point out that if one tries to plot η_- by adding π to the negative value, one encounters a discontinuous behavior unless the Hartree value (at $W_{11} = 1$) is taken to be 3.864 instead of the usual value of 0.722. Thus, if the Hartree result is taken (as is usual) to be 0.722, then it is necessary to use the negative values of η_- for lower values of W_{11} .

Finally, In Table I we give some specific values of $\ell_{\pm}$ to facilitate more quantitative comparisons with other methods and between $\ell_{\pm}$ at other values of W_{II} .

IV. Comments and Discussion

In this paper we have presented numerical values of scattering lengths and phase shifts for electron-hydrogen atom scattering computed using the new coupled channel T operator equations. Particular emphasis in our study has been placed on understanding the role of the channel coupling array W that appears in these equations. In order to bring out its effects, we have chosen to restrict our eigenfunction expansion basis set to include only the $1s$ hydrogenic state and the S -wave relative motion angular state. It appears that the results support a number of interesting conclusions, although more study with larger basis sets will be required to completely establish these.

The use of arbitrary values of the channel coupling array parameter is extremely dangerous. We have found that by varying this parameter, one may obtain any value for $\ell_{\pm}$ whatsoever. Furthermore, although we have seen what might appear to be a bound state appear in the singlet state where one is known to exist, we have also found a bound state in the triplet state where we believe there are none. Thus, it is possible to draw invalid conclusions if one does not treat channel coupling carefully. Nonetheless, a study of the effects of varying the channel coupling array parameters can lead to useful insight into calculations. For example, by being able to study the variation of $\ell_{\pm}$ as functions of the channel coupling (in a direct and simple fashion) we obtain a guide to understanding such numerical parameters as the scattering phase shifts for the system. Furthermore, it is suggested that deeper understanding of other methods may potentially be obtained by noting the values of W_{11} which lead to results equal to those obtained by the other methods. For example, it appears that for singlet scattering, $W_{11} \cong 0.5$ corresponds to a description similar to that one obtains in the static-exchange (Hartree-Fock) procedure. This seems not unreasonable as this W_{11} should correspond to some sort of equal weighting of direct and exchange

aspects of the problem. However, it is also clear that the correspondence is not a hard and fast one (since the triplet results for $W_{11} \approx 0.5$ do not closely correspond to the triplet static-exchange results).

The results obtained using the (mathematically) important channel permuting array,^{5,7-9} $W_{11} = 0$, $W_{21} = 1$, are particularly encouraging. In fact, careful examination of Figs. 1-4 reveals that this choice of W_{11} , W_{21} leads to the best results possible (for the basis set of the 1s hydrogen state and only S-waves) if one considers both the singlet and triplet scattering. To see that this is indeed the case, we call attention again to Figs. 1 and 2 for δ_+ and δ_- (the same conclusions follow when one considers the phase shifts). In Fig. 1, we notice that the best agreement of δ_+ with Schwartz's accurate result occurs for $W_{11} < 0$. In Fig. 2, we see that the best agreement of δ_- with Schwartz's accurate result occurs for $W_{11} > 0$. It therefore appears that the point $W_{11} = 0$ will lead to the best results for both δ_+ and δ_- considered together. This does not mean, of course, that the channel permuting array choice of W must lead to accurate results but rather only that if one wants to obtain similar error in

δ_+ and δ_- , then the channel permuting array is preferable to all other choices of W. However, it is gratifying to note that the absolute agreement of δ_+ and δ_- for the channel permuting array is extremely good since δ_+ differs by only 4.3% and δ_- by only 17.5% from Schwartz's values. (These differences in percentages reflect, of course, the differences in the magnitudes of δ_+ and δ_- . Thus, one may reasonably hope that this choice of W (in the absence of information to the contrary) will be an excellent one to use in general applications where one has not the time (nor inclination) to carry out such extensive studies of the dependence of results on the W array elements.

This latter comment leads us naturally to consider a fundamental question: given any particular scattering system undergoing transitions from states of one channel Hamiltonian to those of another, how are the values of the W_{ij} to be chosen? It would seem that the safest answer is that W should be chosen to ensure connected, iterated kernels under the assumption that exact solutions of the full set of coupled equations are to be obtained. For the case of N channels we have shown that there are $(N-1)!$ channel permuting arrays which guarantee connected, $(N-1)!$ iterated kernels, and also that these different channel permuting arrays are equivalent, since they correspond to $(N-1)!$ different ways of assigning channel labels.

Suppose, however, that exact calculations are not feasible and approximate ones are to be done, in particular the bound state approximation for the various G_i^+ is to be used. This is the approximation by which G_i^+ is expressed as a sum over only bound states of the subsystems in channel i , the 1s approximation of this work being an example. As noted elsewhere,⁷ such an approximation reduces the disconnected diagram problem. In practice this means that choices for W other than the channel permuting arrays can be made in the approximate equations without leading to the divergence problem. However, our results in the present study suggest that it is safe to introduce such approximations only into an exact system of equations to which standard numerical methods can be applied. It is then, and only then, that one may rigorously justify such approximations. Thus, even though in the singlet case, the best agreement with Schwartz's result occurs for $W_{11} \approx -0.2$, it is clear that much worse results are obtained, at this W_{11} , for triplet scattering parameters. Furthermore, it is clear from Figs. 1 and 2 that essentially any value of $\epsilon_{\pm}$ can be obtained as W_{11} is varied from 0 to 1.2. By contrast, our present results strongly suggest that use of the channel permuting array (so as to assure the applicability of standard solution

procedures) leads to the best results in the sense discussed above. Hence, we argue that it is likely the only safe choices of W to use are limited to those which produce connected, iterated kernels for the exact set of coupled equations,

Summarizing, the calculations of this work involve writing

$$G_i^+ \approx \frac{|\varphi_{1s}(j) \rangle \langle \varphi_{1s}(j)|}{E - E_{1s} - K_i + i\epsilon} \quad (23)$$

where $|\varphi_{1s}(j) \rangle$ is the hydrogenic ground state with energy E_{1s} and K_i is the kinetic energy operator for particle i . This has ensured that any choice for W_{11} leads to a connected, iterated kernel in Eq. (16). If we did not know that $W_{11} = 0$ was the channel permuting array choice, we might have guessed that any arbitrary value of W_{11} might give satisfactory results. But, as we have seen, the best results for $\ell_{\pm}$ and for $\eta_{\pm}$ occur for $W_{11} = 0$, which is as expected on the basis of our arguments in the preceding paragraphs. In a sense, the calculations discussed in this paper may be taken as the strongest corroborative evidence for always working with choices for W that guarantee connected, iterated kernels for the general set of equations given by Eq. (1).

In conclusion, we remark that calculations are planned which will include more states in the expansion basis for G_i^+ and which will therefore test these ideas and the coupled channel T operator approach more fully.

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Table IRepresentative Values of Scattering Lengths for Various W_{11}

W_{11}	Singlet ℓ_+	Triplet ℓ_-
-0.4	5.792	2.267
0	6.230*	2.077*
0.4	7.376	1.745
0.8	17.253	0.598
0.9	193.568	-0.658
1.0	-9.442	-9.442
1.1	-2.140	+7.655
1s-2s (Hartree-Fock)	+7.5	+2.33
1s-2s-2p (H-F)	6.74	1.89
Variational (Schwartz)	5.96	1.77

*These values of ℓ_+ correspond to the choice of W_{11} , W_{21} denoted in previous work as a channel permuting array.^{3,6-7} Thus, this particular W array plays a special role in two and more channel applications of the coupled T formalism and we attach therefore special significance to these results. That is, it is the channel permuting array which leads to connected integral equation kernels upon iteration.

Figure Captions

- Figure 1. The singlet scattering length ℓ_+ is plotted as a function of W_{11} over the range $-0.3 \leq W_{11} \leq 1.3$. The point denoted A is that at which ℓ_+ vanishes; the point $\otimes$ denotes the Hartree scattering length; the point $\bullet$ denotes the Hartree-Fock scattering length. All calculations are for the 1s hydrogen basis set.
- Figure 2. The triplet scattering length ℓ_- is plotted as a function of W_{11} over the range $-0.3 \leq W_{11} \leq 1.4$. The points A and $\otimes$ are as in Fig. 1.
- Figure 3. The singlet phase shift is plotted as a function of W_{11} over the range $-0.3 \leq W_{11} \leq 1.1$. The relative kinetic energy is 0.01 Ryd. The points $\otimes$ and $\bullet$ are as in Fig. 1.
- Figure 4. The triplet phase shift is plotted as a function of W_{11} over the range $0 \leq W_{11} \leq 1.0$. The relative kinetic energy is 0.01 Ryd. The point $\otimes$ is as in Fig. 1.

FIG. 1

FIG. 2

FIG. 4

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