Channel coupling arrays and the reduction method in many-body scattering

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A differential equation formulation of the multichannel coupled equations of Kouri and Levin describing rearrangement scattering is given. The different channels are linked together in these equations through the presence of the channel coupling array W. It is shown that the earlier results of Hahn, derived using the reduction method, follow directly from the multichannel coupled equations by making specific choices of the array W. These particular W's guarantee that the iterated kernels of the coupled equations are connected in those channels which are explicitly considered, so that standard numerical techniques can be applied to their solution.

Several years ago, one of us (Y.H.) developed a new technique known as the reduction method for treating many-body scattering problems.[1] It consists of rewriting the Schrödinger equation in matrix form, with certain interactions present in the total Hamiltonian removed from each row or column. The method has been used, for example, to discuss direct reactions[2] and distortion potentials for many-body scattering.[3]

A detailed discussion of the contents of the method is given in Ref. 3 in terms of Green's functions and their partitions, while both the Faddeev equations and the Watson scattering equations are shown to follow rather simply from the general reduction procedure. The main feature of this approach from a practical point of view is of course that the set of coupled scattering equations in the rigorous formulations can be greatly simplified such that the resulting set of equations can often be solved with a reasonable amount of effort and accuracy. By sacrificing the complete connectedness of the iterated kernels and by employing the channel projection operators, we can construct a simple framework in which the strongly coupled direct channels may be treated.

More recently, the other two of us (D.J.K. and F.S.L.) have introduced another method[4] for treating many-body scattering, based on the use of the channel coupling array W which links together the T operators describing transitions between different rearrangement channels.[5] The matrix W, whose elements are initially undetermined apart from a normalization condition, can be chosen so as to guarantee that in an N-channel scattering problem, the $(N-1)$st iterate of the kernel of the coupled equations for the T operators is connected.[6] The resulting equations have been used, e.g., to study e^-+H scattering below the $n=2$ threshold[7] and to formulate optical potentials for many-body scattering.[8]

Unlike the approaches of Faddeev and others to three-body and/or many-body scattering,[9] both of the preceding methods are based on the explicit use of the channel interactions (and/or ancillary distorting potentials) occurring in the many-body Hamiltonian describing the system under consideration. Because the starting point of these two methods is the same (i.e., use of channel interactions), they must be closely related. The purpose of this note is to show that the equations of Hahn,[1] for both the cases of $N=2$ and $N=3$ as examples, follow from particular choices of the channel array elements W_{ij} used in the new equations of Kouri and Levin,[4] for the two-channel and three-channel problems. The method of Kouri and Levin may thus be regarded as another means for realizing the equations of the reduction method[1,3] and also as a means for providing further justification[3] for using the approach of the reduction method.

The procedure we follow here is to derive the equations of Refs. 4 and 6 using the exact formal solution to the usual Lippmann-Schwinger equation, rather than starting with the T operator equations[4,6]; next we show that the transposed matrix operator may be used to generate solutions to the many-body scattering problem, and then, by specific choice of the elements W_{ij}, we derive the results of Hahn. We close with a brief discussion of choices of W for $N>3$.

Let H be the total Hamiltonian for the system, and let H_i be the channel Hamiltonian in channel i.

H_i describes the internal states of the subsystems (or clusters of particles) forming channel i, and also their relative motion. We also introduce distortion potentials Y_i in channel i, so that the relative motion could be distorted wave, rather than plane wave. If $Y_i = 0$, then $V_i = H - H_i$ is the channel perturbation, while if $Y_i \neq 0$, then $V_i - Y_i$ is the channel perturbation, as in Refs. 1 and 3.

Assuming $Y_i \neq 0$, the states of H_i are denoted $|\chi_E^{\pm}(i)\rangle$:

$$(H_i + Y_i)\,|\chi_E^{(\pm)}(i)\rangle = E\,|\chi_E^{(\pm)}(i)\rangle\,, \tag{1}$$

where E is the sum of the kinetic energy in the channel plus the internal energies of the clusters. Scattering amplitudes for transitions between channels k and j are determined from

$$A_{jk} = \langle \chi_E^{(-)}(j)\,|\,T_{jk}(E+i0)\,|\,\chi_E^{(+)}(k)\rangle + \langle \Phi_j\,|\,Y_j\,|\,\chi_E^{(+)}(k)\rangle\,\delta_{jk}\,, \tag{2}$$

where the T_{jk} are operators derived below.

The full scattering state generated from $|\chi_E^{+}(k)\rangle$ is $|\Psi_E^{(+)}(k)\rangle$:

$$|\Psi_E^{(+)}(k)\rangle = |\chi_E^{(+)}(k)\rangle + G^{(+)}(V_k - Y_k)\,|\chi_E^{(+)}(k)\rangle\,, \tag{3}$$

where $G^{(+)} = (E + i\epsilon - H)^{-1}$ is the full, outgoing-wave Green's function. To derive an integral equation for $|\Psi_E^{(+)}(k)\rangle$, one usually expresses $G^{(+)}$ via a Lippmann-Schwinger equation involving a particular channel Green's function $G_i^{(+)} = (E + i\epsilon - H_i)^{-1}$:

$$G^{(+)} = G_i^{(+)} + G_i^{(+)}(V_i - Y_i)G^{(+)}\,. \tag{4}$$

Straightforward substitution of (4) into (3) leads, as is well known, to difficulties involving homogeneous equations when $i \neq k$. The resulting equation is not connected, nor is the dependence on the channels other than i included except via the continuum states in $G_i^{(+)}$. (The argument of the Green's functions will be suppressed in the remainder of this work.)

We finesse these problems by coupling all channels together using the channel coupling array W, whose elements W_{ij} are initially restricted only by the normalization condition

$$\sum_i W_{li} = 1 \quad \text{or} \quad \sum_i W_{il} = 1\,, \tag{5}$$

where i and l run over all N channel labels.

We multiply both sides of (4) by W_{li} and sum on i to give

$$G^{(+)} = \sum_i W_{li}\,[G_i^{(+)} + G_i^{(+)}(V_i - Y_i)G^{(+)}]\,, \tag{6}$$

which partitions $G^{(+)}$ over all the channels by means of the parameters W_{li}. *The index l is free to be chosen as is convenient.*

Substitution of (6) into (3) gives

$$|\Psi_E^{(+)}(k)\rangle = |\chi_E^{(+)}(k)\rangle + \sum_i W_{li}\,G_i^{(+)}(V_k - V_i + Y_i - Y_k)\,|\chi_E^{(+)}(k)\rangle + \sum_i W_{li}\,G^{(+)}(V_i - Y_i)\,|\Psi_E^{(+)}(k)\rangle\,. \tag{7}$$

The product $G_i^{(+)}[V_k - V_i + Y_i - Y_k]\,|\chi_E^{(+)}(k)\rangle$, in limit $\epsilon \to 0^+$, apart from the distortion potentials, has been shown by Lippmann[10] to be equal to $-\bar{\delta}_{ik}\,|\chi_E^{(+)}(k)\rangle$, where $\bar{\delta}_{ik} = 1 - \delta_{ik}$. If Y_i and Y_k depend only on relative coordinates between clusters, then Lippmann's result still holds:

$$\lim_{\epsilon \to 0^+} G_i^{(+)}(V_k - V_i + Y_i - Y_k) = -\bar{\delta}_{ik}\,, \tag{8}$$

when acting on states $|\chi_E^{(+)}(k)\rangle$.

We now assume that (8) holds in (7), which becomes

$$|\Psi_E^{(+)}(k)\rangle = W_{lk}\,|\chi_E^{(+)}(k)\rangle + \sum_i W_{li} G_i^{(+)}(V_i - Y_i)\,|\Psi_E^{(+)}(k)\rangle\,. \tag{9}$$

Use of the limiting procedure has not led to a homogeneous equation, and it can be shown[4] that the solution to (9) in limit $\epsilon \to 0^+$ is just Eq. (3).

Let us now define *channel scattering states* $|\psi_E^{(j)}(k)\rangle$ by

$$|\Psi_E^{(+)}(k)\rangle = \sum_j W_{lj}\,|\psi_E^{(j)}(k)\rangle\,. \tag{10}$$

Substituting (10) into (9) and noting that the W_{li} are arbitrary immediately leads to

$$|\psi_E^{(j)}(k)\rangle = |\chi_E^{(+)}(k)\rangle\,\delta_{jk} + G_j^{(+)}(V_j - Y_j)\sum_i W_{li}\,|\psi_E^{(i)}(k)\rangle \tag{11}$$

as a set of coupled equations for the channel scattering states. In differential form, the set (11) reads (lim $\epsilon \to 0^+$):

$$(E - H_j - Y_j)\,|\psi_E^{(j)}(k)\rangle = (V_j - Y_j)\sum_i W_{li}\,|\psi_E^{(i)}(k)\rangle\,. \tag{12}$$

If we consider the cases $N=2$ and $N=3$, and substitute the values of W_{ij} given below [Eqs. (36) and (41)] into Eq. (12), we find that the result is simply the transpose of Hahn's equations. While these transposed equations are valid ones, it is also possible to obtain precisely Hahn's equations. What we need in place of the term $(V_j - Y_j)W_{li}$ in Eq. (12) is its transpose, viz., $W_{jl}(V_i - Y_i)$. An equation involving the term $W_{jl}(V_i - Y_i)$ can be de-

rived from the Green's function,[3] or directly from the Schrödinger framework.[2] However, we will derive it here[4,6] using the equations for the T operators, thus showing the interrelationship between the two formulations. (See also the following paper.)

The operator T_{jk} describing transitions between channel k and channel j is defined by

$$T_{jk}\,|\,\chi_E^{(+)}(k)\rangle = (V_j - Y_j)\,|\,\Psi_E^{(+)}(k)\rangle\,. \tag{13}$$

On multiplying both sides of (9) by $(V_j - Y_j)$ from the left, and using (13), we find a set of coupled integral equations for the T_{jk}:

$$T_{jk} = (V_j - Y_j)W_{lk} + (V_j - Y_j)\sum_i W_{li}\,G_i^{(+)}\,T_{ik}\,. \tag{14}$$

This is the same set of integral equations for the T_{jk} derived from the definition of the transition amplitude[4]:

$$T_{jk} = (V_j - Y_j) + (V_j - Y_j)G^{(+)}(V_k - Y_k)\,. \tag{15}$$

On the energy shell, matrix elements of the solution to (14) are equal to those of (15).

We may reexpress (14) in matrix form:

$$T = \mathcal{U} + \mathcal{U}\mathcal{G}T\,, \tag{16}$$

where

$$\mathcal{U}_{jk} = (V_j - Y_j)W_{lk} \tag{17}$$

and

$$\mathcal{G}_{jk} = G_j^{(+)}\delta_{jk}\,. \tag{18}$$

The formal solution to (16) is

$$T = \mathcal{U} + \mathcal{U}\,\mathcal{g}\,\mathcal{U}\,, \tag{19}$$

where

$$\mathcal{g}^{-1} = \mathcal{G}^{-1} - \mathcal{U} \tag{20}$$

and $\mathcal{g}$ obeys

$$\mathcal{g} = \mathcal{G} + \mathcal{G}\mathcal{U}\mathcal{g} = \mathcal{G} + \mathcal{g}\mathcal{U}\mathcal{G}\,. \tag{21}$$

Hence, it follows from (20) and (21) that T also obeys a left-handed equation,

$$T = \mathcal{U} + T\mathcal{G}\mathcal{U}\,. \tag{22}$$

The set of equations given by (11) is recovered from (16) by defining a Møller wave operator matrix Ω by

$$T = \mathcal{U}\Omega$$

which leads, via (16) to

$$\Omega = 1 + \mathcal{G}\mathcal{U}\Omega\,; \tag{23}$$

Eq. (23), when acting on $|\,\chi_E^{(+)}(k)\rangle$, gives (11).

Equations (16)–(23) were previously derived[4] from Eq. (15), the "post" form of the T operator. However, it is well known that an equivalent operator to T_{jk} of (15) is the "prior" form, given by

$$\hat{T}_{jk} = (V_k - Y_k) + (V_j - Y_j)G^{+}(V_k - Y_k)\,. \tag{24}$$

We have also used this equation as a starting point to derive alternate coupled equations, similar to (14). In matrix form, these latter equations are[4]

$$\hat{T} = \mathcal{U}^T + \mathcal{U}^T\mathcal{G}\,\hat{T}\,, \tag{25}$$

or in detail,

$$\hat{T}_{jk} = W_{jl}(V_k - Y_k) + W_{jl}\sum_i (V_i - Y_i)G_i^{(+)}\,\hat{T}_{ik}\,. \tag{26}$$

Matrix elements of $\hat{T}_{jk}$ defined by (26) agree with those of T_{jk} defined by (14) when both are taken on the energy shell.[4] Hence, one can use either the set (25) or the set (16) to compute scattering amplitudes.

Defining an alternate matrix of Møller wave operators $\hat{\Omega}$ using

$$\hat{T} = \mathcal{U}^T\hat{\Omega}$$

and substituting into (25), we get

$$\hat{\Omega} = 1 + \mathcal{G}\mathcal{U}^T\hat{\Omega} \tag{27}$$

or

$$\hat{\Omega}_{jk} = \delta_{jk} + \sum_i G_j^{(+)}W_{jl}(V_i - Y_i)\hat{\Omega}_{ik}\,. \tag{28}$$

Operating on $|\,\chi_E^{(+)}(k)$ with both sides of (28) defines a new set of scattering states $|\,\hat{\psi}_E^{(j)}(k)\rangle$ obeying

$$|\,\hat{\psi}_E^{(j)}(k)\rangle = |\,\chi_E^{(+)}(k)\rangle\,\delta_{jk} + G_j^{(+)}W_{jl} \times \sum_i (V_i - Y_i)\,|\,\hat{\psi}_E^{(i)}(k)\rangle\,. \tag{29}$$

Equation (29) is the desired result. Multiplying both sides of (29) by $(G_j^{(+)})^{-1}$ and taking limit $\epsilon \to 0^+$ gives

$$(E - H_j - Y_j)\,|\,\hat{\psi}_E^{(j)}(k)\rangle = W_{jl}\sum_i (V_i - Y_i)\,|\,\hat{\psi}_E^{(i)}(k)\rangle\,. \tag{30}$$

It is this form from which the equations of Hahn[1] can be easily derived. We stress that both sets of equations, (11) and (30), are valid means of computing scattering parameters; their only difference is in the channel coupling interactions.

Up to this point, the parameters W_{jl} (or W_{lj}) are merely arbitrary elements in a scheme for coupling all the channels together. While any W_{jl} satisfying $\sum_j W_{jl} = 1$ are in principle valid choices, in fact the requirement that the iterated kernels of Eqs. (25), (28), or (29) be connected, places quite rigid limitations on the choices of the W_{jl}, and thus reduces their apparent arbitrariness. A general class of W's for the N-channel problem, denoted the channel permuting arrays, has been dis-

cussed elsewhere[6] and shown to lead to the $(N-1)$st iterate of the kernels of the above mentioned equations being connected. In addition, we have also shown that for the case $N=3$, there is a choice of W leading to the *first* iterate of the kernel being connected.[11] We now use this latter choice for $N=3$, and the channel permuting choice for $N=2$, in Eq. (36) and show that they give the equations of Ref. 1.

For $N=2$, the channel permuting array is obtained by setting $l=i$ for each term of the sum, and then choosing

$$W_{11}=W_{22}=0\,,\qquad W_{12}=W_{21}=1\,. \tag{31}$$

The choice $l=i$ is allowed since l is free to be chosen as we wish. Substituting (31) into (30) and suppressing the initial channel label k then leads to

$$(H_1+Y_1-E)\,|\,\hat{\psi}_E^{(1)}\rangle=-(V_2-Y_2)\,|\,\hat{\psi}_E^{(2)}\rangle$$

and (32)

$$(H_2+Y_2-E)\,|\,\hat{\psi}_E^{(2)}\rangle=-(V_1-Y_1)\,|\,\hat{\psi}_E^{(1)}\rangle\,,$$

which are Hahn's equations for $N=2$, which he obtained via the reduction method.

For $N=3$, we shall first specify the notation in more detail. Assuming only pairwise interactions, we have

$$H_i=H_0+V_{jk}\equiv H_0+V^{(i)}\,, \tag{33}$$

where H_0 is the sum of kinetic energies. Thus, we find

$$V_i=H-H_i=V^{(j)}+V^{(k)},\quad i\neq j,\quad i\neq k\,,$$

and using the quantity $\bar{\delta}_{ij}$, we may write

$$V_i=\sum_{n=1}^{3}V^{(n)}\bar{\delta}_{in}\,. \tag{34}$$

For simplicity, we set the distortion potentials $Y_i=0$, and then consider a typical term from the right-hand side in Eq. (30):

$$W_{jl}V_i=W_{jl}\sum_{n=1}^{3}V^{(n)}\bar{\delta}_{in}\,. \tag{35}$$

To obtain the $N=3$ (Faddeev) equation,[1] and also an integral equation [such as (29)] whose first iterated kernel is connected, we set $l=n$ for each n in the sum in (35) and then choose[11]

$$W_{jn}=\delta_{jn}\,. \tag{36}$$

With this choice, Eq. (30) becomes

$$(E-H_j)\,|\,\hat{\psi}_E^{(j)}\rangle=\sum_{i=1}^{3}V^{(j)}\bar{\delta}_{ij}\,|\,\hat{\psi}_E^{(i)}\rangle\,, \tag{37}$$

where the initial channel index k is again suppressed.

Written out as a matrix equation, (37) is

$$\begin{pmatrix}H_1-E & V_{23} & V_{23}\\ V_{13} & H_2-E & V_{13}\\ V_{12} & V_{12} & H_3-E\end{pmatrix}\begin{pmatrix}|\,\hat{\psi}_E^{(1)}\rangle\\ |\,\hat{\psi}_E^{(2)}\rangle\\ |\,\hat{\psi}_E^{(3)}\rangle\end{pmatrix}=0\,, \tag{38}$$

which is the desired equation. This is the differential form of the Faddeev equations in which only bound-pair channels appear.

Notice that both the choices of W_{ij} given by Eqs. (31) and (36) obey $\sum_j W_{jn}=1$. Furthermore, we can use each of these choices in the set of equations (12), to give results quite similar to those derived above. In the $N=2$ case, we would find the right-hand sides of Eq. (32) interchanged, while in the $N=3$ case, the matrix operator of (38) would be replaced by its transpose. Both of these equations resulting from the use of (12) are of course also valid starting points for computations.

In addition to the use of (36) in the $N=3$ case, we could also have employed a channel permuting array. There are two such,[6,11] which are transposes of each other, one of them being

$$W=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}. \tag{39}$$

Use of (39) in (30), with $Y_i=0$, leads to $(l=i)$

$$\begin{pmatrix}H_1-E & V_2 & 0\\ 0 & H_2-E & V_3\\ V_1 & 0 & H_3-E\end{pmatrix}\begin{pmatrix}|\,\hat{\psi}_E^{(1)}\rangle\\ |\,\hat{\psi}_E^{(2)}\rangle\\ |\,\hat{\psi}_E^{(3)}\rangle\end{pmatrix}=0\,, \tag{40}$$

where we recall from (34) that $V_i=V^{(k)}+V^{(j)}$. This is yet another valid starting point for computations in the $N=3$ problem. Furthermore, we can easily show that the components $|\,\hat{\psi}_E^{(i)}\rangle$ satisfy the same basic relation that is the "touchstone" of Hahn's approach. To establish this result, we simply add up the three equations summarized in the matrix equation (40):

$$\sum_{i=1}^{3}(H_i-E)\,|\,\hat{\psi}_E^{(i)}\rangle+\sum_i V_i\,|\,\hat{\psi}_E^{(i)}\rangle=0\,. \tag{41}$$

We then make use of Eqs. (33) and (34) to write (41) as

$$(H_0-E)\sum_{i=1}^{3}|\,\hat{\psi}_E^{(i)}\rangle+\sum_{i=1}^{3}V^{(i)}\,|\,\hat{\psi}_E^{(i)}\rangle+\sum_{i,j}\bar{\delta}_{ij}V^{(j)}\,|\,\hat{\psi}_E^{(i)}\rangle=0\,, \tag{42}$$

or finally

$$(H_0+V-E)\sum_i|\,\hat{\psi}_E^{(i)}\rangle=0\,. \tag{43}$$

From this we conclude that the total wave function $|\psi\rangle$ is given by

$$|\psi\rangle = \sum_{i=1}^{3} |\hat{\psi}_E^{(i)}\rangle . \tag{44}$$

This is Hahn's starting expression, and shows rigorously that for the $N=3$ case, the basic equation of the reduction method is recovered using *any* of the W arrays that lead to connected iterated kernels (i.e., either channel permuting arrays or the array that leads to Faddeev-like T equations.[5,11] It also shows, incidentally, that the eigenstates of $\hat{H}$ given by

$$\hat{H} = \begin{pmatrix} H_1 & V_2 & 0 \\ 0 & H_2 & V_3 \\ V_1 & 0 & H_3 \end{pmatrix}$$

are identical to those of the ordinary Schrödinger Hamiltonian $H = H_0 + V$. *There are no spurious solutions.*

Analogous to (40) in the N-channel case is the equation

$$\begin{pmatrix} H_1 - E & V_2 & 0 & 0 & \cdots \\ 0 & H_2 - E & V_3 & 0 & \cdots \\ 0 & 0 & H_3 - E & V_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ V_1 & 0 & 0 & 0 & \cdots \end{pmatrix} \begin{pmatrix} |\hat{\psi}_E^{(1)}\rangle \\ |\hat{\psi}_E^{(2)}\rangle \\ |\hat{\psi}_E^{(3)}\rangle \\ \vdots \\ |\hat{\psi}_E^{(N)}\rangle \end{pmatrix} = 0 . \tag{45}$$

In the N-channel case, there are $(N-1)!$ channel permuting arrays[6]; Eq. (45) is just one example of the $(N-1)!$ resulting equations, distinguished by permutations of the labels of the channels.

Both (40) and (45) may be regarded as alternate realizations of the equations of the reduction method for arbitrary N. The flexibility of the channel coupling array technique is evident from these examples. As shown elsewhere,[7] the ability of these equations to produce accurate numerical results has been demonstrated for the case of $l=0$, $e^- + H$ scattering in the approximation of retaining only the ground state of hydrogen in expanding the channel Green's function. Further calculations to test the accuracy and thus the potential applicability to other scattering systems are underway.

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