A NEW METHOD IN THE THEORY OF MANY-BODY SCATTERING

D.J. Kouri*, Max-Planck-Institut für Strömungsforschung, 3400 Göttingen, Federal Republic of Germany, and F.S. Levin†, Physics Department, Brown University, Providence, R.I. 02912

We have recently derived new sets of coupled equations for the T operators and for the K operators describing many-body scattering. The key to the method is the channel coupling array W, whose seemingly arbitrary elements are fixed by requiring the iterated kernel of the coupled equations to be connected. Unitary approximations may be introduced with relative ease, since the T and K operators are related by a damping equation and matrix elements of the K operators are real. In addition, the equations are free of spurious solutions and have the correct unitarity structure. This talk will be concerned mainly with a derivation of the equations; a discussion of the properties of the arrays W and of how their elements may be chosen so as to ensure connected iterated kernels; some aspects of the solutions in the N-channel case, including the formulation of a direct channel optical potential operator; connections with other formulations; and numerical applications, particularly to $e^- + H$ scattering.

* Present address: Departments of Chemistry and Physics, University of Houston, Houston, Texas 77004.

† Work supported in part by the U.S. Atomic Energy Commission.

UNE METHODE NOUVELLE DANS LA THEORIE DE LA DIFFUSION A PLUSIEURS CORPS

D.J. Kouri*, Max-Planck-Institut für Strömungsforschung, 3400 Göttingen, République Fédérale d'Allemagne, et F.S. Levin†, Département de Physique, Université Brown, Providence, R.I. 02912

Récemment, nous avons dérivé nouvelles ensembles des équations couplées pour les opérateurs T and les opérateurs K décrivent la diffusion a plusieurs corps. L'aspect essentiel de la méthode est la matrice de canal couplé W, dont apparemment arbitraire éléments sont décidé par la demande quel le noyau itéré des équations couplées soit connexe. Les approximations unitaires peuvent être introduit avec simplicité, depuis les opérateurs T et K sont connexe par un équation Heitler et les éléments des opérateurs K sont réels. Aussi, il n'y a pas les résoudres faux de les équations couplées (il n'y a pas la maladie Federbush). Finalement, les nouvelles équations sont la vraie structure unitarité.

Cette conférence traitera d'une derivation des équations; les propriétés des matrices W et méthodes de choisir leurs éléments afin de garantir quel le noyau itéré des équations est connexe; des aspects des résoudres pour le cas général, comprendrent la formualtion d'un opérateur de potentiel optique dans le canal direct; connexions avec autres formulations; et des applications numériques, particulièrement a le diffusion des électrons par les atomes de hydrogène.

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

A NEW METHOD IN THE THEORY OF MANY-BODY SCATTERING

D. J. Kouri*, Max-Planck-Institut für Strömungsforschung, 3400 Göttingen, Federal Republic of Germany, and P. S. Levin[†], Physics Department, Brown University, Providence, R. I. 02912

It is reasonable to expect that any method for describing many-body scattering processes should satisfy at least four conditions: (1), the dynamics must be properly taken into account, either via interactions or t matrices; (2), the kernel of the equation used in the method must have (finite) iterates that are connected; (3), the theory must have the requisite analytic structure, including proper treatment of threshold behavior and the correct unitarity (discontinuity) relations; and finally, (4), the effects of symmetries must be included. In addition, satisfaction of two other conditions is desirable, though not strictly necessary; (5), the equations should be free from spurious solutions [in Amado's terminology¹⁾, the equations should not suffer from Federbush disease^{2,3)}]; and (6), it should be possible to introduce unitary approximations in a relatively simple way.

The first four conditions may be summarized as follows. If the matrix equations for the operators of interest are of the form [z = a complex energy parameter]

$$U(z) = B(z) + C(z) U(z) \quad , \quad (1)$$

where B is the driving term and C is the kernel of the equation, then: B must properly represent the dynamics; C^M must be connected, for some $M \geq 1$;

$$\text{Im } U(E + i0) = -\pi U(E + i0) \tilde{A}(E) U(E - i0) \quad , \quad (2)$$

where E is the energy of interest and $\tilde{A}$ is an on-shell projector; and effects of symmetries such as the Pauli principle must be either included in (1) or readily taken into account. Lack of Federbush disease means that $(1 - C)$ is zero only at solutions of the relevant Schrödinger equation, while one way of satisfying condition (6) is that an auxiliary (real) operator $Y(E)$ can be found such that (a) U and Y are related via a damping equation, e.g.,

$$U(E + i0) = Y(E) - i\pi Y(E) \tilde{A}(E) U(E + i0) \quad , \quad (3)$$

and (b) $Y(E)$ itself should obey a simple equation, e.g.,

$$Y(E) = B(E) + R(E) Y(E) \quad , \quad (4)$$

where R is a real operator, usually the real part of $C(z)$. In the nonrelativistic case considered here, we may assume that $U(z) = U^*(z^*)$, and that U is either equal to or is

linear in the transition amplitude of interest.

The first many-body theory to satisfy conditions (1) - (4) was that of Faddeev⁴⁾ for the case where $n = 3$ [here n = number of particles, N = number of arrangement channels in the sense of Eckstein⁵⁾ or Newton⁶⁾]. Other formulations, such as that of Alt, Grassberger and Sandhas⁷⁾ are well known; we do not need to consider any of them in detail. Extensions to the case of arbitrary n were first discussed by Yakubovskii⁸⁾ and more recently for example by Bencze⁹⁾, by Karlsson and Zeiger¹⁰⁾ and by Redish¹¹⁾. In all of these works, the terms corresponding to B in Eq. (1) are t operators in n -body Hilbert space for 2, 3, and up to $(n - 1)$ -body subsystems. Furthermore, the kernel C is normally a product of B and another operator: $C(z) = B(z) D(z)$. One may identify three shortcomings to these methods. First, for many systems of interest, the relevant t operators may not be available. Second, and closely related to the first, even if on-shell values of some of the t -operators are known, their off-shell values generally are not known, and one must proceed using models. Thirdly, and of relevance to this work, is the fact that the t operators are complex, so that even if $R(E) = \text{Re } C(E + i0)$, $Y(E)$ of (4) will not be real because $B(E)$ is not real. This means that unitary approximations cannot be introduced in a simple way [in particular, using (3)]. Cahill¹²⁾ and Kowalski¹³⁾, among others, have shown how to deal with this problem via hierarchies of coupled, integral equations for the case $n = 3$, but such solutions, while they do exist, are not simple. We know of no comparable studies for arbitrary n using as a basis the n -body formalisms noted above.

In contrast to these approaches using t operators, we have recently developed a new method for treating the n -body problem^{14,15)} which not only allows unitary approximations to be introduced in a simple fashion (at least from our point of view) but also satisfies the five other conditions listed above. In this treatment, the terms in our equations corresponding to the $B(E)$ of equation (1) are the channel interactions rather than t operators, so that the auxiliary operators $Y(E)$ of eq. (4) are real. An obvious shortcoming is that the formalism cannot be applied directly to hard-core potentials. However, most potentials in non-relativistic problems seem at worst to be soft-core, and in addition, it is generally true as implied above that it is the potential and not the t operators for which there is the most information. In the case of models, a potential is usually postulated first and its t -matrix elements determined second. Finally, by working directly with potentials, problems involving coulomb interactions can be handled relatively simply. An example is the electron-hydrogen scattering system, which despite its having been the object of study for more than 4 decades, is a problem that has not yet been solved. This is the first system to which our method has been applied: so far the results are extremely encouraging¹⁶⁻¹⁸⁾; results of these calculations will be discussed below.

The key to our method is an $N \times N$ matrix W , denoted the channel coupling array, which links the arrangement channels together. Elements of W are fixed by requiring that the coupled equations in which they occur have a connected, iterated kernel (we

assume that the potentials in H are sufficiently well-behaved that the iterated kernels of our equations are compact). In our earlier work^{14,15)}, coupled equations were developed by beginning with the post-prior definition⁶⁾ of transition operators for arrangement collisions, but more recently we have derived our results directly from the Schrödinger equation¹⁹⁾. In addition we have shown that our equations do not suffer from Federbush disease¹⁹⁾ and have also established the relation between our results and those derived by Rahn²⁰⁾ using the reduction technique. For simplicity, we use here the post-prior T operator approach to discuss our work.

To fix notation, consider a model three-body problem consisting of three distinguishable particles (A,B,C) interacting via pair potentials. For simplicity, the mass of particle B is taken as infinitely heavy. The Hamiltonian H is then the sum of the two kinetic energy operators and the three interactions:

$$H = \underbrace{K_A + K_C}_{H_0} + \underbrace{V_{AB} + V_{AC} + V_{BC}}_V \quad (5)$$

We are interested in scattering processes initiated say, by A incident on a bound state of B and C: $A + BC$. The pair interactions are assumed to go to zero sufficiently rapidly as the pair separation becomes large. Thus there are four arrangement channels:

(1) $A + BC \rightarrow A + BC$	elastic
(2) $A + BC \rightarrow AB + C$	charge-exchange
(3) $A + BC \rightarrow B + AC$	pickup
(0) $A + BC \rightarrow A + B + C$	breakup

Corresponding to these four channels are four partitions of the Hamiltonian into channel Hamiltonians H_j and channel perturbations V_j ($H = H_j + V_j$):

$$H_1 = H_0 + V_{BC} \quad , \quad V_1 = V_{AB} + V_{AC}$$

$$H_2 = H_0 + V_{AB} \quad , \quad V_2 = V_{AC} + V_{BC}$$

and similarly for H_3 and V_3 , H_0 and $V_0 = V$.

In the general n -body, N -channel problem, we also have

$$H = H_j + V_j \quad , \quad 1 \leq j \leq N \quad (6)$$

If no restriction to pairwise interactions is assumed. The eigenstates of H_j , corresponding to observable, asymptotic states, will be denoted $|\phi_E(j)\rangle$, where E is the total energy. These correspond to plane wave relative motion of the subsystems or

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

fragments forming the channel j and also describe their internal bound states.

Amplitudes for transitions between states $|\phi_E(k)\rangle$ and $\langle\phi_P(j)|$ are determined⁶⁾ by taking matrix elements of the (post - form) rearrangement transition operator T'_{jk} :

$$T'_{jk}(E + i0) = V_j + V_j G(E + i0) V_k, \quad (7)$$

where $G(z) = (z - H)^{-1}$ is the full resolvent operator. We also define $G_i(z)$ by $G_i(z) = (z - H_i)^{-1}$; G and G_i are related by

$$G(z) = G_i(z) + G_i(z) V_i G(z) \quad (8)$$

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

We shall develop a set of coupled, integral equations for the T'_{jk} [this can also be done for the (prior-form of the) operators⁶⁾ $\hat{T}'_{jk} = V_k + V_j G V_k$, but is not necessary for this development]. If we set $i = k$ in (9) and substitute it in (7), we get ($z = E + i0$)

$$T'_{jk}(E + i0) = V_j + T'_{jk}(E + i0) G_k(E + i0) V_k. \quad (10)$$

This is a standard⁶⁾ integral equation for T'_{jk} which suffers from the familiar drawback of not being connected; in addition, it does not have an analytic behavior that leads to the correct unitarity relation. In order to write out a more appropriate equation, we introduce the $N \times N$ channel coupling array, whose elements are initially restricted only by

$$\sum_{i=1}^N W_{il} = 1 = \sum_{i=1}^N W_{li}. \quad (11)$$

Multiplying both sides of (8) by W_{li} and summing on i gives

$$G(z) = \sum_{i=1}^N W_{li} [G_i(z) + G_i(z) V_i G(z)] \quad (12)$$

where the index l may be chosen at our convenience.

Equation (12) partitions $G(z)$ over all the arrangement channels. The elements W_{li} will determine which channels are explicitly coupled together.

Substitution of (12) into (10) gives

$$\begin{aligned} T'_{jk}(E + i0) = & V_j + V_j \sum_i W_{li} G_i(E + i0) (V_k - V_i) \\ & + V_j \sum_i W_{li} G_i(E + i0) T'_{ik}(E + i0). \end{aligned} \quad (13)$$

The key point in the derivation is now to notice that $T'_{jk}(E + i0)$ will always act on

states $|\phi_E(k)\rangle$, so that Lippmann's²¹⁾ equality can be used:

$$G_1(E + i0)(V_k - V_i) = \delta_{ik} - 1 \equiv -\bar{\delta}_{ik} \quad , \quad (14)$$

when acting on initial two-body states $|\phi_E(k)\rangle$. Use of (14) in (13) leads to

$$T_{jk}^-(E + i0) = V_j W_{jk} + V_j \sum_i W_{ji} G_1(E + i0) T_{ik}^-(E + i0) \quad . \quad (15)$$

We now define new operators $T_{jk}(z)$ which obey (15) for all z , and equal the $T_{jk}^-(E + i0)$ for $z = E + i0$:

$$T_{jk}(z) = V_j W_{jk} + V_j \sum_i W_{ji} G_1(z) T_{ik}(z) \quad . \quad (16)$$

Eq. (16) is the desired result. In matrix form it reads

$$T(z) = \mathcal{V} + \mathcal{V} \mathcal{G}(z) T(z) \quad (17)$$

where $\mathcal{V}_{ij} = V_i W_{ij}$, $\mathcal{G}_{ij}(z) = \delta_{ij} G_1(z)$. The preceding derivation, because it relies on eq. (14), has been questioned. However, not only is (14) a valid result when $|\phi_E(k)\rangle$ is a two body state, but as noted above, we have recently derived eq. (15) directly from the Schrödinger equation, without making use of (14) at all, thus justifying (though unnecessarily) our use of (14). However, when $|\phi_E(k)\rangle$ is not a two-body state, (14) no longer holds, and different equations result. We shall not consider such cases here.

The structure of (17) is such that the operators $T_{jk}(z)$ can satisfy the six conditions stated above. Let us consider connectedness first. The kernel of (17) is $\mathcal{V}\mathcal{G}(z)$, whose matrix element is $V_i W_{ik} G_k(z)$. By proper choice of the elements of W , a connected, iterated kernel can be obtained. For the 3-body problem, we have found a choice such that the first iterate of $\mathcal{V}\mathcal{G}(z)$ is connected¹⁵⁾, as in the Faddeev formalism. For arbitrary N , we have found a general class of $(N-1)!$ W 's denoted channel permuting arrays (CPA), such that the $(N-1)$ st iterate of the kernel is connected¹⁴⁾. Tobocean²²⁾ first gave a prescription for choosing a W that would guarantee that the $(N-1)$ st iterate of $\mathcal{V}\mathcal{G}$ was connected; his prescription is an example of a CPA. The general method for specifying W in this case is to set $k = j$ in (16) and then select N of the $W_{ij} = 1$ (all others = 0), one in each row and column with rows and columns linked successively, as follows:

$$\begin{aligned} W_{ii} &= 0 \quad , \\ W_{ij} &= 1 \text{ or } W_{ji} = 1 \text{ but not both,} \\ W_{lm} &= 1 \rightarrow W_{mn} = 1 \quad . \end{aligned}$$

The first two conditions prevent only one or two T_{jk} being coupled together, while the last helps ensure connectedness of the $(N - 1)$ st iterate. The channel permuting W 's are such that $(W^N)_{ij} = \delta_{ij}$. It is easy to see that, although each of the $(N - 1)!$ CPA's is a representation of the permutation group of order N , these W 's (along with the N unit matrix) form neither a group nor a semi-group except for the cases $N = 2$ and $N = 3$.

We shall not give the proofs that the CPA's guarantee connectedness of the $(N - 1)$ st iterate or that there are $(N - 1)!$ of them. Instead we give a few examples and then write out the general set of equations for a specific choice. For $N = 2$ and 3 , the following are the (unique) CPA's:

$$\sqrt{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}, \quad \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

In the general case, we select as the initial channel $k = 1$; for W_{ij} we choose^{14,22)} $W_{ij} = \delta_{j,i+1}$, $1 \leq i \leq N-1$; $W_{N1} = 1$; all others equal zero. Eq. (16) becomes

$$\begin{aligned} T_{11}(z) &= V_1 G_2(z) T_{21}(z) \\ T_{21}(z) &= V_2 G_3(z) T_{31}(z) \\ &\vdots \\ T_{N-1,1}(z) &= V_{N-1} G_N(z) T_{N1}(z) \\ T_{N1}(z) &= V_N + V_N G_1(z) T_{11}(z) \end{aligned} \quad (18)$$

Equation (18) is not in the usual form of coupled equations we are familiar with; nevertheless, it is a valid form. In particular, the symmetrized version of (18) has yielded unitary, S-wave $e^- + N$ scattering amplitudes while another set, similar to but not identical with (16), gave explicitly non-unitary amplitudes in the same problem¹⁶⁾. These results have been interpreted¹⁷⁾ in light of the existence of the K operator and damping equations corresponding to (17) and their lack in other formulations of many-body scattering, even those utilizing the W array²²⁾.

Before commenting on the unitarity properties of our equations, we consider a further point connected with the specific set (18), viz, only the last equation appears to have a Born term. This is, of course, only an apparent lack, since it is evident that by back substitution, the N equations of (18) may be decoupled, and each of them will display driving terms.

Before displaying the uncoupled equation for T_{11} , it is necessary to consider some analytic properties of our equations, since they are not yet in a form which properly

takes account of unitarity restrictions. Eq. (16) [or (17)] is obtained from (15) simply by replacing $E + i0$ by z . We wish to determine if the matrix $\mathcal{G}(z)$ has the same analytic properties as the collection of its matrix elements $\{G_i(z)\}$, each taken individually. The answer is no: as shown in a paper contributed to this Conference²³⁾, the resolvent $G_i(z)$ behaves differently when considered as an integral part of the equations for $T(z)$ [recall $\mathcal{G}_{ij}(z) = G_i(z)\delta_{ij}$] than when examined in isolation. The difference becomes noticeable when examining the discontinuity of $\mathcal{G}(z)$, $D\mathcal{G}(z)$, across the right hand cuts. Unless special precautions are taken, there will be multiple contributions from cuts occurring in more than one of the $G_i(z)$. Since $D\mathcal{G}(z) = 2i \operatorname{Im} \mathcal{G}(z)$, multiple counting is avoided by the simple device of multiplying each $G_i(z)$ by the projection operator $P(i)$ onto the set of bound internal states in channel i :

$$\operatorname{Im} \mathcal{G}_{ij}(z) \rightarrow \operatorname{Im} \tilde{\mathcal{G}}_{ij}(z) \equiv \delta_{ij} [\operatorname{Im} G_i(z)] P(i).$$

By Cauchy's theorem, we also find²³⁾

$$\operatorname{Re} \mathcal{G}_{ij}(z) \rightarrow \operatorname{Re} \tilde{\mathcal{G}}_{ij}(z) \equiv \delta_{ij} [\operatorname{Re} G_i(z)] P(i) ,$$

so that we may in general replace $\mathcal{G}(z)$ in eq. (17) by $\tilde{\mathcal{G}}(z)$, where

$$\tilde{\mathcal{G}}_{ij}(z) = \delta_{ij} G_i(z) P(i) \equiv \delta_{ij} \tilde{G}_i(z) . \quad (19)$$

This means that $T(z)$ is now defined by

$$T(z) = \mathcal{V} + \mathcal{V} \tilde{\mathcal{G}}(z) T(z) , \quad (20)$$

thus ensuring that $T(z)$ obeys the proper unitarity relation²⁴⁾, viz.,

$$\operatorname{Im} T(E + i0) = -\pi T(E + i0) \tilde{\Delta}(E) T(E - i0) , \quad (21)$$

where $\tilde{\Delta}_{ij}(E) = \delta_{ij} \delta(E - H_j) P(j)$. The change $\mathcal{G}(z) \rightarrow \tilde{\mathcal{G}}(z)$ is, as we have shown²⁴⁾, consistent with the effective orthogonality conditions found by Rahn to hold in multi-particle scattering²⁵⁾.

In the form (17), $T(z)$ has the solution $T(z) = \mathcal{V} + \mathcal{V} \mathcal{Y}(z) \mathcal{V}$, where $\mathcal{Y}(z) = [\mathcal{G}^{-1}(z) - \mathcal{V}]^{-1}$. In addition, a matrix of K operators had been introduced^{14,15)} through $K(E) = \mathcal{V} + \mathcal{V} \mathcal{G}^P(E + i0) K(E)$, where $\mathcal{G}^P(E + i0) = \operatorname{Re} \mathcal{G}(E + i0)$, such that T and K were related by the damping equation^{14,13)} $T(E + i0) = K(E) - i\pi K(E) \Delta(E) T(E + i0)$.

e, $\Delta_{ij}(E) = \delta_{ij} \delta(E - H_j)$, so that $\tilde{\Delta}_{ij}(E) = \Delta_{ij}(E) P(j)$. This latter damping equation is incorrect, since there is multiple counting of the contributions from many of the unitarity cuts. With the new results, we find $T(z) = \mathcal{V} + \mathcal{V} \tilde{\mathcal{Y}}(z) \mathcal{V}$, where $\tilde{\mathcal{Y}}(z) = [\tilde{\mathcal{G}}^{-1}(z) - \mathcal{V}]^{-1}$, and also new K -operator equations and damping relations:

$$K(E) = \mathcal{V} + \mathcal{V} \tilde{G}^P(E + i0) K(E) \quad (22)$$

nd

$$T(E + i0) = K(E) - i\pi K(E) \tilde{A}(E) T(E + i0) \quad (23)$$

Eq. (23) is clearly compatible with the unitarity relation (21), while eq. (22) allows for the introduction of unitary approximations in a simple way.

The implication of this modification is that in carrying out calculations, only bound internal states of the subsystems in each channel need be considered as intermediate states. The effects of a two-body breakup (continuum) state of one of the subsystems in an m -body channel are included in the contributions from bound states in an $(m + 1)$ -body channel. As a result, the complexity of calculations can be greatly reduced. There is another point of interest in this connection. Our method counts contributions from unitarity cuts correctly by restricting the $G_1(z)$ as above. The same effect is obtained in other many-body scattering theories⁷⁻¹¹ by the device of using the n -body, free-particle Green's function $G_0(z) = (z - H_0)^{-1}$ only, but with the entire collection of 2-, 3-, $(n - 1)$ -body t operators, which latter have the effects of all cuts other than the n -body free-particle one built in.

With the preceding modification, we may now consider the uncoupled equations for T_{11} , obtained by back-substitution of the equations from (18), modified by $G_1 \rightarrow \tilde{G}_1$. The result is:

$$T_{11}(z) = U_1^{(N)}(z) [1 + \tilde{G}_1(z) T_{11}(z)] \quad (24)$$

where

$$U_1^{(N)} \equiv V_1 \tilde{G}_2(z) V_2 \tilde{G}_3(z) V_3 \dots \tilde{G}_N(z) V_N \quad (25)$$

is a quantity we have denoted¹⁵ the direct-channel, optical-potential operator. It is a z -(energy-) dependent, complex, non-local, connected operator, expressing the physical result that flux may go into channels other than $k = 1$. This has interesting implications for the theory of the optical model; in particular, even if the energy is too low to excite states in channel 1, it may be possible to have transitions to states in channels other than $j = 1$, as for example in (d,p) reactions. In such cases, the optical potential will be complex even though in channel 1 only the ground state can be seen experimentally.

We now turn to the question of the effects of the Pauli principle. We have recently studied a model identical-particle problem in which one particle is scattered by a system of $(n - 1)$ identical particles under the condition that the final state consists of $(n - 1)$ particles bound together plus one free particle²⁴. In this case, channel labels are identical to particle labels, and the amplitude is given, for

ample, as matrix elements of the operator $\tilde{T} = T_{11} - (n - 1)P_{21}T_{21}$, where 1 (or 2) labels the unbound particle and P_{21} is the two-particle transposition operator. In this notation, 1 is the "direct" channel and 2 is the "exchange" channel. An integral equation for $\tilde{T}$ based on eq. (16) and the symmetry of the problem is²⁴

$$\tilde{J} = [V_1 W_{11} - (n-1)P_{21}V_2 W_{21}](1 + \tilde{G}_1 \tilde{J}) \quad (26)$$

where the energy dependence is suppressed. For the case $n = 2$, (26) reduces to the general form of the equation solved in the $e^- + H$ case which gave unitary amplitudes¹⁶⁻¹⁸⁾. The preferred choice for W_{ij} is $W_{11} = 0$, $W_{21} = 1$, although other values are allowed in this case because of the presence of $\tilde{G}_1$. For this choice, the "direct" driving term $V_1 W_{11}$ vanishes, leaving only the exchange term in (26). The results of approximate $e^- + H$ calculations based on (26) for the case $n = 2$, $V_1 = -e^2/r_1 + e^2/r_{12}$, are very encouraging, despite the lack of the usual Born term when $W_{11} = 0$. We emphasize that these equations, despite a possible superficial resemblance to the more familiar Hartree-Fock type of coupled equation used in electron-atom scattering²⁶⁾, are in fact not only different in appearance, but represent a completely different approach to the physics of identical particle scattering problems. The results presented below for low energy $e^- + H$ scattering parameters calculated in the approximation of retaining only the 1s hydrogenic ground state as an expansion basis for evaluating $\tilde{G}_1$ are corroborative evidence for this conclusion.

The first calculations done for the $e^- + H$ system that gave unitary amplitudes using the W array were¹⁶⁾ for the values $W_{11} = 0$, $W_{21} = 1$ - $W_{11} = 1$. Singlet and triplet phase shifts from this and other calculations are compared in Tables 1 and 2. The results are seen to compare extremely well with the phase shifts computed from both the close-coupling approximation²⁷⁾ and the (lower bound) variational method²⁸⁾. For a detailed discussion see ref. 16 and 17.

Given these successes, additional low energy computational studies were made, in particular to examine the dependence of the singlet and triplet $e^- + H$ scattering lengths and $E = 0.1$ Rydberg phase shifts on W_{11} . A representative set of results is given in Table 3 for the scattering lengths $a^\pm$ (defined here as $\lim_{k \rightarrow 0} [+k \cot \eta^\pm]^{-1}$, where $\eta^\pm$ (η^-) is the singlet (triplet) phase shift). The preferred choice of $W_{11} = 0$ is indicated by an asterisk, and results of several other calculations are included for comparison. Notice that a^+ and a^- must be considered together when examining these results, since we see that variation of W_{11} can yield a value for either one of $a^\pm$ close to, or even less than, Schwartz's variational result²⁸⁾ while the other value ($a^\mp$) can then be arbitrary, both in magnitude and sign. (Schwartz's (upper bound) values are generally regarded as the biblical numbers against which all other calculations are to be measured.) The best pair occurs for the preferred values $W_{11} = 0$, $W_{21} = 1$.

More detailed results are given in Figure 1 for a^+ ($-0.3 \leq W_{11} \leq 1.3$) and in Figure 2 for a^- ($-0.3 \leq W_{11} \leq 1.4$). The use of W_{11} can be thought of as providing, in certain sense, an effective-potential description of the scattering. The points A are where this effective potential turns from repulsive to attractive, while the singular points occur at the onset of a bound state at zero energy. The behavior for

large, negative W_{11} seems smooth; analytic fits to these curves, extrapolated to $W_{11} = -\infty$ show no indication of further poles or zeros. It is tempting to associate the pole in a^+ with the well-known H^- , singlet bound state, but the occurrence of a pole in a^- where no bound, triplet H^- states exist, makes this association, at present, merely an interesting speculation. The $E = 0.1$ Rydberg phase shifts $\eta^\pm$ are shown in Figures 3 and 4. Their behavior corresponds quite closely to that of $a^\pm$; in particular, $\eta^\pm$ goes to zero at the points A where $a^\pm$ changes sign. A more detailed discussion of these calculations is given in ref. 18; other calculations, both for the $e^- + H$ and for the nuclear 3-body systems are in progress. As noted above, the results presented here are favorable numerical evidence that our method, even though it leads to unfamiliar equations, is a promising means for treating multi-channel scattering problems.

* Alfred P. Sloan Foundation Fellow, 1972-74; Alexander von Humboldt-Stiftung Senior Fellow, 1973-74. Permanent address: Departments of Chemistry and Physics, University of Houston, Houston, Texas 77004.

† Work supported in part by the U.S. Atomic Energy Commission. Address until June, 1975: Physics Department, University of Surrey, Guildford, Surrey GU2 5XH, England.

References

1. R. D. Amado, in *Elementary Particle Physics and Scattering Theory*, ed. by M. Chretien and S. S. Schweber (Gordon and Breach, New York, 1970).
2. P. Federbush, *Phys. Rev.* 148 (1966) 1551.
3. R. G. Newton, *Phys. Rev.* 153 (1967) 1562; J. V. Noble, *ibid.*, 148 (1966) 1553; 161 (1967) 1495.
4. L. D. Faddeev, *Sov. Phys.-JETP* 12 (1961) 1014; *Mathematical Aspects of the Three-Body Problem* (D. Davey and Co., New York, 1965).
5. H. Eckstein, *Phys. Rev.* 101 (1956) 880.
6. R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).
7. E. O. Alt, P. Grassberger, and W. Sandhas, *Nucl. Phys.* B2 (1967) 181.
8. O. A. Yakubovski, *Sov. Journ. Nucl. Phys.* 5 (1967) 937.
9. G. Bencze, *Nucl. Phys.* A210 (1973) 568.
10. B. R. Karlsson and E. M. Zeiger, *Phys. Rev.* D9 (1974) 1761.
11. E. Redish, *Phys. Rev.* C10 (1974) 67.
12. R. T. Cahill, *Nucl. Phys.* A194 (1972) 599.
13. K. L. Kowalski, *Phys. Rev.* D5 (1972) 395; D6 (1972) 3705; D7 (1973) 1806.
14. D. J. Kouri and F. S. Levin, *Bull. Am. Phys. Soc.* 19 (1974) 489; *Phys. Letts.* 50B (1974) 421.
15. D. J. Kouri and F. S. Levin, submitted for publication.
16. D. J. Kouri, M. Craigie and D. Secrest, *J. Chem. Phys.* 60 (1974) 1851.
17. D. J. Kouri, F. S. Levin, M. Craigie, and D. Secrest, *J. Chem. Phys.* 61 (1974) 17.
18. D. J. Kouri, F. S. Levin, M. Craigie, and D. Secrest, submitted for publication.
19. Y. Hahn, D. J. Kouri, and F. S. Levin, *Phys. Rev. C*, (in press) October, 1974.
20. Y. Hahn, *Phys. Rev.* 169 (1968) 794; *Nucl. Phys.* A132 (1969) 353; Y. Hahn and K. M. Watson, *Phys. Rev.* A5 (1972) 1718.
21. E. A. Lippmann, *Phys. Rev.* 102 (1956) 256.
22. W. Tobocman, *Phys. Rev.* C9 (1974) 2466.
23. D. J. Kouri and F. S. Levin, Unitarity Modifications of the Coupled Channel T and K Operators for Many-Body Scattering (Proceedings of this Conference), and Ref. 24.
24. D. J. Kouri and F. S. Levin, submitted for publication.
25. Y. Hahn, *Physics Letters*, 30B (1969) 595; *Phys. Rev.* C3 (1971) 1432.
26. Eg., N. F. Mott and H. S. Massey, *Theory of Atomic Collisions*, 3rd edition, (Oxford Univ. Press, Oxford, 1964).
27. P. G. Burke and K. Smith, *Rev. Mod. Phys.* 34 (1962) 458.
28. C. Schwartz, *Phys. Rev.* 124 (1961) 1468.

Table 1

Singlet $e^- + H$ Phase Shifts					
E(Ryd)	Hartree ²⁷⁾	Static-Exchange ²⁷⁾	Close-Coupled ²⁷⁾	W Array ¹⁶⁾	Variational ²⁷⁾
0.01	0.721	2.396	2.491	2.541	2.553
0.04	0.973	1.871	1.974	2.039	2.067
0.09	1.046	1.508		1.646	1.696
0.25	1.045	1.031	1.082	1.080	1.202
0.36	1.021	0.869	0.93	0.871	1.041

Table 2

Triplet $e^- + H$ Phase Shifts					
E(Ryd)	Hartree ²⁷⁾	Static-Exchange ²⁷⁾	Close-Coupled ²⁷⁾	W Array ¹⁶⁾	Variational ²⁷⁾
0.01	0.730	2.908	2.935	2.935	2.939
0.04	0.973	2.679	2.715	2.737	2.717
0.09	1.046	2.461	2.50	2.554	2.500
0.25	1.045	2.070	2.096	2.264	2.105
0.36	1.022	1.901	1.92	2.170	1.933

Table 3

Dependence of $e^- + H$ Scattering Lengths on W_{11}		
W_{11}	a^+	a^-
-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
Strong coupling ²⁷⁾	7.5	2.33
Close coupling ²⁷⁾	6.74	1.89
Variational ²⁷⁾	5.96	1.77

FIG. 1

FIG. 2

FIG. 3

FIG. 4