

Arrangement-channel quantum mechanics: A general time-dependent formalism for multiparticle scattering

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A general time-dependent formulation of many-body, multichannel scattering using the channel-coupling-array theory is presented. The formalism is based on the use of the channel-component states, previously introduced by Hahn, Kouri, and Levin. These states obey a set of non-Hermitian matrix equations, the non-Hermiticity arising from the presence of the channel-coupling array W . Despite the lack of Hermiticity, it is shown that the eigenvalues will always be real if the channel-component states obey a fixed-phase convention under time reversal. Use of the channel-component states leads in a straightforward way to an interaction picture and a single S operator. The analog of the usual two-body (single-channel) result connecting the time-dependent and time-independent descriptions is demonstrated. It is also shown that the channel-component states have the remarkable property that only the component in channel j gives rise to (two-body) outgoing waves in that channel: Components in channels $m \neq j$ do not yield outgoing waves in channel j . This is explicitly seen from the time-dependent development, but is inherent in the time-independent description. Such a property is known for the Faddeev decomposition in the three-body case; the present work extends and generalizes this result for the case of an arbitrary number of particles. In particular, the present formulation is seen to yield precisely the Faddeev equations for the three-body problem.

I. INTRODUCTION

In this article, we present a time-dependent formulation of many-body scattering based on the channel-coupling-array theory.¹ Unlike much of the earlier work involving this theory, where the coupled equations for the various transition operators were emphasized,^{1,2} the approach followed here uses the wave-function decomposition into *channel components* introduced by Hahn, Kouri, and Levin.³ Two major conclusions are reached. First, and in contrast to previous expectations,⁴ an interaction picture for multichannel scattering can be formulated. This immediately leads to a single S operator for rearrangement collisions. Second, in the limit $t \rightarrow \infty$, it is shown that only the j th channel component of the wave function contributes to the amplitude for transitions to two-body states in channel j . This is in contrast to the result based on an analysis using the complete Schrödinger wave function which contributes to the scattering in every channel.

The study of time dependence given herein is abstract, in that various choices of the channel-coupling array W are not introduced, except as illustrative examples in Secs. III A and V. Specific realizations of the W 's, and their concomitant sets of coupled equations for transition op-

erators and wave functions, are given elsewhere.¹⁻⁶ Our purpose here is to develop a general time-dependent formulation which will hold for any choice of W , although applications will involve only those W leading to connected kernel equations.

In previous work, discussion of wave functions has mainly concerned the properties of the *channel-scattering states*,⁵ which have been shown to be equal to the Schrödinger state when W is chosen to be a channel-permuting array.⁵ Although this feature allows one to establish some interesting properties of the channel-scattering states (e.g., Ref. 5 and Sec. II B), the fact that each channel-scattering state contributes to the scattering in every channel makes them less useful for our present purposes than the channel-component states. Hence our main development is based on these latter states. A discussion of relevant properties of each kind of state is given in Sec. II.

The channel-component states obey³ a set of coupled equations with a non-Hermitian Hamiltonian matrix H : $H^\dagger \neq H$. It is therefore important to work only with eigenvalues of H that are real. We show in Sec. III that if H is invariant under rotations and time reversal, and the phases of the time-reversal channel-component states are fixed, then H has *real* eigenvalues. This is the key to

further development, especially the introduction of the Schrödinger and interaction pictures, also introduced in Sec. III.

Section IV is devoted to a proof that the channel-component states behave asymptotically as described above, and then to establishing an S operator for the multichannel case. Section V summarizes and discusses the results of this paper.

A few remarks on conceptual aspects of this paper may, in addition to the preceding comments on organization, be appropriate at this point. The theory derived in this work is based on a non-Hermitian matrix formulation of many-body scattering theory. This should not come as a surprise to anyone familiar with recent developments in this field, beginning with the pioneering work of Faddeev, since it is possible to transform many of the equations derived so far for various (three-, four-, ..., N -body) transition operators into non-Hermitian, time-independent equations for wave functions or state vectors of one kind or another. Because we are interested specifically in time dependence, we work with state-vector (wave-function) components, and the non-Hermiticity occurs almost *ab initio*. The W -array method is, we believe, a "natural" way of doing this because of its generality.^{1-3,5} However, the introduction of *any* correct, connected, non-Hermitian, time-dependent theory of many-body scattering seems to us to be in itself a natural procedure, in the following sense. The Schrödinger equation for an n -body system is not a very suitable equation for describing multichannel effects, a point emphasized by the various approaches to n -body scattering theory based on T -matrix rather than the Schrödinger equation methods. Since Schrödinger methods are not easily extended (at least directly) to include multichannel effects, schemes that do so, even if they involve non-Hermiticity, are of interest. Introducing non-Hermitian matrix methods clearly enlarges the arena in which results can be sought. In order to ensure contact with ordinary quantum mechanics as well as to avoid certain ill-defined limits (see Sec. IIIA), one must endeavor to select a particular subset of results in the enlarged space corresponding to the non-Hermitian H , viz., those solutions with real eigenvalues. It is not hard to prove³ that any *exact* solution of the H problem is also a solution of the Schrödinger (\bar{H}) problem, so that eigenvalues will indeed be real. As insurance, particularly in the case of approximate solutions, we show in Sec. III that imposition of the usual symmetries of time-reversal and rotational invariance that are assumed to hold for H guarantees that the eigenvalues of \bar{H} are indeed real. Since for remote times in the past (exact or approximate) initial

states can be generated which are well defined under these two symmetry operations, then a one-to-one correspondence with ordinary quantum mechanics is maintained, and the present theory provides a satisfactory time-dependent description of many-body scattering. It is this fact, coupled with the multichannel nature of the description, that causes us to believe that the non-Hermitian matrix approach is a "natural" one.

The main body of this paper begins with a very brief summary of previous results from the channel-coupling-array theory that are relevant. Even though our development is based exclusively on the channel-component states, we discuss both them and the channel-scattering states. This is done mainly for contrast but also to develop certain interesting results and to establish procedural methods based on what are probably more familiar aspects of the channel-coupling-array theory. Readers for whom such a review is unnecessary or who wish to follow the development of channel-component states only may skip immediately to Eq. (17) or possibly even to Sec. III. That is, the matrix notation of Eqs. (25)–(31) and Eqs. (32)–(34) could be regarded as providing the basic theoretical foundation. It is interesting to note that Eqs. (21) and (22) lead to a complex scheme of coupled, second-order, integro-differential radial equations with specific boundary conditions, for which existence theorems may be hard to prove. If instead we consider the first-order equation (34) as the starting point, with the boundary condition (53), then proof of an existence theorem is not a problem. Furthermore, from (72) we have that the desired solution to (21) and (22) is just the solution to (34) at $t=0$, thereby finessing the potential existence theorem problems connected with the time-independent equations.

Finally, we note that the theory is formulated mainly in terms of plane-wave relative motion states of sharp energy E . In actuality, the strong limit procedures of Secs. III and IV require that the initial states be represented by wave packets rather than plane waves. We shall only resort to wave packets where necessary by implication, preferring to present results based on the less rigorous but didactically simpler notion of plane waves. Places where rigor would require wave packets are noted in the text.

II. PRELIMINARIES

A. Transition operators

State vector equations have been introduced in the channel-coupling-array theory in two ways, corresponding to the integral equations for the transition operators $T_{jR}(z)$ and $\bar{T}_{jR}(z)$ discussed in

previous work.^{1,5} These latter equations are

$$T_{jk}(z) = V_j W_{jk} + V_j \sum_m W_{lm} G_m(z) T_{mk}(z) \quad (1)$$

and

$$\hat{T}_{jk}(z) = W_{jl} V_k + \sum_m \hat{T}_{jm}(z) G_m(z) W_{ml} V_k, \quad (2)$$

where the notation is as follows. The subscripts j, k, m, l (etc.) refer to the arrangement channels of the n particles forming the systems of interest: It is assumed that each channel is defined through its asymptotic (bound) states. Associated with these asymptotic states are partitions of the full n -particle Hamiltonian into a channel Hamiltonian and a channel perturbation as follows:

$$H = H_j + V_j = H_k + V_k = \dots \quad (3)$$

Here H_j describes the internal and unperturbed relative motion states of the m clusters forming channel j ($2 \leq m \leq n$), and V_j is the set of inter-cluster interactions, assumed to go to zero rapidly enough when the intercluster c.m. separations become infinite so as to allow asymptotic states to be defined.⁴ These asymptotic states are the internally bound eigenstates of the various channel Hamiltonians H_j . In general we write

$$H_j |\Phi_j(E)\rangle = E |\Phi_j(E)\rangle,$$

where E is the total energy.

The $G_j(z)$ are the channel- j resolvents, defined as usual by

$$G_j(z) = (z - H_j)^{-1}, \quad (4)$$

with z being a complex energy parameter. In the limit $z \rightarrow E \pm i0$ we have

$$\lim_{z \rightarrow E \pm i0} G_j(z) = G_j(\pm), \quad (5)$$

where $G_j(\pm)$ are the familiar outgoing (+) and incoming (-) wave Green's functions for channel j . Finally, the W_{ij} are elements of the channel-coupling array W , normalized in Eq. (1) to $\sum_j W_{ij} = 1$ and in Eq. (2) to $\sum_l W_{lj} = 1$. The index l occurring in Eqs. (1) and (2) is free to be chosen as is convenient. In general, the W are selected so as to lead to kernels for (1) and (2) that are connected after a finite number of iterations. For an N -channel problem, the $(N-1)!$ channel-permuting arrays (CPA's) lead to connectivity after $(N-1)$ iterations.^{1,5}

The derivation of Eqs. (1) and (2) is based on Lippmann's identity, which for (1) takes the equivalent forms^{1,2,5}

$$G_j(\pm)(V_j - V_k) = -\delta_{jk} + 1 \quad (6)$$

and

$$G_j(\pm)G_k^{-1}(\pm) = \delta_{jk},$$

while for (2) it reads

$$(V_k - V_j)G_k(\pm) = -\delta_{jk} + 1$$

and

$$G_j^{-1}(\pm)G_k(\pm) = \delta_{jk},$$

where \pm stands for $E \pm i0$ with E being the total energy. These latter sets of equations are to be interpreted as operator identities, valid only for Eq. (6) when acting to the right on two-body states $|\Phi_k(E)\rangle$ and only for Eq. (7) when acting to the left on two-body states $\langle\Phi_j(E)|$. Hence, on-shell matrix elements of $T_{jk}(+)$ and $\hat{T}_{jk}(+)$ are the transition amplitudes of interest only when k in the case of Eqs. (1) and (6) and j in the case of Eqs. (2) and (7) label two-body channels. When these requirements are not met, matrix elements of the operators $U_{jk}^{(+)}(+)$ and $U_{jk}^{(-)}(+)$ must be determined instead,⁶ where

$$U_{jk}^{(+)}(+) = \sum_m T_{jm}(+)G_m(+)G_k^{-1}(+) \quad (8)$$

and

$$U_{jk}^{(-)}(+) = \sum_m G_j^{-1}(+)G_m(+)\hat{T}_{mk}(+). \quad (9)$$

From (6) and (7), it follows that

$$U_{jk}^{(+)}(+) = T_{jk}(+)$$

when acting to the right on a state $|\Phi_k(E)\rangle$ in a two-body channel k , and

$$U_{jk}^{(-)}(+) = \hat{T}_{jk}(+)$$

when acting to the left on a state $\langle\Phi_j(E)|$ in a two-body channel j . Thus, while T_{jk} and \hat{T}_{jk} are well-defined operators through Eqs. (1) and (2), their direct interpretation as transition operators is limited as above.

B. Wave functions

1. Channel-scattering states

Let us now consider time-independent wave-function equations. We discuss the set corresponding to Eq. (1) first; it has been derived in several ways, e.g., the methods of Hahn, Kouri, and Levin² and Kouri and Levin.⁵ We shall compare the two methods, as this comparison is extremely useful for our subsequent discussion.

Proceeding directly from Eq. (1), we define channel-scattering states $|X_{mk}\rangle$ by

$$T_{jk}(+)|\Phi_k(E)\rangle = V_j \sum_m W_{im} |X_{mk}\rangle. \quad (10)$$

Operating on $|\Phi_k(E)\rangle$ with both sides of Eq. (1) (in $\lim z = E + i0$) and then using Eq. (10) in the resulting relation leads to

$$V_j \sum_m W_{jm} |X_{mk}\rangle = V_j W_{jk} |\Phi_k(E)\rangle + V_j \sum_{m,m'} W_{jm} G_m(+V_m W_{jm'}) |X_{m'k}\rangle. \quad (11)$$

The arbitrariness of the W_{jm} implies that (11) is equivalent to

$$|X_{mk}\rangle = |\Phi_k(E)\rangle \delta_{mk} + G_m(+V_m) \sum_{m'} W_{jm'} |X_{m'k}\rangle. \quad (12)$$

It is simple to show that $|X_{mk}\rangle$ of (12) asymptotically yields as a transition amplitude just the relevant on-shell matrix element of T_{mk} obeying Eq. (1).

In view of this latter remark, it is of interest to determine the relation of the $|X_{mk}\rangle$ with the scattering (Schrödinger) wave function $|\Psi\rangle$, which is that solution of $(E-H)|\Psi\rangle=0$ obeying

$$|\Psi\rangle = |\Phi_k(E)\rangle + (E+i0-H)^{-1} V_k |\Phi_k(E)\rangle. \quad (13)$$

The desired relation is

$$|\Psi\rangle = \sum_m W_{jm} |X_{mk}\rangle. \quad (14)$$

As shown in the last of Refs. 2, this is proved using Lippmann's identity (6) as well as Eq. (14) in (13), which establishes that $|X_{mk}\rangle$ of (14) also obeys (12).

Equation (14) may appear ambiguous, in that l has not been specified. We therefore take W to be a CPA; in this case,⁵ there is one value of unity in each row and column (with no repetitions and all $W_{ii}=0$). Suppose we now systematically let l run over the values 1, 2, ... up through the total number of channels coupled together. For any given l , the sum on m will be limited to only one term: that value m_l for which $W_{jm_l}=1$ (recall that $\sum_m W_{jm}=1$). It now follows that for a CPA, (14) is equivalent to

$$|X_{m_k}\rangle \equiv |\Psi\rangle, \quad \text{all } m. \quad (15)$$

That is, the *channel-scattering states* $|X_{mk}\rangle$ are each identical to the Schrödinger scattering state, and the channel subscript m is simply a *mnemonic* device indicating which complete set of eigenstates (of H_m) should be used in expanding $|\Psi\rangle$ as it appears in particular places in (12) or its differential equation equivalent, derived below.

Equation (15) is identical to a similar result proved earlier,⁵ also in the context of CPA's. However, notice that (15) will hold for any W having only one value of unity in each row and column with no repetitions. Thus, even for a W not leading to connected equations, such as the unit matrix, Eq. (15) still holds.

Equation (12) is a set of coupled equations, which,

when written out in detail with $k=1$ and all $|X_{m_1}\rangle$ replaced by $|\Psi\rangle$ reads $(\sum_m W_{jm}=1)$

$$\begin{aligned} |\Psi\rangle &= |\Phi_1(E)\rangle + G_1(+V_1) |\Psi\rangle, \\ |\Psi\rangle &= G_2(+V_2) |\Psi\rangle, \\ |\Psi\rangle &= G_3(+V_3) |\Psi\rangle, \\ &\dots \end{aligned} \quad (16)$$

In this form, the coupled equations obeyed by $|X_{mk}\rangle = |\Psi\rangle$ may be more familiar. For the three-body problem, (16) is precisely the set of three two-body equations shown by Glöckle⁷ to specify $|\Psi\rangle$ uniquely. For an arbitrary number of particles n , it is the set proposed by Tobocman² as a basis for analyzing multichannel nuclear reactions. It is also a set discussed by Sandhas⁸ as providing a unique solution to the n -body scattering problem. In differential form, obtained by multiplying both sides of the i th equation in (16) by $G_i(+)^{-1}$, it is the set of coupled equations derived by Kouri and Levin⁵ for n -particle, N -two-body-channel scattering.

Equation (16) is *not* the set we shall consider as the basis for our time-dependent description of the next section, because the identification $|X_{mk}\rangle = |\Psi\rangle$ means that each $|X_{mk}\rangle$ of (14), since it is the full Schrödinger wave function, lacks the special asymptotic property we derive below for the channel-component states $|\psi_j\rangle$ [Eq. (78)]. We have presented the preceding analysis partly as a guide to a similar one in the next section, and partly to make explicit the fact that the $|X_{mk}\rangle$ are an alternate to, although for our present purposes less useful than, the set of channel-component states $\{|\psi_j\rangle\}$ introduced below: There is more than one way, for arbitrary W , to introduce wave functions, and the properties of these different wave functions will differ, as we shall see. We comment here on two aspects of the set (16). The first is the question of uniqueness: What is the minimum number of equations needed for an n -particle problem to ensure that $|\Psi\rangle$ as defined by (16) is unique? For $n=3$, the answer is three, viz., the set of three two-body-channel equations, as was shown by Glöckle.⁷ Because of the use of Lippmann's identity in deriving (12) from (1) via (10) and also from (13), this answer is correct only when $|\Phi_1(E)\rangle$ is an initial state in a two-body channel, but we shall assume only such initial states in this discussion. The logical extension of Glöckle's result to the case of arbitrary n is that (16) must contain at least the N_2 equations corresponding to the set of N_2 two-body channels. To our knowledge, a rigorous proof of this statement, for example along the lines of Glöckle's proof, has not been given. That the set of N_2 two-body channels is the mini-

mum number is strongly implied by the analysis of Benoist-Gueutal,⁶ who showed that the $T_{jk}(z)$ would not satisfy unitarity if the set of defining equations (1) were smaller in size than $N_2 \times N_2$, as above. Since (16) uniquely leads to (1), the implication is thereby established. Unfortunately, a connection between unitarity (i.e., the discontinuity relation) and uniqueness has not been demonstrated; a rigorous proof would thus be an interesting result to derive.

The set (16) has been obtained essentially by use of an off-shell transformation, viz., Lippmann's identity, Eq. (6). While this fact seems not to have been recognized previously, it is of no consequence when exact solutions to (16) are determined, since they yield as amplitudes precisely the correct, on-shell matrix elements of the $T_{jk}(+)$ of Eq. (1). However, when only approximate solutions are, or can be, obtained, Lippmann's identity plays a different role. One particular consequence of it is that in most channels, when one-body distorting (optical) potentials are introduced, the lowest-order contribution to the approximate amplitude will *not* be the distorted wave Born approximation, even though multistep processes will be included (in higher-order contributions) in an approximate way. The effects of Lippmann's identity on exact and approximate amplitudes will be discussed in detail in a forthcoming article,⁹ but it is useful to recall that approximate solutions of (16) need not yield standard results.

2. Channel-component states

The channel-scattering states $|X_{mk}\rangle$, because they each are equal to the Schrödinger wave function $|\Psi\rangle$, must asymptotically contain outgoing waves in all channels. As such, the $|X_{mk}\rangle$ and Eq. (16) are not the most convenient quantities to consider for the purposes of a time-dependent development of many-body scattering. We choose instead to work with the *channel-component states* $|\psi_j\rangle$, first introduced in the present context by Hahn, Kouri, and Levin,³ although these states are analogous to similar ones used earlier by Eyges,¹⁰ Hahn,¹¹ and Diestler and Krüger.¹² As in Sec. IIB1 two derivations of the equations obeyed by the $|\psi_j\rangle$ are given, one starting from the Schrödinger equation, the other based on Eq. (2). The former derivation slightly generalizes that given in Ref. 3, and we begin with it.

The Schrödinger equation is

$$(E - H)|\Psi\rangle = 0. \quad (17)$$

In view of the partitionings (3), we seek an expansion of $|\Psi\rangle$ into channel-component states $|\psi_j\rangle$ via

$$|\Psi\rangle = \sum_j |\psi_j\rangle, \quad (18)$$

with the channel subscript j corresponding, in a manner to be determined subsequently, to the partition $H = H_j + V_j$. No orthonormality assumption is made about the $|\psi_j\rangle$; in fact, we fully expect that $\langle\psi_j|\psi_k\rangle \neq 0$, $j \neq k$. Note that, unlike (14), Eq. (18) expresses $|\Psi\rangle$ as a linear combination of the $|\psi_j\rangle$ without intervening weights [i.e., no elements of a W array occur in (18)].

Substituting (18) into (17) yields

$$\sum_j (E - H_j - V_j)|\psi_j\rangle = 0, \quad (19)$$

where $H = H_j + V_j$ has been used. Introducing the elements W_{mi} obeying $\sum_m W_{mi} = 1$ allows V_j to be written as

$$V_j = \sum_m W_{mi} V_i,$$

so that (19) is equivalent to

$$\sum_j \left[(E - H_j)|\psi_j\rangle - \sum_m W_{ji} V_m |\psi_m\rangle \right] = 0, \quad (20)$$

where in the double summation, there has been a relabeling of subscripts. The $|\psi_j\rangle$ are now *defined* to be that solution of (20) obeying

$$(E - H_j)|\psi_j\rangle = \sum_m W_{ji} V_m |\psi_m\rangle, \quad (21)$$

subject to the outgoing-wave boundary conditions implied by

$$|\psi_j\rangle = |\Phi_k(E)\rangle \delta_{jk} + G_j(+) \sum_m W_{ji} V_m |\psi_m\rangle, \quad \text{all } j. \quad (22)$$

Before relating this latter set of equations to those derived directly from Eq. (2), we note several points. Equation (21) is a generalization of the set of equations derived in Ref. 3, to which it reduces simply by choosing $l = m$ in each term of the sum on the right side of (21). The arbitrariness in l allows this to be done. Second, Eq. (22) differs from Eq. (12) in what may appear to be a minor matter, viz., $W_{ji} V_m$ in (22) is replaced by its transpose in (12). However, as we shall see, this difference is a profound and important one, since $|\psi_j\rangle \neq |X_{jk}\rangle$. Third, the derivation of (22) has not employed Lippmann's identity, and so it might be regarded as a more fundamental set than (12) or even (16). We now show, starting from Eq. (2), which does depend on Eq. (7), that (22) leads to the operators \hat{T}_{jk} . Because of this, Eq. (22) cannot be regarded as more fundamental than (12).

The derivation of (22) from (2) proceeds in two stages. First we note that Eq. (2) defines the same set of operators $\{\hat{T}_{jk}\}$ as does

$$\hat{T}_{jk}(z) = W_{ji}V_k + \sum_m W_{ji}V_m G_m(z) \hat{T}_{mk}(z). \quad (23)$$

Proof of the equivalence of (22) and (23) follows the method given in Sec. IV of Ref. 5 and we do not repeat it here. The second stage of the derivation parallels that given in Sec. II B 1 for Eq. (12). We introduce $|\psi_i\rangle$ via

$$\hat{T}_{jk}(+)|\Phi_k(E)\rangle = \sum_i W_{ji}V_i|\psi_i\rangle, \quad (24)$$

substitute (24) into (23), and then use the arbitrariness of the W_{ji} to obtain Eq. (22). This is an *a posteriori* justification for using the symbols $|\psi_i\rangle$ in (24). It should be clear by inspection that the set of integral equations (23) for the \hat{T}_{jk} is obtained from (22) by the simple off-shell expansion $E + i0 - z$.

In the sense of also providing amplitudes which involve Lippmann's identity, the sets (21) and (22) cannot be considered to be more fundamental than Eqs. (12) or (16). They are merely an alternate form, which if solved exactly yield the \hat{T}_{jk} , and we already know from Ref. 5 that exact, on-shell matrix elements of $T_{jk}(+)$ and $\hat{T}_{jk}(+)$ are identical. The difference between the sets of equations for the $|X_{mk}\rangle$ and the $|\psi_i\rangle$ lies in the nature of the expansion (18) and the properties of the $|\psi_i\rangle$, which we establish in part through the time-dependent analysis of the next section. Finally, we remark that the question of uniqueness noted in subsection B, i.e., the size of the set (16), is reflected in the present case in the number and kind of channels to be included in (18).

III. TIME-DEPENDENT EQUATIONS

A. Time-reversal properties

Before introducing and examining the structure of our time-independent formalism, we reexpress Eq. (21) in a more compact matrix notation. Define H to be a matrix Hamiltonian operator having components H_{jk} given by

$$(\underline{H})_{jk} = H_{jk} = (\underline{H}_0)_{jk} + (\underline{V})_{jk} = H_j \delta_{jk} + W_{ji}V_k, \quad (25)$$

which defines $V_{jk} = W_{ji}V_k$ and $H_{0,jk} = H_j \delta_{jk}$. Also, let $|\underline{\psi}\rangle$ be a column vector with components $|\psi_j\rangle$. Then (21) is equivalent to

$$\underline{H}|\underline{\psi}\rangle = E|\underline{\psi}\rangle, \quad (26)$$

while Eq. (22) reads in this new notation

$$|\underline{\psi}\rangle = |\underline{\phi}\rangle + \underline{G}_0(+) \underline{V}|\underline{\psi}\rangle, \quad (27)$$

where $|\underline{\phi}\rangle$ is a column vector containing $|\Phi_k(E)\rangle$ in row k and zeros elsewhere and $\underline{G}_0(+)$ is a diagonal matrix of channel Green's functions:

$$\underline{G}_0(+) = (E + i0 - \underline{H}_0)^{-1}. \quad (28)$$

In terms of the matrix Green's function $\underline{G}(+)$ defined by

$$\underline{G}(+) = (E + i0 - \underline{H})^{-1} \quad (29)$$

and obeying

$$\underline{G}(+) = \underline{G}_0(+) + \underline{G}_0(+) \underline{V} \underline{G}(+) \quad (30a)$$

$$= \underline{G}_0(+) + \underline{G}(+) \underline{V} \underline{G}_0(+), \quad (30b)$$

the solution to (27) may be written as

$$|\underline{\psi}\rangle = |\underline{\phi}\rangle + \underline{G} \underline{V} |\underline{\phi}\rangle. \quad (31)$$

The analogy with standard two-body results is evident, as noted elsewhere.^{1,2,5}

Just as Eq. (21) [or (25)] was derived from (17), so a time-dependent set of coupled equations can be derived from the time-dependent Schrödinger equation for $|\Psi(t)\rangle$ ($\hbar = 1$),

$$i \frac{\partial |\Psi(t)\rangle}{\partial t} = H |\Psi(t)\rangle. \quad (32)$$

Let $|\psi_j(t)\rangle$ be a time-dependent state analogous to $|\psi_j\rangle$ of Eq. (18), and let

$$|\underline{\Psi}(t)\rangle = \sum_j |\psi_j(t)\rangle \quad (33)$$

be the analogous expansion. If (33) is now substituted into (32) and the same steps are followed as occur between Eqs. (18) and (21), we find the matrix result

$$i \frac{\partial |\underline{\psi}(t)\rangle}{\partial t} = \underline{H} |\underline{\psi}(t)\rangle, \quad (34)$$

where the notation used above is followed.

Equation (34) is the basic, time-dependent result on which all further analysis is based. We shall assume henceforth that \underline{H} is at least an $N_2 \times N_2$ matrix, where N_2 is the number of two-body channels. The channel labels will thus include at least all two-body channels unless otherwise specified. Through the elements of \underline{W} , Eq. (34) couples together the various channel-component states $|\psi_j(t)\rangle$. As a concrete example of the detailed structure of this set of equations, we consider the $n=3$, $N_2=3$ case, and choose a channel-permuting array of the form (see Tobocman,¹ Kouri and Levin^{1,5})

$$\underline{W} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. \quad (35)$$

Setting $l=k$ in $V_{jk} = W_{ji}V_k$ and using (35) in (34) yields

$$\left(i \frac{\partial}{\partial t} - H_1 \right) |\psi_1(t)\rangle = V_2 |\psi_2(t)\rangle,$$

$$\left(i \frac{\partial}{\partial t} - H_2\right) |\psi_2(t)\rangle = V_3 |\psi_3(t)\rangle,$$

$$\left(i \frac{\partial}{\partial t} - H_3\right) |\psi_3(t)\rangle = V_1 |\psi_1(t)\rangle.$$

The cyclic nature of the coupling due to the channel-permuting array is evident from this example.

We shall discuss the time evolution of the $|\underline{\psi}(t)\rangle$ by means of time-evolution operators, e.g., $U(t, t_0) = \exp[-i\overline{H}(t-t_0)]$. Unlike the usual approach to this analysis involving the Schrödinger equation Hamiltonian H in $\exp[-iH(t-t_0)]$, there could be serious problems associated with \overline{H} when $\lim t, t_0 \rightarrow \pm\infty$ is taken. The reason is that \overline{H} is not Hermitian, while H is: $\overline{H}^\dagger \neq \overline{H}$, $H^\dagger = H$. That is, H_j and V_j are as usual assumed to be Hermitian for all partitions, but the presence of W in $V_{jk} = W_{ji}V_k$ means that $V^\dagger \neq V$, and thus that $\overline{H}^\dagger \neq \overline{H}$. This is easily seen in the $n=3$, $N_2=3$ example defined by Eq. (35). However, if it can be shown that only the real eigenvalues of \overline{H} enter, then taking the preceding limits will introduce no singularities, the resulting operator will be as well defined as in the standard approaches to a time-dependent theory, and we can proceed with the development. We shall now show how to ensure reality of the E in Eq. (26) [or (27)].

We do this by first assuming that \overline{H} is invariant under time reversal and rotations, and then imposing the effects of these symmetries on the solutions $|\underline{\psi}\rangle$ of \overline{H} . This is especially important when approximations are introduced, though we shall not be concerned with these here. Since H (and all its partitions) are assumed invariant under time reversal, then

$$\overline{H}\overline{\tau}^\dagger = \overline{H}, \quad (36)$$

where $\overline{\tau}$ is the (antilinear) time-reversal operator. Invariance of H under rotations means that the Schrödinger state $|\Psi\rangle$ is characterized by angular momentum J and projection M : $|\Psi\rangle \equiv |\Psi(JM)\rangle$. The time-reversed state is $\overline{\tau}|\Psi(JM)\rangle$, and we choose its phase so that

$$\overline{\tau}|\Psi(JM)\rangle = (-1)^{J-M}|\Psi(J-M)\rangle. \quad (37)$$

This is one of the standard phase conventions for time-reversal-invariant systems as discussed for example by Lane and Thomas¹⁴ or Rodberg and Thaler.¹³ Notice that if the system has only axial symmetry, then $|\Psi\rangle$ will be characterized only by the projection M on that axis, but a phase convention similar to (37) can still be introduced, as discussed by Bohr and Mottelson.¹⁴

Let us now apply these considerations to \overline{H} and $|\underline{\psi}\rangle$. By assumption, $\overline{\tau}H_j\overline{\tau}^\dagger = H_j$ and $\overline{\tau}V_j\overline{\tau}^\dagger = \overline{V}_j$ for all j , and $\overline{\tau}W_{jk}\overline{\tau}^\dagger = W_{jk}$ because the W_{jk} are all real. Therefore we find the important result that

$$\overline{\tau}H\overline{\tau}^\dagger = \overline{H}. \quad (38)$$

Furthermore, because H_j , V_j , and W_{jk} are all scalars under rotations, every $|\psi_j\rangle$ and thus $|\underline{\psi}\rangle$ can be characterized by unique J and M . It is clear that the same value of J and M must occur on each side of Eq. (18) since eigenfunctions belonging to different irreducible representations of the rotation group are orthogonal. That is, while $\langle\psi_j(JM)|\psi_k(JM)\rangle \neq 0$, we do have

$$\langle\psi_j(JM)|\psi_k(J'M')\rangle = 0$$

$$= \langle\psi_j(JM)|\Psi(J'M')\rangle, \quad J' \neq J, \quad M' \neq M,$$

and hence

$$|\Psi(JM)\rangle = \sum_j |\psi_j(JM)\rangle. \quad (39)$$

The behavior of $|\underline{\psi}\rangle$ under $\overline{\tau}$ is not so straightforward. From (37) it follows that

$$\overline{\tau} \sum_j |\psi_j(JM)\rangle = (-1)^{J-M} \sum_j |\psi_j(J-M)\rangle,$$

but the nonorthogonality of $|\psi_j\rangle$ and $|\psi_k\rangle$ (for the same value of J and M) does not allow us to conclude that¹⁵

$$\overline{\tau}|\psi_j(JM)\rangle = (-1)^{J-M}|\psi_j(J-M)\rangle$$

holds for each j . However, if this condition does hold, then (37) follows automatically from it. Furthermore, this also is a sufficient condition for \overline{H} to have real eigenvalues. Therefore we choose the phase of each channel-component state $|\psi_j(JM)\rangle$ by demanding that

$$\overline{\tau}|\psi_j(JM)\rangle = (-1)^{J-M}|\psi_j(J-M)\rangle. \quad (40)$$

Equation (40) is an extremely weak condition. But, since the original Schrödinger equation problem satisfies (36) and (37), it is an obvious requirement to impose on the $|\psi_j\rangle$, particularly since \overline{H} obeys (38). We are "simply" limiting the solutions of the extended problem to those that obey the same physical conditions as $|\Psi\rangle$ itself. By doing so, we ensure that the eigenvalues of (26) are real. An alternate way of stating this is that (26) may admit both real and complex eigenvalue solutions. Imposition of (40) selects the real ones.

To establish reality, we first notice that from (40) it follows that

$$\overline{\tau}|\underline{\psi}(JM)\rangle = (-1)^{J-M}|\underline{\psi}(J-M)\rangle. \quad (41)$$

Hence, applying $\overline{\tau}$ to both sides of (26) gives

$$\overline{\tau}\overline{H}\overline{\tau}^\dagger \overline{\tau}|\underline{\psi}(JM)\rangle = E^* \overline{\tau}|\underline{\psi}(JM)\rangle$$

or

$$\overline{\tau}\overline{H}\overline{\tau}^\dagger |\underline{\psi}(J-M)\rangle = E^* |\underline{\psi}(J-M)\rangle, \quad (42)$$

where we have assumed a JM dependence for $|\underline{\psi}\rangle$ as in (40) and have used the antilinear nature of τ . Using (38) in (42), we find that

$$\underline{H}|\underline{\psi}(J-M)\rangle = E^*|\underline{\psi}(J-M)\rangle. \quad (43)$$

Proof of the reality of E in (26) is now trivial. We project both sides of (26) onto $\langle\underline{\psi}(JM)|$ to find

$$\langle\underline{\psi}(JM)|\underline{H}|\underline{\psi}(JM)\rangle = E\langle\underline{\psi}(JM)|\underline{\psi}(JM)\rangle, \quad (44)$$

where we again assume a JM dependence for $|\underline{\psi}\rangle$. Similarly, projecting both sides of (43) onto $\langle\underline{\psi}(J-M)|$ gives

$$\langle\underline{\psi}(J-M)|\underline{H}|\underline{\psi}(J-M)\rangle = E^*\langle\underline{\psi}(J-M)|\underline{\psi}(J-M)\rangle. \quad (45)$$

Subtraction of the members of (45) from (44) leads to

$$\begin{aligned} & [\langle\underline{\psi}(JM)|\underline{H}|\underline{\psi}(JM)\rangle - \langle\underline{\psi}(J-M)|\underline{H}|\underline{\psi}(J-M)\rangle] \\ & = E\langle\underline{\psi}(JM)|\underline{\psi}(JM)\rangle - E^*\langle\underline{\psi}(J-M)|\underline{\psi}(J-M)\rangle. \end{aligned} \quad (46)$$

Since H and \underline{H} are scalar operators under rotations, the Wigner-Eckart theorem immediately implies that the two matrix elements on the left-hand side of (46) are equal as are the two on the right-hand side. Hence (46) reduces to

$$(E - E^*)\langle\underline{\psi}(JM)|\underline{\psi}(JM)\rangle = 0. \quad (47)$$

Since the matrix element in (47) is a sum of normalization integrals ($\sum_n \langle\underline{\psi}_n|\underline{\psi}_n\rangle$), not all of which can be assumed to vanish simultaneously (indeed, we assume that $\langle\underline{\psi}_n|\underline{\psi}_n\rangle \neq 0$, all n), we then find that

$$E = E^*,$$

which provides the desired proof of reality. Clearly the same procedure can be followed to establish the reality of the eigenvalues of H .

Reality of the eigenvalues of H holds under the condition that the $|\underline{\psi}_j\rangle$ obey (40). Notice that it is sufficient that the continuum solutions of (26) [or (27)] obey (40) for each total angular momentum partial wave for E to be real. No other conditions need apply. Since \underline{H} or any operator function of \underline{H} will always be applied to such continuum solutions, then it is clear that quantities such as $\exp[iH(t-t_0)]$ and their limiting values for $t, t_0 \rightarrow \pm\infty$ will be as well behaved as $\exp[iH(t-t_0)]$ in more standard treatments of time-dependent scattering theory.

B. Schrödinger picture

By assumption, H and thus \underline{H} is independent of time. We may therefore introduce a time-evolution operator $\underline{U}(t, t_0)$ such that

$$|\underline{\psi}(t)\rangle = \underline{U}(t, t_0)|\underline{\psi}(t_0)\rangle. \quad (48)$$

The requirements that $\underline{U}(t, t) = \underline{I}$, where \underline{I} is the unit matrix, and that (48) obey (34) immediately give

$$\underline{U}(t, t_0) = e^{-i\underline{H}(t-t_0)}, \quad (49)$$

in complete analogy with standard results. Equations (44) and (45) help to define a matrix Schrödinger picture, while the analysis of the preceding section ensures that (49) is a well-defined quantity in the space of interest.

Unperturbed channel states $|\underline{\varphi}\rangle$ can be introduced in analogy to the $|\underline{\psi}\rangle$. They obey

$$\underline{H}_0|\underline{\varphi}\rangle = E|\underline{\varphi}\rangle, \quad (50)$$

with $|\underline{\varphi}\rangle$ of Eq. (27) being one example of a $|\underline{\varphi}\rangle$. Notice that if more than one row in $|\underline{\varphi}\rangle$ is nonzero, each component $|\underline{\varphi}_j\rangle$ of $|\underline{\varphi}\rangle$ is defined to have total (real) energy E . Because \underline{H}_0 is diagonal, time-dependent states $|\underline{\varphi}(t)\rangle$ can be introduced in a trivial manner:

$$\begin{aligned} |\underline{\varphi}(t)\rangle & = e^{-iEt}|\underline{\varphi}\rangle \\ & = e^{-i\underline{H}_0t}|\underline{\varphi}\rangle. \end{aligned} \quad (51)$$

The time-evolution operator $\underline{U}_0(t, t_0)$ for the $|\underline{\varphi}(t)\rangle$ is essentially given in (51):

$$\underline{U}_0(t, t_0) = e^{-i\underline{H}_0(t-t_0)}. \quad (52)$$

We now examine the time dependence of $|\underline{\psi}(t)\rangle$ following the usual assumption of two-body scattering theory¹³ that at a remote time t_0 in the past, $|\underline{\psi}(t_0)\rangle$ is given by

$$\begin{aligned} |\underline{\psi}(t_0)\rangle & = e^{-i\underline{H}_0t_0}|\underline{\phi}\rangle \\ & = e^{-iEt_0}|\underline{\phi}\rangle. \end{aligned} \quad (53)$$

At a later time t we have from (48) that

$$|\underline{\psi}(t)\rangle = e^{-i\underline{H}(t-t_0)}e^{-i\underline{H}_0t_0}|\underline{\phi}\rangle. \quad (54)$$

Our interest is in times $t=0$, $t_0 \rightarrow -\infty$. The analysis of Chandler and Gibson¹⁶ indicates that

$$|\underline{\psi}(t=0)\rangle = \underline{\Omega}^*|\underline{\phi}\rangle, \quad (55)$$

with the matrix Møller operator $\underline{\Omega}^*$ defined by¹⁷

$$\underline{\Omega}^* = \text{s-lim}_{t \rightarrow -\infty} e^{i\underline{H}t}e^{-i\underline{H}_0t}. \quad (56)$$

In a similar fashion, the operator $\underline{\Omega}^{-\dagger}$, defined by (56) but with $t \rightarrow +\infty$ and s-lim replaced by w-lim, can be introduced, as in Sec. IV.

From Eq. (55) it now follows that

$$\begin{aligned} |\underline{\psi}(t)\rangle & = \underline{U}(t, 0)\underline{\Omega}^*|\underline{\phi}\rangle \\ & = e^{-i\underline{H}t}\underline{\Omega}^*|\underline{\phi}\rangle. \end{aligned} \quad (57)$$

Also, the operator $\underline{\Omega}^*$ can as usual^{13,16} be shown to obey an intertwining relation,

$$\underline{H}\underline{\Omega}^* = \underline{\Omega}^*\underline{H}_0, \quad (58)$$

which implies that (57) is equal to

$$|\underline{\psi}(t)\rangle = e^{-iEt}\underline{\Omega}^+|\underline{\phi}\rangle \equiv e^{-iEt}|\underline{\psi}(t=0)\rangle. \quad (59)$$

We thus obtain the important result that $|\underline{\psi}(t)\rangle$ has the same energy dependence as $|\underline{\phi}(t)\rangle$. For wave packets, (59) would be replaced by an integral over the same coefficients as found in the wave packet describing $|\underline{\phi}(t)\rangle$. These manipulations all follow from the analysis of subsection A, which allows us to use $\exp(iHt)$ freely since all states ($|\underline{\phi}\rangle$ and $|\underline{\psi}\rangle$) on which \underline{H} acts are assumed where necessary to obey the time-reversal condition (41).

C. Interaction picture

An interaction picture can be introduced in a straightforward way analogous to the usual procedure in two-body scattering, essentially because our matrix formalism is constructed in precise analogy to the two-body case. The *interaction* vector of states $|\underline{\chi}(t)\rangle$ is defined by

$$|\underline{\chi}(t)\rangle = e^{iH_0 t}|\underline{\psi}(t)\rangle, \quad (60)$$

and $\underline{U}_I(t, t_0)$, the time-evolution operator in the interaction picture, is given by

$$\begin{aligned} \underline{U}_I(t, t_0) &= e^{iH_0 t}\underline{U}(t, t_0)e^{-iH_0 t_0} \\ &= e^{iH_0 t}e^{-iH(t-t_0)}e^{-iH_0 t_0}, \end{aligned} \quad (61)$$

where \underline{U}_I governs the time evolution of $|\underline{\chi}(t)\rangle$:

$$|\underline{\chi}(t)\rangle = \underline{U}_I(t, t_0)|\underline{\chi}(t_0)\rangle. \quad (62)$$

It is straightforward to show that $\underline{U}_I(t, t_0)$ obeys

$$\begin{aligned} i \frac{\partial \underline{U}_I(t, t_0)}{\partial t} &= e^{iH_0 t}\underline{V}e^{-iH_0 t}\underline{U}_I(t, t_0) \\ &\equiv \underline{V}(t)\underline{U}_I(t, t_0). \end{aligned} \quad (63)$$

In integral form, (63) reads

$$\underline{U}_I(t, t_0) = \underline{I} - i \int_{t_0}^t dt' \underline{V}(t')\underline{U}_I(t', t_0), \quad (64)$$

and an equivalent form can also be derived:

$$\underline{U}_I(t, t_0) = \underline{I} - i \int_{t_0}^t dt' \underline{U}_I(t, t')\underline{V}(t'). \quad (65)$$

These results are analogs of the familiar results of two-body scattering theory.¹³

In the interaction picture for remote times t_0 , $|\underline{\chi}(t_0)\rangle$ is equal to $e^{+iH_0 t_0}|\underline{\phi}(t_0)\rangle$, or

$$|\underline{\chi}(t_0)\rangle = |\underline{\phi}\rangle, \quad t_0 \ll 0.$$

For later times we find

$$|\underline{\chi}(t)\rangle = \underline{U}_I(t, t_0)|\underline{\phi}\rangle. \quad (66)$$

Our interest again is in times $t=0$, $t_0 \rightarrow -\infty$, and the development in Sec. III B leads us to

$$|\underline{\chi}(t=0)\rangle = \underline{\Omega}_I^+|\underline{\phi}\rangle, \quad (67)$$

where again following the analysis of Chandler and Gibson¹⁶ we have defined $\underline{\Omega}_I^+$ by

$$\begin{aligned} \underline{\Omega}_I^+ &= s\text{-}\lim_{t \rightarrow -\infty} \underline{U}_I(0, t) \\ &= s\text{-}\lim_{t \rightarrow -\infty} e^{iHt}e^{-iH_0 t} \equiv \underline{\Omega}^+. \end{aligned} \quad (68)$$

Let us now apply the strong-limit procedure of (68) to both sides of Eq. (64). We find that

$$\underline{\Omega}_I^+ = \underline{I} - i \int_{-\infty}^0 dt' \underline{V}(t')\underline{U}_I(t', -\infty), \quad (69)$$

where $\underline{U}_I(t', -\infty)$ is to be interpreted as $s\text{-}\lim_{t_0 \rightarrow -\infty} \underline{U}_I(t', t_0)$. Applying both sides of (69) to $|\underline{\phi}\rangle$ gives

$$|\underline{\chi}(t=0)\rangle = |\underline{\phi}\rangle - i \int_{-\infty}^0 dt' e^{iH_0 t'} \underline{V} e^{-iH_0 t'} |\underline{\chi}(t')\rangle. \quad (70)$$

If we substitute Eq. (60) for $|\underline{\chi}(t')\rangle$ in (70), and note that $|\underline{\chi}(t=0)\rangle = |\underline{\psi}(t=0)\rangle$, then (70) becomes

$$|\underline{\psi}(t=0)\rangle = |\underline{\phi}\rangle - i \int_{-\infty}^0 dt' e^{-iH_0 t'} \underline{V} |\underline{\psi}(t')\rangle.$$

Use of Eq. (59) in this latter result now gives

$$|\underline{\psi}(t=0)\rangle = |\underline{\phi}\rangle - i \int_{-\infty}^0 dt' e^{-i(E-H_0)t'} \underline{V} |\underline{\psi}(t=0)\rangle. \quad (71)$$

The integral in (71) is a familiar one occurring in scattering theory, and we treat it in the usual way through insertion of the standard ϵ factor¹³ to give

$$|\underline{\psi}(t=0)\rangle = |\underline{\phi}\rangle + \underline{G}_0(+)\underline{V}|\underline{\psi}(t=0)\rangle, \quad (72)$$

where $\underline{G}_0(t)$ is defined by Eq. (28). Equation (72) is precisely the same as Eq. (27), thus establishing the expected result that $|\underline{\psi}(t=0)\rangle$ is the solution of Eq. (26). Had we used (65) rather than Eq. (64), the end result would have been the replacement of (72) by Eq. (31). The introduction of an interaction picture thus not only leads to results in complete analogy to those of two-body scattering, but is consistent with the results derived from the \hat{T} -operator equation.

IV. MULTICHANNEL S OPERATORS

The S operator S will be shown to be given by the product $\underline{U}(t, 0)\underline{U}(0, t_0) = \underline{U}_I(t, 0)\underline{U}_I(0, t_0)$ in the limit as $t \rightarrow +\infty$ and $t_0 \rightarrow -\infty$, with matrix elements to be evaluated between initial and final asymptotic states. In particular, for $\underline{\Omega}^+$ defined by (56) and $\underline{\Omega}^{-\dagger}$ by¹⁶

$$\underline{\Omega}^{-\dagger} = \text{w-lim}_{t \rightarrow \infty} e^{iH_0 t} e^{-iH t},$$

\underline{S} will be¹⁷

$$\underline{S} = \underline{\Omega}^{-\dagger} \underline{\Omega}^{\dagger}. \quad (73)$$

To determine \underline{S} in the above form, we must establish two results. First, it must be shown that the present formalism leads to amplitudes determined by (73), and second, these amplitudes must be shown to be identical to the usual S-matrix elements. In achieving this, we shall establish some interesting properties of the channel-component states.

The standard approach,¹³ modified as in Ref. 16, determines an S-matrix element \bar{S}_{jk} through evaluation of

$$\bar{S}_{jk} = \lim_{t \rightarrow \infty} \langle \Phi_j(E') | e^{iH_j t} | \Psi(t) \rangle, \quad (74)$$

where $|\Psi(t)\rangle$ is generated from the asymptotic state $|\Phi_k(E)\rangle$, although we have suppressed the k dependence of $|\Psi(t)\rangle$. For the channels of interest here, \bar{S}_{jk} can be shown to be¹³

$$\bar{S}_{jk} = \delta_{jk} \delta_{\gamma'\gamma} - 2\pi i \delta(E - E') \langle \Phi_j(E) | \hat{T}_{jk}(E + i0) | \Phi_k(E) \rangle, \quad (75)$$

where γ' (γ) is the complete set of quantum numbers including the energy, characterizing the state $|\Phi_j(E)\rangle$ [$|\Phi_k(E)\rangle$]. To emphasize this aspect of the asymptotic states $|\Phi_j(E)\rangle$ we shall rewrite them in a different notation:

$$|\Phi_j(E)\rangle \rightarrow |\varphi_j(\gamma)\rangle, \text{ etc.} \quad (76)$$

Note that (75) contains matrix elements of \hat{T}_{jk} because this operator is known⁵ to give the correct, on-shell transition amplitude. If j does not denote a two-body channel, \hat{T}_{jk} must be replaced by $U_{jk}^{(-)}$

of Eq. (9).

We shall now show that if (33) is substituted into (74), then

$$\bar{S}_{jk} = S_{jk} \equiv \lim_{t \rightarrow \infty} \langle \varphi_j(\gamma') | e^{iH_j t} | \psi_j(t) \rangle, \quad (77)$$

i.e., that

$$\begin{aligned} I_{jm} &\equiv \lim_{t \rightarrow \infty} \langle \varphi_j(\gamma') | e^{iH_j t} | \psi_m(t) \rangle \\ &= \bar{S}_{jk} \delta_{jm}. \end{aligned} \quad (78)$$

Hence, in limit $t \rightarrow \infty$, only the component $|\psi_j(t)\rangle$ occurring in $|\Psi(t)\rangle = \sum_m |\psi_m(t)\rangle$ contributes to the scattering in channel j . The generalization of this result will yield Eq. (73).

To prove our claim, we use the interaction picture. From Eqs. (64) and (66), and the arguments leading to (71), we find that

$$|\underline{\chi}(t)\rangle = |\underline{\phi}\rangle - i \int_{-\infty}^t dt' e^{-i(E-H_0)t'} \underline{V} |\underline{\psi}(t'=0)\rangle, \quad (79)$$

where $\lim_{t \rightarrow -\infty}$ has been assumed in applying $U_I(t', -\infty)$ to $|\underline{\phi}\rangle$. Next, use of (60) in (79) leads to

$$|\underline{\psi}(t)\rangle = e^{-iH_0 t} |\underline{\phi}\rangle - i e^{-iH_0 t} \int_{-\infty}^t dt' e^{-i(E-H_0)t'} \underline{V} |\underline{\psi}(t'=0)\rangle. \quad (80)$$

Finally, the fact that H_0 is diagonal in channel indices means that (80) is equivalent to

$$\begin{aligned} |\psi_m(t)\rangle &= e^{-iH_m t} |\varphi_k(\gamma)\rangle \delta_{mk} \\ &\quad - i e^{-iH_m t} \int_{-\infty}^t dt' e^{-i(E-H_m)t'} \\ &\quad \times \sum_{m'} W_{m1} V_{m'} |\psi_{m'}(t'=0)\rangle. \end{aligned} \quad (81)$$

Substituting (81) into the definition of I_{jm} , Eq. (78), we find that

$$I_{jm} = \lim_{t \rightarrow \infty} \langle \varphi_j(\gamma') | e^{iH_j t} e^{-iH_m t} | \varphi_k(\gamma) \rangle \delta_{mk} - i \lim_{t \rightarrow \infty} \langle \varphi_j(\gamma') | e^{iH_j t} e^{-iH_m t} \int_{-\infty}^t dt' e^{-i(E-H_m)t'} \sum_{m'} W_{m1} V_{m'} |\psi_{m'}(t'=0)\rangle \rangle. \quad (82)$$

The desired result follows from (82) by making use of Lippmann's identity. We first note that the integral in (82) can be evaluated by using the usual¹³ ϵ convergence factor to give

$$\int_{-\infty}^t dt' e^{-i(E-H_m)t'} = e^{-i(E-H_m)t} G_m(+), \quad (83)$$

exactly as in the derivation of Eq. (72), where we had $t=0$. Substitution of (83) into (82) leads to

$$I_{jm} = \lim_{t \rightarrow \infty} \left\{ \langle \varphi_j(\gamma') | e^{iH_j t} e^{-iH_m t} | \varphi_k(\gamma) \rangle \delta_{mk} - i \langle \varphi_j(\gamma') | e^{-i(E-H_j)t} G_m(+) \sum_{m'} W_{m1} V_{m'} |\psi_{m'}(t'=0)\rangle \right\}. \quad (84)$$

Next we insert the factor $G_j(+)\mathcal{G}_j^{-1}(+) = 1$ to the left of $G_m(+)$ in (84), and then use (83) with the subscript m replaced by j to rewrite (84) as

$$I_{jm} = \lim_{t \rightarrow \infty} \left\{ \langle \varphi_j(\gamma') | e^{iH_j t} e^{-iH_m t} | \varphi_k(\gamma) \rangle \delta_{mk} - i \langle \varphi_j(\gamma') | \int_{-\infty}^t e^{-i(E-H_j)t'} dt' \mathcal{G}_j^{-1}(+) G_m(+) \sum_{m'} W_{m1} V_{m'} |\psi_{m'}(t'=0)\rangle \right\}. \quad (85)$$

Now consider the limit in (85). The first term will vanish unless $j=k$ and $\gamma=\gamma'$, as the usual wave-packet arguments show.¹³ The second term contains an integral which yields the factor $2\pi\delta(E-H_j)$. Hence we find that

$$I_{jm} = \delta_{jk}\delta_{m\bar{k}}\delta_{\gamma\gamma'} - 2\pi i\delta(E-E') \left\langle \varphi_j(\gamma') \left| G_j^{-1}(+)G_m(+) \sum_{m'} W_{m'l} V_{m'} \right| \psi_{m'}(t=0) \right\rangle,$$

where we have used $\langle \varphi_j(\gamma') | H_j = \langle \varphi_j(\gamma') | E'$ to move the δ function outside of the matrix element and also $\delta(E-E')$ to set the arguments of $G_j^{-1}(+)$ and $G_m(+)$ equal to each other. Lippmann's identity in the form of Eq. (7) now yields the final result

$$\begin{aligned} I_{jm} &= \delta_{jm} \left\{ \delta_{jk}\delta_{\gamma\gamma'} - 2\pi i\delta(E-E') \left\langle \varphi_j(\gamma') \left| \sum_{m'} W_{m'l} V_{m'} \right| \psi_{m'}(t=0) \right\rangle \right\} \\ &= \delta_{jm} \left\{ \delta_{jk}\delta_{\gamma\gamma'} - 2\pi i\delta(E-E') \langle \Phi_j(E) | \hat{T}_{jk}(+) | \Phi_k(E) \rangle \right\} \\ &= \delta_{jm} \bar{S}_{jk}, \end{aligned} \tag{86}$$

where we have used $\delta_{jk}\delta_{m\bar{k}} = \delta_{jm}\delta_{j\bar{k}}$ to get the first line of (86), Eqs. (24) and (76) to go to the second line, and the definition (75) for \bar{S}_{jk} .

The last line of (86) is just Eq. (78), and so our claim is now verified. Note that the result is valid *only* if $|\varphi_j(\gamma')\rangle$ is a two-body state, since only then does Lippmann's identity hold. As long as only two-body final states are used in forming the matrix elements, we may write $S_{jk} = \bar{S}_{jk}$ as the matrix element of the operator \hat{S}_{jk} defined by

$$\hat{S}_{jk} = \delta_{jk} - 2\pi i\delta(E-H_j)\hat{T}_{jk}(E+i0), \tag{87}$$

a definition we use after next establishing Eq. (73).

To verify (73), we note first that (57) in component form reads

$$|\psi_j(t)\rangle = \sum_m (e^{-iHt})_{jm}(\underline{\Omega}^+)_{m\bar{k}} |\varphi_k(\gamma)\rangle, \tag{88}$$

where we have assumed that $|\phi\rangle$ has only one non-zero element, viz., $|\varphi_k(\gamma)\rangle$. Substitution of (88) into (77) yields

$$\begin{aligned} S_{jk} &= \lim_{t \rightarrow \infty} \left\langle \varphi_j(\gamma') \left| e^{iH_j t} \sum_m (e^{-iHt})_{jm}(\underline{\Omega}^+)_{m\bar{k}} \right| \varphi_k(\gamma) \right\rangle \\ &= \lim_{t \rightarrow \infty} \left\langle \varphi_j(\gamma') \left| \sum_m (e^{iH_0 t} e^{-iHt})_{jm}(\underline{\Omega}^+)_{m\bar{k}} \right| \varphi_k(\gamma) \right\rangle \\ &= \left\langle \varphi_j(\gamma') \left| \sum_m (\underline{\Omega}^+)_{jm}(\underline{\Omega}^+)_{m\bar{k}} \right| \varphi_k(\gamma) \right\rangle, \end{aligned} \tag{89}$$

where we have used the fact that H_0 is diagonal in channel indices and also the definition of $\underline{\Omega}^+$ introduced above Eq. (73). This last result clearly

$$I_{jm} = \delta_{jm}\delta_{jk}\delta_{\gamma\gamma'} - 2\pi i\delta(E-E') \left\langle \varphi_j(\gamma') \left| G_j^{-1}(+)G_m(+) \sum_{m'} W_{m'l} V_{m'} \right| \psi_{m'}(t=0) \right\rangle. \tag{92}$$

The S matrix element $S_{jk} = \bar{S}_{jk}$, from Eq. (74), now becomes

$$\begin{aligned} S_{jk} &= \sum_m I_{jm} \\ &= \delta_{jk}\delta_{\gamma\gamma'} - 2\pi i\delta(E-E') \left\langle \varphi_j(\gamma') \left| \sum_m G_j^{-1}(+)G_m(+) \hat{T}_{m\bar{k}}(+) \right| \varphi_k(\gamma) \right\rangle \\ &= \delta_{jk}\delta_{\gamma\gamma'} - 2\pi i\delta(E-E') \langle \Phi_j(E) | U_{jk}^{(-)}(+) | \Phi_k(E) \rangle, \end{aligned} \tag{93}$$

establishes that S_{jk} is the *double* jk matrix element of \underline{S} as given by (73), which is the result we set out to prove. That is, to find S_{jk} , we first form

$$\hat{S}_{jk} = (\underline{S})_{jk}, \tag{90}$$

where \hat{S}_{jk} is given in Eq. (87), and then evaluate

$$S_{jk} = \langle \varphi_j(\gamma') | \hat{S}_{jk} | \varphi_k(\gamma) \rangle. \tag{91}$$

The fact that \underline{S} is an operator matrix in channel space means that we could reformulate the preceding in terms of single "superoperators" defined in a new vector channel space $\mathcal{H}^{(N)}$ given by $\mathcal{H}^{(N)} = \mathcal{H} \otimes \mathcal{H} \otimes \dots \otimes \mathcal{H}$ (N factors), where \mathcal{H} is the usual Hilbert space of the eigenstates of H , and N is the number of channels. We have not done this because there seems to be at present no special advantage to be gained by it.¹⁸

Our basic assumption so far has been that the channel labels run over the set of two-body channels. Indeed this assumption was necessary to derive Eq. (78), since we employed Lippmann's identity [Eq. (7)] to obtain the final line of Eq. (86). We now examine the case when the final channel index refers to an m -body channel, $m \geq 3$. In this case, Lippmann's identity (7) does not hold; instead we get

$$G_j^{-1}(+)G_m(+) = 1 + (V_j - V_m)G_m(+),$$

which could be used in Eq. (9) to help evaluate $U_{jk}^{(-)}(+)$. Since Eq. (7) cannot be used, we find that I_{jm} becomes

where we have used Eqs. (24) and (9), and have again reintroduced the states $|\Phi\rangle$. This result is no surprise, in that it indicates the consistency of our procedure: When j is not a two-body channel, the correct transition operator is $U_{jk}^{(+)}(+)_{-}$, and the preceding analysis simply shows how this latter operator is obtained.

We conclude this section by noting two properties of S . First, by construction (i.e., reality of W), we have that the usual results¹³ of time-reversal invariance follow from the present formalism. Second, as long as the set of channels used in defining H , and thus S , contains at least the set of two-body channels, then the relation (87) plus the analysis of Benoist-Gueutal⁶ suffices to show that the usual discontinuity relations are obeyed. Hence, the present formulation of many-body scattering theory leads to results consistent with those of more standard formulations.¹³ The fact that we are able to formulate a single S operator is completely in accord with the results of Faddeev for the three-body problem¹⁹ and, e.g., that of Taylor¹³ for the arbitrary n -body problem. The existence of an interaction picture for multichannel scattering seems not to have been shown in detail before.

V. DISCUSSION

In the preceding sections, we have shown that channel-component states $|\psi_m(t)\rangle$ can be used as the basis for a time-dependent many-body scattering theory. Time-evolution operators can be formulated leading to an interaction picture and single S operator exactly as in the two-body case. Furthermore, the usual connection^{13,16} between the time-independent and time-dependent descriptions has been made. In particular, we have shown that $|\psi_m(t=0)\rangle$ and $|\psi_m\rangle$ of the time-independent analysis (Sec. II B 2) are identical. We now examine some consequences of this relation, based on the results of Sec. IV.

We consider the total (Schrödinger) state $|\Psi\rangle$ first. In two-body (single-channel) scattering, $|\Psi\rangle$ obeys a Lippmann-Schwinger equation and manifestly contains only outgoing scattered waves asymptotically.¹³ In the n -body, N -channel case, the physical boundary condition on $|\Psi\rangle$ is that it contains only outgoing scattered waves asymptotically in each open arrangement channel. One object of many-body scattering theory is to provide a formulation in which this aspect of $|\Psi\rangle$ is ensured and manifest, as it is for example in the channel-coupling-array theory.¹ The fact that $|\Psi\rangle$ must have this property means that

$$(2\pi)^{3/2} \langle \vec{r}_j, \vec{\varphi}_j(\gamma') | \Psi \rangle \underset{r_j \rightarrow \infty}{\sim} e^{i\vec{p}_k \cdot \vec{r}_k} \delta_{jk} \delta_{\gamma\gamma'} + f_{\gamma'j, \gamma k}(\vec{p}_j, \vec{p}_k) e^{i\vec{p}_j \cdot \vec{r}_j / r_j}, \quad (94)$$

where $|\vec{\varphi}_j(\gamma')\rangle$ is the product of internal bound states present in $|\varphi_j(\gamma')\rangle$, $\vec{r}_j(\vec{r}_k)$ and $\vec{p}_j(\vec{p}_k)$ are the relative coordinate and momentum of the two clusters in channel $j(k)$, and $f_{\gamma'j, \gamma k}$ is the relevant scattering amplitude.

Suppose we now were to attempt to calculate $f_{\gamma'j, \gamma k}$. Apart from the very real problem associated with the fact that we would be dealing with a many-body scattering system, there is an interesting conceptual problem that one can usually ignore in a practical calculation because only (internal) bound states of two-body channels are normally included in such calculations.²⁰ The conceptual problem is that of ensuring that only the state $|\vec{\varphi}_j(\gamma')\rangle$ actually contributes to $f_{\gamma'j, \gamma k}$. This is a nontrivial problem as the following two examples show. First, suppose that one attempts to approximate $|\Psi\rangle$ using a single Lippmann-Schwinger equation, for example

$$|\Psi\rangle = |\varphi_k(\gamma)\rangle + G_k(+)(V_k|\Psi\rangle), \quad (95)$$

where k is the initial arrangement channel. This is an approximation in the sense that such an equation does not define a unique solution to the Schrödinger equation. The eigenstates of H_k form an expansion set for use in (95), and it is evident that to find $f_{\gamma'j, \gamma k}$ from (95), one must use, in principle, all such eigenstates in computing $|\Psi\rangle$. In this case then, bound and continuum states in channel k , and not merely $|\vec{\varphi}_j(\gamma')\rangle$ alone, contribute to the scattering amplitude of interest. An alternate way of stating this is merely to note that $G_k(+)$ gives rise to outgoing waves asymptotically in (open arrangement) channels other than k .

The other example involves approximations to $|\Psi\rangle$ obtained by expanding it in selected states of various channel Hamiltonians, as in the nonorthogonal basis expansion (using states from two-body channels) associated with the coupled reaction channel method discussed e.g., by Udagawa, Wolter, and Coker.²⁰ We assume that only two channels, j and k , need be considered, and we here let the expansion states include two-body and three-body states of both j and k . Because $[H_j, H_k] \neq 0$, $j \neq k$, it is evident that even if $|\vec{\varphi}_j(\gamma')\rangle$ is a two-body state, three-body states of H_k will in general make a contribution to $f_{\gamma'j, \gamma k}$, unless special precautions are taken. Such precautions are nontrivial to impose for $n \geq 3$, as has been noted in another context.²¹

The point of the preceding remarks is that even though *in principle* $f_{\gamma'j, \gamma k}$ is uniquely defined by the projection of $|\Psi\rangle$ onto $\langle \vec{\varphi}_j(\gamma') |$, in practical calculations for many-body scattering systems, states other than $|\vec{\varphi}_j(\gamma')\rangle$ may contribute to $f_{\gamma'j, \gamma k}$, essentially because of the complicated nature of the many-channel scattering problem and the fact

that eigenstates of H_j and H_k are not orthogonal, i.e., $[H_j, H_k] \neq 0$, $j \neq k$. Thus, in formulations of many-body scattering theory in which various H_m (and their associated eigenstates) occur, it is of interest to try to determine from $|\Psi\rangle$ the sources of outgoing waves in the different arrangement channels. This problem has been briefly commented on in a slightly different context by Schwager,²² and a heuristic method for such a determination has recently been given by Redish, Tandy, and L'Huillier.²³ The results of the preceding sections show that this is accomplished within the present formulation of many-body scattering theory in an exceedingly simple way. That is, if the channel-component formulation of the channel-coupling-array theory is used to describe multichannel scattering, as in Sec. II B 2 (and Sec. III A for the time-reversal property), then *only* $|\bar{\varphi}_j(\gamma')\rangle$ need be considered in determining $f_{\gamma',j,\gamma k}$, even if m -body states ($m \geq 3$) from channels other than j are used to calculate $|\Psi\rangle$. That is,

$$\langle \bar{\mathbf{F}}_j, \bar{\varphi}_j(\gamma') | \psi_m \rangle \xrightarrow{r_j \rightarrow \infty} 0, \quad m \neq j.$$

This property follows from the time-dependent analysis of the preceding section, where we showed that *only* $|\psi_j(t)\rangle$ contributes to S_{jk} . To see this, we first note that $|\psi_j(t=0)\rangle$ is identical to the usual time-independent state $|\psi_j\rangle$. Second, it yields asymptotically the same matrix element $\langle \varphi_j(\gamma') | \hat{T}_{jk}(E+i0) | \varphi_k(\gamma) \rangle$ as occurs in S_{jk} [determined from $|\psi_j(t)\rangle$]. But, since this matrix element is the coefficient of $|\bar{\varphi}_j(\gamma')\rangle$ in the asymptotic form of $|\psi_j\rangle$, the preceding property is established. Notice that this property is an intrinsic one, and is thus independent of the presence or absence of m -body states in any arrangement channel other than j .

The time-dependent analysis serves to dramatize this property of the $|\psi_m\rangle$. We note that it also follows from consideration of the expansion (18), Eqs. (21) and (22), and the fact that (22) yields the \hat{T}_{jk} via Eq. (24). That is, among the set $\{|\psi_m\rangle\}$ used in (18), only $|\psi_j\rangle$ yields (ultimately) the scattering amplitude $f_{\gamma',j,\gamma k}$. Hence, the decomposition (18) plus the equation obeyed by the $|\psi_m\rangle$ are a unique way to determine scattering amplitudes. This is in obvious contrast to the results obtained from use of the channel-scattering states, where each $|X_{mk}\rangle$ contributes outgoing waves in all open channels.

These comments help to clarify the meaning of the expansion (18). We noted below Eq. (18) that the subscript j corresponded to the partition $H = H_j + V_j$. The previous implication of this correspondence is now established since $|\psi_j\rangle$ yields \hat{T}_{jk} . \hat{T}_{jk} is the operator for making transitions

from states in channel k to those in channel j , and channel j is defined by the asymptotic states of H_j , which asymptotic states themselves are defined under the assumption that the V_j go to zero sufficiently rapidly.^{4,13} We may therefore describe $|\psi_j\rangle$ as that portion of $|\Psi\rangle$ which yields the two-body scattering amplitudes for transitions to states in channel j . That is, $|\psi_j\rangle$ is the only portion of $|\Psi\rangle$ where the two-body bound-state components $|\bar{\varphi}_j\rangle$ have asymptotically nonvanishing coefficients.

Given that $|\psi_j\rangle$ essentially describes the behavior of $|\Psi\rangle$ in channel j , we see that (18) may be considered as an "expansion" of $|\Psi\rangle$ in the non-orthogonal bases corresponding to the different (two-body) arrangement channels. Thus, while $|\psi_j\rangle$ is not obtained from $|\Psi\rangle$ via an obvious projection operator, it is a clearly identifiable ingredient in (18) and also in the set of Eqs. (21) or (22). In an asymptotic sense, then, $|\psi_j\rangle$ is the portion of $|\Psi\rangle$ present in channel j .

From (22) we see that $|\psi_j\rangle$ contains breakup states of H_j as well; these are necessary to give a complete (exact) representation of $|\psi_j\rangle$ via the eigenstates of H_j . Notice that the eigenstates of H_m , $m \neq j$, could in principle be used to expand the $|\psi_j\rangle$, but that one then loses the advantage of being able to select by inspection the relevant scattering amplitudes $f_{\gamma',j,\gamma k}$ as in an expansion via eigenstates of H_j .

A pair of examples for the case $n=3$, $N_2=3$, i.e., the three-body problem with pair interactions, may help to make these remarks clearer. Introducing the standard cyclic pair notation,

$$V^{(i)} = V_{jk},$$

where V_{jk} is the two-body interaction between particles j and k , we have²⁴

$$V_j = \sum_m \bar{\delta}_{mj} V^{(m)},$$

with $\bar{\delta}_{mj} = 1 - \delta_{mj}$. Then (22) becomes

$$|\psi_m\rangle = |\Phi_k(E)\rangle \delta_{mk} + G_m(+)\sum_{j,m'} W_{mj} \bar{\delta}_{jm'} V^{(j)} |\psi_{m'}\rangle \quad (96)$$

as the relevant set of equations.

In the first example, we make the Faddeev-Lovelace choice^{5,6} for W , which consists in setting $l=j$ in (96) and then choosing $W_{mj} = \delta_{mj}$. This gives

$$|\psi_m\rangle = |\Phi_k(E)\rangle \delta_{mk} + G_m(+)\sum_{m'} \bar{\delta}_{mm'} |\psi_{m'}\rangle. \quad (97)$$

With no loss of generality, we set $k=1$ in (97), leading to

$$\begin{aligned}
|\psi_1\rangle &= |\Phi_1(E)\rangle + G_1(+)V^{(1)}[|\psi_2\rangle + |\psi_3\rangle], \\
|\psi_2\rangle &= G_2(+)V^{(2)}[|\psi_1\rangle + |\psi_3\rangle], \\
|\psi_3\rangle &= G_3(+)V^{(3)}[|\psi_1\rangle + |\psi_2\rangle].
\end{aligned} \tag{98}$$

On using the relation²⁴ $G_i(+)V^{(i)} = G_0(+)t^{(i)}(+)$, where $G_0(+)$ is the three-body free Green's function and $t^{(i)}(+)$ is the $j-k$ pair two-body T matrix in three-body space, we immediately recognize (98) as the set of coupled equations first derived by Faddeev¹⁹ for the three-body problem. It is well known by now²⁵ that the set (98) implies that only in channel m will there be (two-body) outgoing waves corresponding to the bound states of the pair potential $V^{(m)}$. This particular example serves to emphasize the role played by the channel-component states in the present formalism. That is, for the preceding choice of W , the $|\psi_m\rangle$ are precisely the Faddeev wave-function components, whose relation to $|\Psi\rangle$ is just Eq. (18). Notice that if we do not use $G_i(+)V^{(i)} = G_0(+)t^{(i)}$ but retain the channel Green's function $G_i(+)$, then we readily see that through $G_i(+)$, all the bound and continuum states in the potential $V^{(i)}$ enter the description of $|\psi_i\rangle$. However, no matter how $|\psi_j\rangle$ and $|\psi_k\rangle$ might be approximated, $|\psi_i\rangle$ will be the only source of two-body scattering amplitudes in channel i . We again remark that, in differential form, the $|\psi_j\rangle$ of (98) obey a non-Hermitian matrix equation.

The asymptotic property of the $|\psi_m\rangle$ is both manifest and familiar when presented in the Faddeev form, Eq. (98). But this is a property *independent* of the choice among those W 's leading to connected kernel equations, as we have demonstrated in the preceding sections. Our second example establishes this through the choice of the channel-permuting array, Eq. (35), for W . Setting $k=1$ in (96) and using (35) now gives

$$\begin{aligned}
|\psi_1\rangle &= |\Phi_1(E)\rangle + G_1(+)[V^{(1)} + V^{(3)}]|\psi_2\rangle, \\
|\psi_2\rangle &= G_2(+)[V^{(1)} + V^{(2)}]|\psi_3\rangle, \\
|\psi_3\rangle &= G_3(+)[V^{(2)} + V^{(3)}]|\psi_1\rangle.
\end{aligned} \tag{99}$$

The set (99) is clearly very different in appearance from (98), although it is only an alternate representation of the dynamics. Since it is the combination $G_i(+)V^{(i)}$ that is supposed to ensure only outgoing waves in each of the relevant channels for the Faddeev equations, the set (99) might appear to require a detailed analysis in order to establish the sources of outgoing waves in the various channels because of the presence of the factors $G_i(+)V^{(j)}$, $j \neq i$. Or, noting that (99) can

be reexpressed in the form

$$\begin{aligned}
|\psi_1\rangle &= |\Phi_1(E)\rangle + G_1(+)V_2|\psi_2\rangle, \\
|\psi_2\rangle &= G_2(+)V_3|\psi_3\rangle, \\
|\psi_3\rangle &= G_3(+)V_1|\psi_1\rangle,
\end{aligned} \tag{100}$$

then it is the set of channel interactions $\{V_i\}$ that might not seem to provide the necessary cutoffs in coordinate space to prevent $|\psi_i\rangle$ from contributing outgoing waves in channels j or k . (Similar remarks might be thought to hold for the general n, N case also.) It is certainly true for the similar but not identical set (16) that outgoing waves for all channels *will* be contained in each $|X_{mk}\rangle = |\Psi\rangle$. But there is an important difference between (16) and (100): The factors $G_i(+)V_i$ (same subscript) always appear in (16) and *never* appear in (100). This difference is indeed crucial. In Eq. (100), we find that the factors $G_j(+)V_{j+1}$ occur, so that any particular channel interaction will not recur in an iteration of (100) until all other channel interactions have appeared. It is just this characteristic of the CPA that guarantees connectedness of the iterated kernel in general, and which in the present case serves to ensure that only channel j contributes outgoing (two-body) waves to $|\psi_j\rangle$. In the context of the Tandy, Redish, and L'Huillier heuristic method for determining outgoing waves in many-body wave functions,²³ this property of (100) and its N -channel ($N \geq 3$) generalization is equivalent to the statement that there is a lack of primary singularities in any channels other than the one of interest, and hence that each $|\psi_j\rangle$ has the desired connectivity properties.²⁶

These two $n=3, N_2=3$ examples also illustrate an important property of the expansion (18), viz., that the $|\psi_j\rangle$ need not be unique. For example, different choices of W do not lead to the same channel components $|\psi_j\rangle$ in each channel j . Instead, equality of channel components will hold only asymptotically. This is obvious from Eqs. (98) and (99), which are not transformable into one another, although exact solutions of each will yield as amplitudes identical matrix elements of the operators \hat{T}_{jk} . The nonuniqueness is also easily seen in the context of identical particle scattering, for example, $e^- + H$ scattering, $n=2, N_2=2$. In this case, $|\Psi\rangle = |\psi_1\rangle + |\psi_2\rangle$ and $P_{12}|\Psi\rangle = -|\Psi\rangle$, where P_{12} is the two-particle transposition operator and 1 and 2 label the two electrons. These two equations imply that $|\psi_2\rangle = -P_{12}|\psi_1\rangle$. From this it follows that if $|\eta_\alpha\rangle$ is the α th state of hydrogen ($\alpha = nlm$), then equal, but arbitrary amounts of the product $|\eta_\alpha(1)\rangle|\eta_\alpha(2)\rangle$ can be added to $|\psi_1\rangle$ and (with opposite sign) to $|\psi_2\rangle$ without changing $|\Psi\rangle$. Nonuniqueness is an obvious consequence of the fact that $[H_j, H_k] \neq 0, j \neq k$, and as

such, is an intrinsic property of systems which can be partitioned in various ways.

We have seen that the $|\psi_j\rangle$ provide an in-principle means for readily supplying the scattering amplitudes in channel j , implying that the formalism presented in this paper seems well suited to a description of multichannel scattering processes. It is both general and, presumably, flexible, and should be applicable to a wide variety of nonrelativistic many-body problems. In particular, we note that not only is there a W giving the Faddeev equations, but there exists²⁷ a choice of W leading to the Bencze-Redish equations,²⁸ thus indicating one aspect of the generality of the channel-coupling scheme. Applications of this formalism to bound-state problems, to identical particle problems, to variational principles, and to various approximation schemes will be discussed in future work.

Note added in proof. R. C. Johnson has pointed out to us that the discussion of reality of the eigenvalues of \underline{H} as stated in Sec. III A is not valid for the case of continuum (scattering) states. The essential point is that the application of Γ in this case produces the complex conjugate of the radial functions, and the occurrence of the complex conjugate cannot in general be included as a phase factor. Nevertheless, one can still prove that the exact eigenvalues of \underline{H} are real, following

the arguments given by Faddeev (Ref. 19). That is, by summing over j and using $\sum_j W_{jj} = 1$ in Eq. (21), we find $\underline{H}\sum_j |\psi_j\rangle = E\sum_j |\psi_j\rangle$. This is just the Schrödinger equation, all of whose eigenvalues E are real. Since these same eigenvalues E also appear in Eqs. (21) or (26), reality of the exact eigenvalues of \underline{H} is thus ensured. (We conjecture that other properties, similar if not identical to those proved by Faddeev in the case $n=3$, also hold for the exact solutions when $n>3$.) We thus conclude that apart from the time-reversal discussion, the analysis and results of this paper are indeed valid for exact solutions of \underline{H} . This is sufficient to establish a general (exact) time-dependent scattering theory. In addition, the time-reversal arguments, which are valid for discrete states, play an important role in the application of the present formalism to bound-state problems, as will be shown elsewhere. We thank Dr. Johnson for a useful discussion and correspondence on time reversal.

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