1983

Scattering theory in arrangement channel quantum mechanics

James W. Evans
Iowa State University, evans@ameslab.gov

D. K. Hoffman
Iowa State University

D. J. Kouri
University of Houston

Follow this and additional works at: http://lib.dr.iastate.edu/physastro_pubs

Part of the Quantum Physics Commons

The complete bibliographic information for this item can be found at http://lib.dr.iastate.edu/physastro_pubs/432. For information on how to cite this item, please visit http://lib.dr.iastate.edu/howtocite.html.

This Article is brought to you for free and open access by the Physics and Astronomy at Iowa State University Digital Repository. It has been accepted for inclusion in Physics and Astronomy Publications by an authorized administrator of Iowa State University Digital Repository. For more information, please contact digirep@iastate.edu.
Scattering theory in arrangement channel quantum mechanics

**Abstract**
The time-independent scattering theory associated with the non-self-adjoint matrix Hamiltonians $H$ of arrangement channel quantum mechanics is presented in detail first using the 3-particle case as an example. A key feature is the biorthogonality of a suitably constructed set of scattering eigenvectors and duals. Channel space Möller operators, $S$- and $T$-matrices are defined and a variety of properties investigated including the way multichannel unitarity is embedded into the theory. Some remarks on the time-dependent theory are also made. A detailed discussion of channel space density matrix scattering theory (of interest, e.g., in reactive kinetic theory) is presented using the Liouville representation. We describe some special cases including the exclusion of breakup and $2\times2$ choices of three particle $H$.

**Keywords**
Scattering theory, Quantum mechanics, Eigenvalues, Operator theory, Kinetic theory

**Disciplines**
Physics | Quantum Physics

**Comments**
Scattering theory in arrangement channel quantum mechanics

J. W. Evans and D. K. Hoffman
Ames Laboratory and Department of Chemistry, Iowa State University, Ames, Iowa 50011

D. J. Kouri
Department of Chemistry, University of Houston—Central Campus, Houston, Texas 77004

(Received 1 June 1982; accepted for publication 17 September 1982)

The time-independent scattering theory associated with the non-self-adjoint matrix Hamiltonians $H$ of arrangement channel quantum mechanics is presented in detail first using the 3-particle case as an example. A key feature is the biorthogonality of a suitably constructed set of scattering eigenvectors and duals. Channel space Möller operators, $S$- and $T$-matrices are defined and a variety of properties investigated including the way multichannel unitarity is imbedded into the theory. Some remarks on the time-dependent theory are also made. A detailed discussion of channel space density matrix scattering theory (of interest, e.g., in reactive kinetic theory) is presented using the Liouville representation. We describe some special cases including the exclusion of breakup and $2 \times 2$ choices of three particle $H$.

PACS numbers: 03.65.Nk, 03.80. + r

1. INTRODUCTION

Inherent difficulties with the standard Lippmann–Schwinger equation approach to many-body scattering theory\(^1\) have recently lead to the development of a variety of alternative approaches.\(^2\) Most of these implement various forms of decomposition of the wavefunction or $T$-matrices to obtain “well behaved” scattering equations. In this work, we present an analysis of the scattering theory pertaining to the “arrangement channel quantum mechanics” (ACQM) approach.\(^3\) Thus, we consider a system of $N$ distinguishable particles characterized by a Hamiltonian $H$ (with center of mass kinetic energy removed) acting on the $N$-particle Hilbert space $\mathcal{H}$. The ACQM theory is characterized by a matrix Hamiltonian $H$ with operator valued components $H_{\alpha\beta}$ where $\alpha, \beta, \ldots$ belong to some subset of arrangement channels (clustering) for the $N$ particles. Typically, $H$ is not self-adjoint (or even normal) but its components satisfy the summation condition\(^4\)

$$\sum_{\beta} H_{\alpha\beta} = H \quad \text{for all } \beta. \quad (1.1)$$

Other constraints will be described later.

The channel space form of the Schrödinger equation becomes

$$\begin{align*}
(H - \lambda)(|\psi\rangle) &= 0 \quad \text{(time independent),} \\
(H - i\hbar \frac{\partial}{\partial t})(|\psi\rangle) &= 0 \quad \text{(time dependent),}
\end{align*} \quad (1.2)$$

where $|\psi\rangle$ is a vector in the channel space $\mathcal{C} = \bigoplus_\alpha \mathcal{H}_\alpha$ with components $|\psi_\alpha\rangle \in \mathcal{H}_\alpha$. Summing over the components of the rhs of these equations and using (1.1), it follows that either $\sum_\alpha |\psi_\alpha\rangle \neq 0$ and satisfies the corresponding Hilbert space equation or $\sum_\alpha |\psi_\alpha\rangle = 0$. In the context of (1.2), the former are called “physical” eigenvectors for which $\lambda = E \in \mathbb{R}$ and the latter “spurious.”

Recently, there have been some extensive investigations into the spectral and semigroup theory for channel space Hamiltonian $H$.\(^5,6\) Although these are expected to be typically scalar spectral having a complete set of physical and spurious eigenvectors, this as yet has only been demonstrated for the Faddeev case (with some technical assumptions).\(^6\) Consequently, it is appropriate to first consider the time-independent scattering theory where we deal directly with $H$-eigenvectors (rather than $e^{i\alpha Ht}$ as in the time-dependent theory). In fact, the original motivation for the introduction of the $H$ operators was to provide a “well behaved” set of time-independent scattering equations amenable to numerical solution.

If we denote by $H_\alpha$ the $\alpha$-channel Hamiltonian so $H = H_s + V^e$ for all $\alpha$ (where $V^e$ consists of those potentials external to channel $\alpha$), then it is natural to make the decomposition

$$H = H_0 + V, \quad (1.4)$$

where $[H_0]_{\alpha\beta} = \delta_{\alpha\beta} H_\alpha$ and $[V]_{\alpha\beta}$ involves potentials guaranteeing (1.1). The operator $V$ is typically chosen so that the kernel of the resulting scattering equation

$$\psi = \phi + G(E) V \psi \quad (1.5)$$

is “well behaved.” Here $(E - H_0)\phi = 0$, $G = \lim_{z \to 0} G(z) \phi = 0$, $G(E) = (z - H_0)^{-1}$. One usually demands that the kernel $G(E)$ is connected after a finite number of iterations\(^5,5,7\) guaranteeing uniqueness of the scattering solutions of (1.5) (to within any normalizable $H$-eigenvectors of the same “imbedded” eigenvalue). This requirement is further motivated by the “fiber compactness assumption”\(^7,8\) that for reasonable potentials connectivity of some iterate leads to compactness of that or a higher (finite) iterate. This guarantees that standard numerical solution techniques are applicable. In our work we further elucidate the role of these conditions.

In Sec. 2, we investigate the scattering theory of both
the eigenvectors and their corresponding duals for a general 3-particle, 3- (2-cluster) channel \( H \) (remembering that \( H \) is not self-adjoint). A biorthogonality property is proved and channel space Möller operators defined. The corresponding \( S \)- and \( T \)-matrices are introduced in Sec. 3 and various properties, including multichannel unitarity, investigated. Some remarks on the corresponding time-dependent theory are made in Sec. 4. A scattering theory for channel space density matrices is presented in Sec. 5 using the Liouville representation. Various expressions for the transition super operator (which is related to the collision operator in the corresponding reactive Boltzmann equations) are provided. In Sec. 6, some modifications of the above 3-particle case and the extension to the \( N \)-particle case are discussed.

2. SCATTERING EQUATIONS FOR EIGENVECTORS OF \( \tilde{H} \) AND THEIR DUALS

For purposes of illustration, in Secs. 2–5 we consider a system of three distinguishable particles labeled 1, 2, 3. Furthermore, we consider only 3 X 3 channel space Hamiltonians \( H \) with components \( H_{\alpha \beta} \) labeled by the two cluster arrangement channels, namely \((1)(2, 3), (2)(1, 3), (3)(1, 2)\). The discussion of Secs. 2–5 will go through with virtually no constraints on the choice of \( \tilde{V} \) other than that the required solutions to the scattering equation (1.5) exist. However, the advantage of the “connected” choices is that any nonuniqueness of the scattering solutions must correspond to spatially confined \( \tilde{H} \)-eigenvectors of the same eigenvalue as may be seen by iteration of the homogeneous equation. This suggests that all the scattering eigenvectors of \( H \) are accounted for by the appropriate inhomogeneous solutions of (1.5) in contrast to the standard Lippmann–Schwinger equations. Clearly, the latter type of nonuniqueness problems will arise for a continuous range of energies if some \( H_{\alpha \alpha} \) can support bound states in channels other than \( \alpha \), and in Appendix A an example is given where \( H_{\alpha \alpha} = H_{\alpha} \) but disconnectivity still leads to such nonuniqueness.

Another consequence of a “connected” choice of \( \tilde{V} \) is a partial interpretational property of the components of \( \tilde{\psi} \). Specifically, it follows that the different two cluster (pair bound state) parts of the Hilbert space wavefunction are contained asymptotically only in the appropriate channel components. This may not hold for a disconnected choice of \( \tilde{V} \) even where \( H_{\alpha \alpha} = H_{\alpha} \) (see Appendix B).

It is convenient to characterize the eigenvectors of \( H \) assuming asymptotic completeness. If \( \alpha = (i k j) \) and bound states \((i k j) \) exist, then \( H \) has weak (scattering) eigenvectors \( |\psi^+_\alpha(\varepsilon)\rangle \) where \(+ /−\) denotes an asymptotically prepared pre-/post-collisional state with \((i k j) \) bound and \((i) \) free. This asymptotic state is denoted \( |\phi_\alpha\rangle \) and is an eigenvector of \( H_{\alpha} \) with the same energy (eigenvalue) as \( \psi^+_\alpha(\varepsilon) \). There are also eigenvectors \( |\psi^-_\alpha\rangle \) where \(+ /−\) denotes that the three particles are prepared pre-/post-collisionally asymptotically free. The asymptotic state here is a plane wave \(|\phi_\alpha\rangle \) of the same energy (eigenvalue) as \( |\psi^-_\alpha(\varepsilon)\rangle \). For simplicity, we will suppress state labels in this work. There may also be true 3-particle bound state eigenvectors \(|\psi_\alpha\rangle \) of \( H \).

We now consider the weak (scattering) eigenvectors and dual eigenvectors of \( \tilde{H} \). We recall that the components of any eigenvector of \( \tilde{H} \) either sum to an \( \tilde{H} \)-eigenvector with the same real eigenvalue (physical) or sum to zero (spurious).\(^{5,6}\)

Also, by taking any eigenvector of \( \tilde{H} \) and constructing the corresponding equal component dual channel space vector, one obtains a dual eigenvector of \( \tilde{H} \) with the same eigenvalue.\(^{5,6}\) The asymptotic 2-cluster scattering eigenvectors \( \psi^+_\alpha \) corresponding to \(|\phi_\alpha\rangle \), with eigenvalue \( E \), satisfy

\[
\psi^+_\alpha = \phi_\alpha + \tilde{G}^+(E) \tilde{V} \psi^+_\alpha ,
\]

where \([\phi_\alpha]\) \(= \delta_{\alpha \beta} \phi_\beta \) so \((E - \tilde{H}_\beta)\phi_\beta = 0 \). We also have linearly independent eigenvectors \( \psi^+_\alpha, j = 1, 2, 3 \), with eigenvalue \( E \), satisfying

\[
\psi^+_\alpha = \phi_\alpha + \tilde{G}^+(E) \tilde{V} \psi^+_\alpha ,
\]

\((E - \tilde{H}_\beta)\psi^+_\alpha = 0 \) and \( \phi_\alpha \sim \phi \) in the notation of Ref. 5. Another significant choice is where one of the \( \psi^+_\alpha \) is physical and the other two spurious, e.g., \( \Sigma_\alpha \theta_\alpha \) is zero \( \tilde{H} = 1, 2 \) and nonzero \( \tilde{H} = 3 \) (so the physical scattering eigenvectors of \( H \) are in 1-1 correspondence with those of \( \tilde{H} \)).\(^{6}\) We term such a choice canonical. By considering all three \( \psi^+_\alpha \) instead of just \( j = 3 \) (which is sufficient to "represent" the \(|\psi^+_\alpha\rangle \) physics), the inhomogeneous terms in (2.1) constitute a complete set of \( \tilde{H}_\alpha \)-eigenvectors. This will allow definition of corresponding channel space Möller operators, independent of \( \theta^\dagger \), on the whole of \( \psi^\dagger \).

The asymptotic 2-cluster dual scattering eigenvectors \( \xi^\dagger \) of \( \tilde{H} \) chosen with all components equal to \( \langle \psi^+_\alpha \rangle \) satisfy

\[
\xi^\dagger = \xi^\dagger + \xi^\dagger \tilde{V} \tilde{G} \xi^\dagger (E),
\]

where \([\xi^\dagger]\) \(= \delta_{\alpha \beta} \phi_\beta \) so \( \xi^\dagger (E - \tilde{H}_\beta) = 0 \). We also construct linearly independent dual eigenvectors \( \xi^\dagger, j = 1, 2, 3 \), satisfying

\[
\xi^\dagger = \xi^\dagger + \xi^\dagger \tilde{V} \tilde{G} \xi^\dagger (E),
\]

\((E - \tilde{H}_\beta)\xi^\dagger = 0 \) and \( \xi^\dagger \sim \phi^\dagger \) in the breakup region. Here \( \phi^\dagger \) are biorthogonal to \( \theta^\dagger \). If we make the above canonical choice of \( \theta^\dagger \), then \( \phi^\dagger \) and \( \xi^\dagger \) have equal components.

In this work, we assume that all of the above integral equations have suitable solutions which do, in fact, correspond to weak eigenvectors of \( \tilde{H} \). The type of analysis required to prove this rigorously is described for 2-particle scattering in Refs. 9 and 10. If there is any nonuniqueness in these equations, it is assumed a single appropriate solution is chosen. It has been observed previously\(^{5,6}\) that after explicitly setting the components of \( \xi^\dagger \) equal, (2.3) reduce to LS–GT equations.\(^{11}\)

Standard manipulations can be performed for the above equations. For example, any solutions \( \psi^+_\alpha \) of

\[
\psi^+_\alpha = \phi^+_\alpha + \tilde{G}^+(E) \tilde{V} \psi^+_\alpha \quad \xi^\dagger (E - \tilde{H}_\beta) = 0 \]

\((E - \tilde{H}_\beta)\xi^\dagger = 0 \) satisfy

\[
\psi^+_\alpha = (1 + \tilde{G}^+(E) \tilde{V}) \phi^+_\alpha \quad \xi^\dagger (E - \tilde{H}_\beta) = 0 \]

\((E - \tilde{H}_\beta)\xi^\dagger = 0 \) respectively. Here \( \tilde{G}^+(E) = \lim_{\varepsilon \to +0} \tilde{G}(E \pm \varepsilon) \), \( \tilde{G}(z) = (z - \tilde{H})^{-1} \) and we have the standard resolvent equations.


Evans, Hoffman, and Kouri 577
\[ G(z) = G_0(z) + G_0(z) L G(z) = G_0(z) + G(z) L G_0(z). \] (2.7)

It is natural to ask whether the scattering eigenvectors and duals constructed above are biorthogonal in a generalized “delta-function” sense. This is readily verified if the dual vector has equal components. It is also anticipated to be true in general since the corresponding inhomogeneous terms in the integral equations are constructed to be biorthogonal. If the scattering eigenvectors of \( H \) described above together with all physical and spurious normalizable eigenvectors of \( H \) form a basis for the channel space (so \( H \) is scalar spectral), then biorthogonality is immediately verifiable.\(^{4,2}\) However, it is possible to show that biorthogonality of the scattering eigenvectors holds without this assumption (Appendix C).

We now define and investigate the properties of the channel space Möller operator from a time-independent perspective. Firstly, \( Q^\pm \) are defined on the entire channel space by

\[ \psi_0^\pm = Q^\pm \phi_0, \quad \psi^\pm = Q^\pm \phi^\pm, \] (2.8)

where the \( \phi \) also include a sum/integral over state labels. Any ambiguity in (2.8) due to normalizable \( H \)-eigenvectors imbedded into the continuum will not affect \( Q^\pm \) in (2.9) regarded as operators on \( \psi \) (since the imbedded eigenvalues are a set of measure zero). We denote \( \mathcal{D}^\pm_\text{scatt} = \text{Range}(Q^\pm) \), the subspace spanned by the corresponding scattering eigenvectors and expect that \( \mathcal{D}^+_\text{scatt} = \mathcal{D}^-_\text{scatt} = \mathcal{D} \) for reasonable systems.\(^{9,10}\) Also \( \mathcal{D}^\pm_\text{scatt} = \text{Range}(Q^\pm_\text{scatt}) \) where

\[ Q^\pm_\text{scatt} = \sum_{\alpha} \psi^\pm_\alpha \xi_\alpha^\pm \xi_\alpha^\pm \] (2.9)

are \( H \)-invariant \( ([Q^\pm_\text{scatt}, H] = 0) \), nonorthogonal projection operators (from biorthogonality). From (2.6) and (2.7) one obtains expressions for \( Q^\pm \) in terms of the energy dependent operators \( Q^\pm (E) \). Explicitly,

\[ Q^\pm (E) = \lim_{\epsilon \to 0} Q(E + \epsilon i) \] (2.11)

where \( Q(E) = 1 + G(z) L = 1 + G_0(z) L G(z) \). (2.12)

Möller operators \( Q^\pm \) associated with the dual scattering eigenvectors are defined on \( \mathcal{D}^\pm_\text{scatt} \) by

\[ \xi^\pm_\alpha = \xi^\pm_\alpha \xi^\pm_\alpha, \quad \xi^\pm_\alpha = \xi^\pm_\alpha \xi^\pm_\alpha Q^\pm. \] (2.13)

Also defining \( Q^\pm \) to be zero on \( \text{Range}(1 - \mathcal{D}^\pm_\text{scatt}) \), we have

\[ Q^\pm = \sum_{\alpha} \psi^\pm \xi^\pm_\alpha \xi^\pm_\alpha + \sum_{\alpha} \phi^\pm_\alpha \xi^\pm_\alpha. \] (2.14)

Of course, \( \text{Range}(Q^\pm) \) is the full channel space. From (2.6) and (2.7) one obtains expressions for \( Q^\pm \) in terms of the energy dependent operators \( Q^\pm (E) \). Explicitly,

\[ \xi^\pm_\alpha Q^\pm = \xi^\pm_\alpha Q^\pm (E_\alpha), \quad \xi^\pm_\alpha Q^\pm = \xi^\pm_\alpha Q^\pm (E_\alpha). \] (2.15)

where \( Q^\pm (E) = \lim_{\epsilon \to 0} Q(E + \epsilon i) \) and

\[ \hat{Q}(z) = 1 + G(z) L = 1 + \hat{Q}(z) L \hat{Q}_0(z). \] (2.16)

It is readily verified, from biorthogonality, that \( \hat{Q}^\pm = L \) and \( \hat{Q}^\pm \) are independent of the choice of \( \{ \phi^\pm \} \) and satisfy the intertwining relations

\[ H Q^\pm = Q^\pm H, \quad \hat{Q}^\pm \hat{U}_\text{scatt} = \hat{U}_\text{scatt} \hat{Q}^\pm. \] (2.17)

3. CHANNEL SPACE \( S^\pm \) AND \( I^\pm \)-MATRICES

For our discussion of \( S^\pm \)-matrices, we invoke the assumption that \( \mathcal{D}^\pm_\text{scatt} = \mathcal{D}^\pm \), which is anticipated to hold for systems of interest. (In the 2-particle scattering theory, this question is analyzed using Möller operators and the corresponding identity termed “weak asymptotic completeness.”\(^{12}\)) We now define channel space scattering operators by

\[ S^\pm = \hat{Q}_0^\mp \hat{Q}^\pm \] (3.1)

It then follows immediately from (2.17) and (2.18) that

\[ S^\pm S^\pm = S^\mp S^\pm = L \] (3.2)

We shall show that although \( S^\pm \) are not unitary (if the breakup channel is open), the identity (3.2) does incorporate the relationships typically associated with “unitarity” for the multichannel reactive scattering problem.\(^{13}\)

First, we make a connection between the matrix elements of \( S^\pm \) and those of the various corresponding Hilbert space operators \( S^\mp_0, S^\pm_0, S^\mp_0, \) and \( S^\pm_0 \) using the obvious notation. Consider first

\[ (S^\pm)_\alpha = (\xi^\pm_\alpha S^\mp_0 \phi_\alpha) = (\xi^\pm_\alpha S^\mp_0 \phi_\alpha) = (\psi^\pm_\alpha \psi^\pm_\alpha) = (S^\mp_0)_{\alpha \beta}. \] (3.3)

where again state labels have been suppressed and we have used the equal component property of \( \xi^\pm_\alpha \) and the summation property of \( \psi^\pm_\alpha \). Further, it follows that

\[ (S^\pm)_\alpha = (S^\pm_\alpha)_{\beta \gamma}. \] (3.4)

For the other cases, it is convenient to use a canonical choice of \( \phi^\pm \) (and thus \( \psi^\pm_\alpha \)) with \( j = 3 \) (say) physical. One may similarly verify that

\[ (S^\pm)_\alpha = (S^\pm_0)_\alpha \delta_{\alpha j}, \] (3.5)

\[ \delta^j_{\alpha j}. \] (3.6)

The matrix elements with \( 0(k) \), \( k \neq 3 \), as the bra are not simply determined. We have the additional relationships

\[ (S^\pm)_\alpha (0(k)) = (S^\pm_0)_{k 0(k)} \phi^\pm_\alpha (0(k)) = (S^\pm_0)_{k 0(k)0(k)}. \] (3.6)

where in the second, we have indicated the interchange of state labels.
It may now be readily verified that $S^\pm$ are not unitary if for this were the case it would require, for example, that when $\theta' = \xi^\dagger$,

$$(\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\alpha) = (\xi^\dagger \bar{S}^\dagger \xi)\phi_\alpha = S_{\alpha\alpha}^\dagger \phi_\alpha$$

for $j = 1, 2, 3, (3.7)$

which contradicts (3.6) noting $\xi_{\alpha}^\dagger \phi_\alpha$ in that expression corresponds to $\Sigma_{\alpha}^\dagger \phi_\alpha$ here.

The multichannel reactive scattering "unitarity" relationships are now readily obtained. Firstly, using (3.2), (3.3), and (3.5) and thus a canonical choice of $\theta'$, we obtain

$$\delta_{\alpha\beta} = (\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta)$$

$$= \sum_j (\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) \langle \xi_{j}^\dagger \bar{S}^\dagger \phi_\beta \rangle$$

$$+ \sum_{\alpha \beta} (\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) \langle \xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta \rangle$$

$$= \sum_j S_{\alpha\beta}^j \phi_\beta$$

$$= 0$$

where only $j = 3$ contributes in the second term. Similarly one obtains

$$(\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) = \sum_j S_{\alpha\beta}^j \phi_\beta + \sum_j S_{\alpha\beta}^0 \phi_\beta,$$

$$= 0$$

$$= 0$$

We remind the reader that for the canonical choice $\phi^\dagger = (1, 1, 1)$ but $\theta' = \xi^\dagger$ can be any vector satisfying $\Sigma_{\alpha}^\dagger \phi_\alpha = 1$.

Finally, in this section, we make the connection between the $S^\pm$-matrices described above and corresponding channel space $\mathcal{T}^\pm$ matrices. Consider first the $S^\pm_{\alpha\beta}$ matrix elements. Now since

$$\xi_{\alpha}^\dagger = \xi_{\alpha}^\dagger \bar{\mathcal{T}}^\pm (E_\alpha) = \xi_{\alpha}^\dagger + \xi_{\alpha}^\dagger \bar{\mathcal{T}}^\pm (E_\alpha)$$

$$= \mathcal{T}^\pm (E_\alpha),$$

we have

$$(\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) = \xi_{\alpha}^\dagger \bar{\mathcal{T}}^\pm (E_\alpha) \phi_\beta$$

$$= \xi_{\alpha}^\dagger \bar{\mathcal{T}}^\pm (E_\alpha) \phi_\beta$$

$$= \delta_{\alpha\beta}$$

where we have used the formal identity from (A3),

$$(\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) = \xi_{\alpha}^\dagger \bar{\mathcal{T}}^\pm (E_\alpha) \phi_\beta.$$ 

Equation (3.13) motivates the definition of channel space $\mathcal{T}^\pm$ matrices,

$$\mathcal{T}^\pm = \mathcal{U} \mathcal{T}^\pm,$$

so then

$$(\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) = \delta_{\alpha\beta} \mp 2\pi i \delta(E_\alpha - E_\beta) \mathcal{T}^\pm \phi_\beta.$$

Instead of decomposing $\phi^\dagger$ in (3.13), analogous to (3.12), one obtains

$$\mathcal{T}^\pm = \mathcal{U} \mathcal{T}^\pm,$$

where

$$\mathcal{T}^\pm = \mathcal{U} \mathcal{T}^\pm.$$

A similar analysis again implementing a canonical choice $\theta'$, with $j = 3$ physical, shows

$$(\xi_{\alpha}^\dagger \bar{S}^\dagger \phi_\beta) = \delta_{\alpha\beta} \mp 2\pi i \delta(E_\alpha - E_\beta) \mathcal{T}^\pm \phi_\beta,$$

where in (3.19), we have decomposed $\xi_{\alpha}^\dagger \phi_\beta$ and in (3.20), $\phi_\alpha^\dagger$, analogous to (3.12).

From (2.11), (2.12), (2.15), and (2.16) one obtains expressions for $\mathcal{T}^\pm$ and $\bar{\mathcal{T}}^\pm$ in terms of energy dependent operators $\mathcal{T}^\pm (E)$. Explicitly, for any choice of $\theta'$,

$$\mathcal{T}^\pm (E_{\alpha}) \phi_\beta = \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta,$$

$$= \mathcal{T}^\pm (E_{\alpha}) \phi_\beta.$$

From (3.21) and (3.22) it follows that $\mathcal{T}^\pm$ and $\bar{\mathcal{T}}^\pm$ coincide on the $H_{\alpha}$-energy-shell [consistent with (3.16) and (3.17)].

A reactive optical theorem is readily derived in a channel space setting from the identities

$$\mathcal{T}^\pm (E + i\epsilon) - \mathcal{T}^\pm (E - i\epsilon) = \mathcal{U} [\mathcal{T}^\pm (E + i\epsilon) - \mathcal{T}^\pm (E - i\epsilon) \mathcal{U} + \epsilon \mathcal{U} \delta(E + i\epsilon) \mathcal{U} - \epsilon \mathcal{U} \delta(E - i\epsilon) \mathcal{U}]$$

$$= \mathcal{U} [\mathcal{T}^\pm (E + i\epsilon) - \mathcal{T}^\pm (E - i\epsilon) \mathcal{U} + \epsilon \mathcal{U} \delta(E + i\epsilon) \mathcal{U} - \epsilon \mathcal{U} \delta(E - i\epsilon) \mathcal{U}]$$

$$= \mathcal{U} [\mathcal{T}^\pm (E + i\epsilon) - \mathcal{T}^\pm (E - i\epsilon) \mathcal{U} + \epsilon \mathcal{U} \delta(E + i\epsilon) \mathcal{U} - \epsilon \mathcal{U} \delta(E - i\epsilon) \mathcal{U}]$$

$$= \mathcal{U} [\mathcal{T}^\pm (E + i\epsilon) - \mathcal{T}^\pm (E - i\epsilon) \mathcal{U} + \epsilon \mathcal{U} \delta(E + i\epsilon) \mathcal{U} - \epsilon \mathcal{U} \delta(E - i\epsilon) \mathcal{U}]$$

$$= \mathcal{U} [\mathcal{T}^\pm (E + i\epsilon) - \mathcal{T}^\pm (E - i\epsilon) \mathcal{U} + \epsilon \mathcal{U} \delta(E + i\epsilon) \mathcal{U} - \epsilon \mathcal{U} \delta(E - i\epsilon) \mathcal{U}]$$

Thus, formally we can write

$$\mathcal{T}^\pm (E) - \mathcal{T}^\pm (E) = -2\pi i \mathcal{T}^\pm (E(\delta(E - H_\alpha) \mathcal{T}^\pm (E)).$$

Finally, we remark that it follows from (3.16), (3.17), (3.19), (3.20), and (3.3) and (3.5) that we have agreement on the $H_{\alpha}$-energy-shell of the matrix elements of $\mathcal{T}^\pm$, $\bar{\mathcal{T}}^\pm$, and those of the corresponding Hilbert space $\mathcal{T}$-matrices for any choice of $\mathcal{U}$.

4. TIME-DEPENDENT SCATTERING THEORY FOR VECTORS AND DUAL VECTORS

Some significant complications occur in the time-dependent channel space scattering theory not present in treatments involving self-adjoint Hamiltonians. In solving the equations

$$i\hbar \frac{\partial}{\partial t} \psi = \mathcal{U} \psi,$$
one must consider the sense in which $i\mathcal{H}$ generates a time evolution group (remembering $\mathcal{H}$ is typically not self-adjoint or even normal). It has been shown, with some weak constraints, that $-\mathcal{H}$ generates a holomorphic semigroup $e^{-t\mathcal{H}}$ in the open right half-plane. However, at present, it has only been proved that this semigroup extends to the imaginary $z$ axis to yield a time-evolution group $e^{-t\mathcal{H}'}$ when $\mathcal{H}'$ is strictly bounded. In contrast, we indicate below that, with some mild technical assumptions, a functional calculus for $\mathcal{H}$ (and thus $e^{-t\mathcal{H}'}$) can always be constructed on a suitable subspace.

Define $\mathcal{P}_{\text{scatt}}$ to be the projection operator associated with $\mathcal{P}_{\text{scatt}}^\pm$ and $\mathcal{P}_{\text{scatt}}$, and their biorthogonal duals for a canonical choice of $\mathcal{P}_{\text{scatt}}^j$ with $j = 3$ physical. If any bound states $|\psi_\alpha\rangle$ of $\mathcal{H}$ are imbedded into $\mathcal{H}$-eigenvectors $\psi_\alpha^+$ and if $\xi^\pm_{\alpha}$ are the corresponding equal component duals, define $\mathcal{P}_{\text{scatt}} = \sum_{\alpha} \xi^\dagger_{\alpha} \xi_{\alpha}$. Further define $\mathcal{P}_{\text{scatt}}^z = \mathcal{P}_{\text{scatt}} - \mathcal{P}_{\text{scatt}}^\pm$, the projection operator associated with spurious scattering solutions; $\mathcal{P}_{\text{scatt}}^z = \mathcal{P}_{\text{bound}} + \mathcal{P}_{\text{scatt}}^\pm$, the physical projection operator of Refs. 4-6 and $\mathcal{P}_{\text{scatt}}^\pm = \mathcal{P}_{\text{bound}} \pm \mathcal{P}_{\text{scatt}}$. All of these are $\mathcal{H}$-invariant. If we assume the eigenvectors associated with $\mathcal{P}_{\text{scatt}}^\pm$ form part of a basis for $\mathscr{H}$, then it must be generalized Besselian from asymptotic considerations (i.e., convergent linear combinations are $L^2$) and is assumed generalized Hilbertian (i.e., all $L^2$ linear combinations are convergent).16

This, in particular, guarantees that the projection operators and Möller operators of Sec. 2 are bounded. Furthermore, $\mathcal{H}$ is real eigenvalue scalar spectral on Range $\mathcal{P}_{\text{scatt}}^\pm$ (and can be regarded as $\cdots$-self-adjoint there where the involution $\cdots$ is associated with the conjugate linear duality mapping taking eigenvectors to dual vectors). Previous corresponding results were stated only for Range $\mathcal{P}_{\text{scatt}}^\pm$. In particular, we have

$$e^{\pm i\mathcal{H}t} \mathcal{P}_{\text{scatt}}^\pm = e^{\pm i\mathcal{H}t} \mathcal{P}_{\text{scatt}}^\pm + \sum_{\alpha} e^{\pm i\mathcal{H}t} \xi^\dagger_{\alpha} \xi_{\alpha}$$

$$+ \sum_{\alpha} e^{\pm i\mathcal{H}t} \xi^\dagger_{\alpha} \xi_{\alpha} \mathcal{P}_{\text{bound}}$$

$$+ \sum_{\alpha} e^{\pm i\mathcal{H}t} \xi^\dagger_{\alpha} \xi_{\alpha} \mathcal{P}_{\text{bound}}$$

which, from the Hilbertian basis assumption, may be shown uniformly bounded on $\mathscr{H}$. If $\mathcal{P}_{\text{scatt}} = \mathcal{P}_{\text{scatt}}^\pm$ is zero as in the Faddeev case5 or if the corresponding subspace is spanned by normalizable spurious eigenvectors of $\mathcal{H}$, then $\mathcal{H}$ is scalar spectral on the whole channel space5 [so, e.g., (4.3) extends accordingly]. Even where this is not the case a functional calculus on the whole channel space may still be available.17

If there are any complex eigenvalue spurious solutions, then $e^{\pm i\mathcal{H}t}$ will not be uniformly bounded.\textsuperscript{5}

Now we give an heuristic discussion of the scattering behavior of vector wave pulses with various asymptotic clusterings. Firstly, let $\psi^\pm_\alpha(t)$ be a wave pulse satisfying (4.1) with channel $\alpha$ stable asymptotic clustering $\mathcal{P}_{\text{att}}^\alpha(t)$ as $t \to \mp \infty$. Clearly $\psi^\pm_\alpha(t)$ is evolved by $\mathcal{H}_0$ and $\langle \psi^\pm_\alpha(t) | \rho \rangle = \delta_{\alpha \rho} | \psi^\alpha_\rho(t) \rangle$. Thus for suitably well-behaved potentials, we expect that

$$\psi^\pm_\alpha(t) \sim \phi^\pm_\alpha(t)$$

as $t \to \mp \infty$, (4.4)

i.e.,

$$e^{-i\mathcal{H}t} \psi^\pm_\alpha(t) = e^{-i\mathcal{H}t} \phi^\pm_\alpha(t),$$

(4.5)

where "$\sim$" indicates strong convergence and where $\mathcal{P}_{\text{scatt}}^\pm$ (or $\mathcal{P}_{\text{bound}}^\pm$) may be inserted explicitly without change. Similarly let $\phi^\pm_\alpha(t)$ be a wave pulse satisfying (4.1) corresponding to the three particles asymptotically free. The asymptotic behavior of the wave pulse $\phi^\pm_\alpha(t)$ is evolved by $\mathcal{H}_0$. Also $\phi^\pm_\alpha(t)$ is evolved by the pure kinetic energy operator. Thus for suitable potentials, we expect that

$$\phi^\pm_\alpha(t) \sim \psi^\pm_\alpha(t)$$

as $t \to \mp \infty$, (4.6)

i.e.,

$$e^{-\mathcal{H}t} \phi^\pm_\alpha(t) = e^{-\mathcal{H}t} \psi^\pm_\alpha(t),$$

(4.7)

From (4.5) and (4.7) we conclude that

$$Q^\pm = \lim_{t \to \pm \infty} e^{\pm i\mathcal{H}t} \mathcal{P}_{\text{att}} e^{-\mathcal{H}t},$$

(4.8)

and if in addition $i\mathcal{H}$ generates a uniformly bounded time evolution group, then also\textsuperscript{5,9}

$$Q^\pm = \lim_{t \to \pm \infty} e^{\pm i\mathcal{H}t} e^{-i\mathcal{H}t}. $$

(4.9)

A rigorous analysis of the conditions on the potentials required for convergence of (4.9) can be made using a modified Cook's method incorporating the uniform boundedness assumption followed by a stationary phase analysis.5,9

It is appropriate here to introduce the channel space interaction picture defined by

$$\psi^\pm_\alpha(t) = e^{i\mathcal{H}t} \phi^\pm_\alpha(t).$$

(4.10)

Then, for example,

$$\psi^\pm_\alpha(0) = Q(t) \phi^\pm_\alpha(t) = Q^\pm \phi^\pm_\alpha(t),$$

(4.11)

$$\phi^\pm_\alpha(0) = Q(t) \psi^\pm_\alpha(t) = Q^\pm \psi^\pm_\alpha(t),$$

(4.12)

where $Q(t) = e^{i\mathcal{H}t} e^{-i\mathcal{H}t}$, and since

$$\psi^\pm_\alpha(t) \to \phi^\pm_\alpha(t), \phi^\pm_\alpha(t) \to \phi^\pm_\alpha(t)$$

(4.13)

for suitable potentials, it then follows that

$$Q^\pm = \lim_{t \to \pm \infty} Q(t)$$

(4.14)

provided $Q(t)$ is uniformly bounded (in agreement with the above analysis).

We consider now the corresponding aspects of the scattering of dual vector wave pulses. If $\xi^\pm_\alpha(t)$ is a wave pulse satisfying (4.2) with channel $\alpha$ stable asymptotic clustering, then clearly

$$\xi^\pm_\alpha(t) = \langle \phi^\pm_\alpha(t) | \rho \rangle$$

(4.15)
In terms of the interaction picture which here takes the form
\[ \hat{\xi}^{\pm}(t) = \hat{\xi}^{\pm}(0)e^{-iH_{0}t}, \]  
(4.16)
we have
\[ \langle \xi_{\alpha}^{\pm}(t) \rangle_{B} \sim \langle \phi_{\alpha}(t) | e^{-iH_{0}t} \delta_{\alpha \beta} \langle \phi_{\alpha}(0) | \rangle \quad \text{as } t \to \mp \infty. \]  
(4.17)

Using obvious notation (4.17) becomes
\[ \hat{\xi}^{\pm}(t) \sim \hat{\xi}^{\pm}(0) \quad \text{as } t \to \mp \infty. \]  
(4.18)

Next let \( \xi^{\alpha}(t) \) be a wave pulse satisfying (4.2) analogous to \( \phi^{\alpha}(t) \) with asymptotically free particles and let \( \xi^{\pm}(t) \) be the corresponding \( U_{0} \)-evolved asymptotic form analogous to \( \phi^{\pm}(t) \). Then in contrast to (4.18) we expect that
\[ \hat{\xi}^{\pm}(t) \sim \hat{\xi}^{\pm}(0), \]  
(4.19)
so
\[ \hat{\xi}^{\pm}(t) \rightarrow \hat{\xi}^{\pm}(0) \quad \text{as } t \rightarrow \mp \infty, \]  
(4.20)
from the same intuitive reasoning as in the \( \phi^{\pm}(t) \) case. Now
\[ \hat{\xi}^{\pm}(0) = \hat{\xi}^{\pm}(t) | e^{+iH_{0}t} - e^{-iH_{0}t} | U_{0} \]  
(4.21)
which suggests (but does not prove) that
\[ \hat{\xi}^{\pm}(0) \rightarrow \hat{\xi}^{\pm}(0) \quad \text{as } t \rightarrow \mp \infty, \]  
(4.22)
if the limit exists. In fact, this identity can only be satisfied if the partial componentwise interpretational property holds for the \( \phi^{\pm}(t) \)'s. In general the limit on the rhs is "less" than \( \hat{\xi}^{\pm} \) corresponding to outgoing 2-cluster flux lost to the wrong channels (see Appendix D).

5. SCATTERING THEORY FOR DENSITY MATRICES
AND THE LIOUVILLE REPRESENTATION

The time-dependent Liouville/Von Neumann equation for a channel space density matrix \( \rho(t) \) has the form
\[ i\hbar \frac{\partial}{\partial t} \rho(t) = [H_{0}, \rho(t)]. \]  
(5.1)
It is convenient to introduce the super-operators
\[ \mathcal{L}_{0} = [H_{0}, ], \quad \mathcal{L} = [\mathcal{L}, ], \]  
(5.2)
\[ \mathcal{L} = \mathcal{L}_{0} + \mathcal{L}^{\pm} = [U_{0}, ]. \]  
(5.3)

A further useful decomposition is illustrated by \( \mathcal{L} = \mathcal{L}^{\pm} - \mathcal{L}^{\pm} \), where \( \mathcal{L} = U_{0} \otimes \mathcal{L} \)
\[ \mathcal{L}^{\pm} = [\mathcal{L}, \mathcal{L}^{\pm}]. \]  
(5.4)
\[ \mathcal{L}^{\pm} = \mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm}, \]  
(5.5)
where \( \mathcal{L}^{\pm} = \mathcal{L} \otimes \mathcal{L}^{\pm} + \mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm} \). The solution to (5.1) can be formally written as
\[ \rho(t) = e^{-\frac{i\hbar}{\mathcal{L}^{\pm}}(\mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm})} \rho(0) e^{-\frac{i\hbar}{\mathcal{L}^{\pm}}(\mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm})}, \]  
(5.6)
where the super-operator \( \mathcal{L}^{\pm}(t) \) is defined by
\[ \mathcal{L}^{\pm} = \mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm}, \]  
(5.7)

In discussing density matrix scattering theory, we shall make use of the interaction picture
\[ \rho(t) = e^{-\frac{i\hbar}{\mathcal{L}^{\pm}}(\mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm})} \rho(0) e^{-\frac{i\hbar}{\mathcal{L}^{\pm}}(\mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm})}, \]  
(5.8)

Consider a time-dependent scattering problem with packet-like, trace-class solution \( \mathcal{Q}^{\pm}(t) \). The asymptotic condition corresponding to (4.13), (4.18), and (4.19) for collisions where the particle clustering is asymptotically resolved (e.g., the chemical composition of a reactive gas is typically precollisionally resolved in the Boltzmann regime) becomes
\[ \mathcal{Q}^{\pm}(t) \rightarrow \mathcal{Q}_{\text{int}}(0). \]  
(5.9)

Here \( \mathcal{Q}_{\text{int}}(0) \) is diagonal with respect to the channel indices of necessity for the partially bound channels and can be so chosen for the breakup channel. The sense of the limit is described below. Formal manipulation of (5.6) yields
\[ \mathcal{Q}^{\pm}(t) = \mathcal{Q}^{\pm}(0) = \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(0), \]  
(5.10)

Thus from (5.2) and (5.9), we have
\[ \mathcal{L}^{\pm} = \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(0), \]  
(5.11)

Thus from (5.2) and (5.9), we have
\[ \mathcal{L}^{\pm} = \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(0), \]  
(5.12)

where \( E_{\pm} \) are the energies of the \( U_{0} \)-eigenbras/kets of \( \mathcal{A} \).

We now mimic the discussion of Snider and Sanctuary to provide scattering equations for the above super-operators. For motivational and notational convenience we first present scattering equations for the channel space \( \mathcal{L}^{\pm} \)'s of the form
\[ \mathcal{T}^{\pm} = \mathcal{L}^{\pm} \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(\mathcal{T}^{\pm}), \]  
(5.13)
where the super-operator \( \mathcal{Q}_{\text{int}}(\mathcal{T}^{\pm}) \) is defined by
\[ \mathcal{Q}_{\text{int}}(\mathcal{T}^{\pm}) = \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(0) \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(0), \]  
(5.14)

Jauch et al. argue, in a Hilbert space scattering theory setting, that a physical statement of the asymptotic condition should involve density matrices with a limit in terms of a certain physical topology (which in their case corresponds to a trace class norm). The limit in (5.6) and (5.8) should be regarded appropriately. If the potentials are such that \( \mathcal{Q}^{\pm} \) and \( \mathcal{Q}^{\pm} \) exist (a stronger condition than the existence of \( \mathcal{Q}^{\pm} \), Ref. 21), then
\[ \mathcal{Q}^{\pm} = \lim_{t \to \mp \infty} e^{+\frac{i\hbar}{\mathcal{L}^{\pm}}(\mathcal{L}^{\pm} \otimes \mathcal{L}^{\pm})} \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}(0). \]  
(5.15)

From the Möller super-operators (5.8), we can define transition super-operators \( \mathcal{L}^{\pm} \), analogous to (3.15) and (3.18), by
\[ \mathcal{L}^{\pm} = \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}^{\pm} \mathcal{Q}^{\pm} \mathcal{Q}_{\text{int}}^{\pm}. \]  
(5.16)

If we define 
\[
\mathcal{L}^\pm (\omega) = \int \mathcal{Q}^\pm (E) d\mathcal{P}_o (E)
\]
where \{\mathcal{P}_o (E)\} is the spectral family of projectors for \(\mathcal{H}_o\), \(d\mathcal{Q}^\pm (E) \equiv d\mathcal{P}_o (E) \otimes d\mathcal{P}_o (E)\), and \(\mathcal{Q}_o (z) = (z - \mathcal{L}_o)^{-1}\).

Thus \(\mathcal{Q}^\pm (E)\) are the spectral components of \(\mathcal{L}^\pm\). Clearly

\[
\mathcal{T}^\pm = \int \mathcal{T}^\pm (E) d\mathcal{P}_o (E).
\]

Returning to the case of the abstract super-operators, \(\mathcal{L}^\pm\) satisfy

\[
\mathcal{L}^\pm = \mathcal{L}^\pm + \mathcal{Q}_o ^\pm (\mathcal{L}^\pm),
\]

where the (super-) super-operator \(\mathcal{Q}_o ^\pm\) satisfies

\[
\mathcal{Q}_o ^\pm (\omega) = \lim_{\epsilon \to 0} \int \int \int \frac{1}{\delta E - \delta E' \pm i\epsilon} d\mathcal{Q}_o (E_k, E_b) \times d\mathcal{Q}_o (E_k, E_b)
\]

\[
= \lim_{\epsilon \to 0} \int \int \frac{1}{\delta E - \delta E' \pm i\epsilon} d\mathcal{Q}_o (E_k, E_b)
\]

\[
= \lim_{\epsilon \to 0} \int \int \frac{1}{\mathcal{Q}_o (\delta E \pm i\epsilon)} d\mathcal{Q}_o (E_k, E_b),
\]

and \(\delta E = E_k - E_b\), etc. Thus \(\mathcal{Q}_o ^\pm (\delta E)\) are the spectral components of \(\mathcal{Q}_o ^\pm\).

It is appropriate to introduce frequency (energy difference) dependent transition super-operators

\[
\mathcal{L}^\pm (\omega) = \lim_{\epsilon \to 0} \frac{1}{\omega \pm i\epsilon}\mathcal{L}(\omega)
\]

where \(\mathcal{L}(\omega)\) satisfies

\[
\mathcal{L}(\omega) = \mathcal{L}^\pm + \mathcal{Q}_o ^\pm (\mathcal{L}(\omega)) \mathcal{L}(\omega) = \mathcal{L}^\pm + \mathcal{Q}_o ^\pm (\mathcal{L}(\omega)) \mathcal{L}(\omega).
\]

Thus

\[
\mathcal{L}^\pm = \int \mathcal{L}^\pm (\delta E) d\mathcal{Q}_o (E_k, E_b),
\]

and \(\mathcal{L}_o A \mathcal{L}^\pm (\omega) = \omega A \mathcal{L}^\pm (\omega)\). Various other relationships can be obtained for the \(\mathcal{L}(\omega)\)'s, \(\mathcal{Q}_o ^\pm (\mathcal{L}(\omega))\)'s, and appropriate Green functions by standard manipulations (the Hilbert space analogs of some of these are given in Ref. 23 and a more complete list presented in Appendix C). We remark that in the treatment of the scattering theory for energy diagonal density matrices, as with application to reactive Boltzmann equations, \(\mathcal{L}^\pm\) reduce to \(\mathcal{L}^\pm\) = \(\lim_{\epsilon \to 0} \mathcal{L}^\pm (\pm i\epsilon)\).

Under certain conditions the analysis of Fano\(^{19}\) may be adapted to provide a contour integral representation for the transition super-operator \(\mathcal{L}(\omega)\). Firstly, we note that if \(\mathcal{Q}_o (z) = (z - \mathcal{L}_o)^{-1}\), \(\mathcal{Q}_o ^* (z) = (z - \mathcal{L}_o)^{-1}\) then

\[
\mathcal{Q}_o (z) = (z - \mathcal{L}_o + \mathcal{L}_o ^* (z) - \mathcal{L}_o + \mathcal{L}_o ^*)^{-1} = \mathcal{Q}_o (z + \mathcal{L}_o ^* (z) - \mathcal{L}_o + \mathcal{L}_o ^*)
\]

\[
= -\mathcal{Q}_o (d_0 - z).
\]

If we define \(\mathcal{L}_1(z), \mathcal{L}_1^* (z)\) as the solutions of

\[
\mathcal{L}(z) = \mathcal{L}_1(z) + \mathcal{L}_1^* (z) = \mathcal{Q}_o (z) \mathcal{Q}_o (z) \mathcal{L}(z),
\]

then, from (5.19), it follows that

\[
\mathcal{L}(z + \mathcal{L}_o ) = \mathcal{L}_1(z) + \mathcal{L}_1^* (z) = \mathcal{L}_1(z) \mathcal{L}_1^* (z) = \ldots = \mathcal{L}_1(z) \mathcal{L}_1^* (z).
\]

Furthermore, since \(\mathcal{Q}_o (z) = \mathcal{Q}_o (z) \mathcal{Q}_o (z) \mathcal{L}(z) = \mathcal{L}_1 \mathcal{L}_1^* (z)\) we conclude also that (cf. Eu\(^{20}\))

\[
\mathcal{L}_1(z + \mathcal{L}_o ) = \mathcal{L}_1(z + \mathcal{L}_o ) \mathcal{L}_1(z + \mathcal{L}_o ) = \ldots.
\]

Secondly, we make use of the fact that since \(\mathcal{L}_1(z) = \mathcal{L}_1(z) \mathcal{L}_1^* (z)\) represents a decomposition of \(\mathcal{L}_1\) into commuting parts, one may show

\[
\mathcal{Q}_o (z) = \frac{1}{2\pi i} \int_\infty ^\pm -i\delta \mathcal{Q}_o (z) \mathcal{Q}_o (z),
\]

where \(\mathcal{Q}_o (z) = \frac{1}{2\pi i} \int_\infty ^\pm -i\delta \mathcal{Q}_o (z) \mathcal{Q}_o (z)\). The analysis parallels that of Hugenholtz\(^{27}\) for operators with discrete spectra but uses an extension of the Dunford functional calculus for the unbounded self-adjoint operator \(\mathcal{H}_o\).

At this stage we assume that \(\mathcal{L}(\omega), \mathcal{L}^* (\omega)\) are analytic off the real \(z\) axis (which, in particular, requires that \(\mathcal{H}_o\) have no complex eigenvalue spurious solutions). Then using the results listed above, the analysis of Fano\(^{19}\) may be modified to show that

\[
\mathcal{L}(z) = \mathcal{L}(z + \mathcal{L}_o ) - \mathcal{L}_1(z + \mathcal{L}_o ) = \mathcal{L}_1(z + \mathcal{L}_o ) \mathcal{L}_1(z + \mathcal{L}_o ) = \ldots
\]

\[
= \frac{1}{2\pi i} \int_\infty ^\pm -i\delta \mathcal{Q}_o (z - \mathcal{L}_o ) \mathcal{Q}_o (z - \mathcal{L}_o ) - \mathcal{L}_1(z + \mathcal{L}_o ) \mathcal{L}_1(z + \mathcal{L}_o ) = \ldots
\]

The analysis of Eu\(^{20}\) may be adapted to give an alternative derivation of (5.27) in which the requirements that \(\alpha (\mathcal{H}_o) \in \mathbb{R}\) and

\[
\frac{1}{2\pi i} \int_\infty ^\pm -i\delta \mathcal{Q}_o (z - \mathcal{L}_o ) \mathcal{Q}_o (z - \mathcal{L}_o ) = \mathcal{Q}_o (z - \mathcal{L}_o ) \mathcal{Q}_o (z - \mathcal{L}_o ) = \mathcal{Q}_o (z - \mathcal{L}_o ) \mathcal{Q}_o (z - \mathcal{L}_o )
\]

are clear.

A somewhat different algebraic expression for \(\mathcal{L}_1(z)\) may also be obtained from an adaption of Eu's work as follows.\(^{20}\) Define

\[
\mathcal{L}_1(z) = \mathcal{L}_1(z) \mathcal{Q}_o (z) \mathcal{L}_1(z),
\]

\[
\mathcal{L}_1^* (z) = \mathcal{L}_1^* (z) \mathcal{Q}_o (z) \mathcal{L}_1^* (z),
\]

so that

\[
\mathcal{L}_1(z) = \mathcal{L}_1(z) - \mathcal{L}_1^* (z).
\]

Substituting (5.31) into (5.29) and (5.30) and using (5.22) and (5.23) to achieve appropriate rearrangements, one obtains

\[
\mathcal{L}_1^* (z) = \mathcal{L}_1^* (z) + \mathcal{L}_1^* (z) - \mathcal{L}_1(z + \mathcal{L}_o ) = \mathcal{L}_1(z + \mathcal{L}_o ) \mathcal{L}_1(z + \mathcal{L}_o ) = \mathcal{L}_1(z + \mathcal{L}_o ) \mathcal{L}_1(z + \mathcal{L}_o ) = \ldots
\]

Iterating (5.32) once decouples the equations for \(\mathcal{L}_1\) and \(\mathcal{L}_2\) leading to the formal solutions

\[ \mathcal{L}_1(z) = (1 + \mathcal{L}(z + \delta \xi) \mathcal{G}_0(z) \mathcal{L}^*(z - \xi) \mathcal{G}_0(z))^{-1} \times \mathcal{L}(z + \delta \xi) - \mathcal{L}(z + \delta \xi) \mathcal{G}_0(z) \mathcal{L}^*(z - \xi) \mathcal{G}_0(z) \]
\[ \mathcal{L}_2(z) = (1 + \mathcal{L}^*(z - \xi) \mathcal{G}_0(z) \mathcal{L}(z + \delta \xi) \mathcal{G}_0(z))^{-1} \times \mathcal{L}^*(z - \xi) - \mathcal{L}^*(z - \xi) \mathcal{G}_0(z) \mathcal{L}(z + \delta \xi) \mathcal{G}_0(z). \] (5.33)

It is elucidating to compare (5.33) with (5.11) acting on an eigenket \( \phi_{a,b} \) of \( \mathcal{L}_o \). Retaining only terms quadratic in the \( T \)'s in (5.33), one obtains
\[ \mathcal{L}_\pm \equiv (E_a - E_b) \phi_{a,b} \]
\[ \simeq \mathcal{T}_\pm (E_a) \phi_{a,b} - \phi_{a,b} \mathcal{T}^\mp (E_b) \]
\[ + \mathcal{T}_\pm (E_a - E_b) + \mathcal{T}_\pm (E_a) \mathcal{G}_0 \mathcal{T}(E_b) \]
\[ - \mathcal{G}_0 \mathcal{T}(E_a) \mathcal{T}^\pm (E_b) \mathcal{T}^\pm (E_b) \mathcal{T}^\pm (E_a) \mathcal{G}_0 \mathcal{T}(E_b). \] (5.34)

Thus, except where \( E_a = E_b, E_a = E_b \), different energies appear in the quadratic terms of (5.34) and (5.35). The difference must be accounted for in the higher order terms of (5.33). Omlsted et al. have further investigated this question (for the Hilbert space analog).

6. RESTRICTIONS, MODIFICATIONS, AND EXTENSIONS

First we consider a restriction of the analysis of the 3-particle problem in previous sections to the case where the breakup channel is strictly closed. Such systems considered here incorporate a true 3-body potential which guarantees that the total potential becomes unbounded in the breakup region (see Fig. 1). The asymptotic \( \{ \phi_{a,b} \} \) for each arrangement channel \( \alpha \) include an infinite number of bound states. Furthermore, there are now no scattering solutions \( \{ \phi_{a,b}^\pm \} \).

For a real system with tightly bound pairs, it may be possible to add a fictitious 3-body potential to strictly exclude breakup at all energies without significantly affecting the nonreactive and rearrangement collision dynamics of tightly bound reactants for a significant range of energies (of course, artificial higher energy bound states are introduced in all channels).

We expect there to be scattering solutions \( \psi_{a,b}^\pm \) as before but the association with integral equations must be reexamined. For type 1B potentials, all infinite wall potentials must appear on diagonal [otherwise (1.1) requires off-diagonal \( \mathcal{H} \) components with regions of \( -\infty \) potential]. This allows construction of incoming spurious solutions with asymptotic parts in the "wrong" channels and allows spurious parts in outgoing parts of physical scattering solutions (thus destroying interpretation). Consequently, we confine our attention to type 1A potentials and BKLT choice of \( \mathcal{H} \) where only appropriate channel potentials (infinitely deep wells) appear on diagonal. Application of the techniques of Appendix B demonstrates that the components of the scattering solution have the desired interpretational features (the appearance of channel Hamiltonians on diagonal in itself is not enough to guarantee the desired interpretational property as may be seen by analysis of the disconnected example of Appendix A). The \( \mathcal{H}_0 \)-eigenvectors \( \{ \phi_{a,b} \} \) by themselves form a basis for \( \mathcal{E} \) so \( \mathcal{Q}^\pm \) are still defined on the whole space and thus, from (3.1) and (3.4) \( \mathcal{S}^\pm \) are unitary (in the usual sense for operators on the Hilbert space \( \mathcal{E} \)).

Consider next a three particle system where there are no (1 2) bound states. We examine a corresponding \( 2 \times 2 \) channel space Hamiltonian \( \mathcal{H} \), where the components are labeled by \( \alpha \beta \) \( \alpha = 1(2) 3, \beta = 1(2) 3 \), having the decomposition \( \mathcal{H} = \mathcal{H}_0 + \mathcal{Y} \) with \( \mathcal{Y}_{0\alpha\beta} = \delta_{\alpha\beta} \mathcal{H}_0 \). Forming the corresponding integral equation, the discussion of Secs. 2-5 may be readily modified to demonstrate the existence of scattering solutions \( \psi_{a,b}^\pm \) with \( \alpha = 1(2) 3 \), \( \beta = 1(2) 3 \), and \( \psi_{a,b}^\pm \) with \( j = 1,2 \) corresponding to \( |\psi_{a,b}^\pm \rangle \) and \( |\psi_{a,b}^\pm \rangle \), respectively. The correspond-

FIG. 1. Potential plots for \( r_{12}, r_{13}, r_{23} \) collinear configurations.
consider an $N$-particle, $m$-cluster system where breakup and recombination are excluded by inclusion of a suitable potential. Again, a BKLT choice with components labeled by $m$-cluster channels will guarantee the desired interpretational properties. Furthermore, these properties are preserved for suitable energies if a spatially confining potential is added (of course, here, if the energy is too high, then the assignment of clustering inside the container becomes fuzzy). These results follow from the type of analysis described in Appendix B.

For comparison with the 3-particle discussion, we finally consider the general $N$-particle problem where one or more of the 2-cluster channels do not correspond to a stable molecule. If the connected $\mathcal{H}$ includes all 2-cluster channels except some of these, then the partial interpretational property for the 2-cluster parts of the scattering wavefunction is satisfied. The scattering equations may, however, exhibit homogeneously spurious wavelike solutions as seen in Appendix F. If no 2-cluster channels are stable, then a BKLT choice of $\mathcal{H}$ with components labeled by stable 3-cluster (and possibly finer) channels will exhibit a partial interpretational property with respect to the 3-cluster part of the scattering wavefunction. There are further obvious extensions of these results.

**APPENDIX A**

We shall use the notation $i = (i| j k \rangle$, $i = 1, 2, 3$ where $\{ i, j, k \} = \{ 1, 2, 3 \}$ and $V_{ij} = V_{ji}$ for the potential internal to channel $i$ so $H_{ij} = T + V_{ij}$, where $T$ is the kinetic energy. Further, $H = H_{ii} + V_{ii}$ for all $i$ where $V_{ii} = V_{i} + V_{k}$ assuming there are no true 3-body forces. We consider the channel space Hamiltonian

$$\mathcal{H} = \begin{pmatrix} H_{11} & V_{12} & V_{13} \\ V_{21} & H_{22} & 0 \\ V_{31} & 0 & H_{33} \end{pmatrix}. \tag{A1}$$

This does not correspond to a connected choice of $V$ since

\[
\begin{pmatrix} (G_0 V_{12})^n \\ (G_0 V_{13})^n \\ (G_0 V_{23})^{n+1} \end{pmatrix} = \begin{pmatrix} (G_{12} V_{12})^n & 0 & 0 \\ 0 & (G_{13} V_{13})^n - (G_{12} V_{12} V_{13})^n & (G_{13} V_{13} V_{23})^n \\ 0 & 0 & (G_{23} V_{23})^n \end{pmatrix}, \quad n \geq 1, \tag{A2}
\]

and the four corner elements each contains terms of the form $(G_{ij} V_{kl})^n$ (after expansion of $G_{ij} V_{kl}$).

In Sec. 2, we discuss the solutions of the inhomogeneous scattering equation (1.5) associated with the decomposition $\mathcal{H} = \mathcal{H}_0 + \mathcal{L}$. To obtain other scattering solutions of $\mathcal{H}$ in (A1) which correspond to homogeneous solutions of (1.5), we make the decomposition $\mathcal{H} = \mathcal{H}_2 + \mathcal{L}^2$, where

$$\mathcal{H}_2 = \begin{pmatrix} T & V_{12} \\ 0 & H_{11} \end{pmatrix}, \quad \mathcal{L}^2 = \begin{pmatrix} V_{11} & V_{12} & V_{13} \\ V_{21} & V_{22} & 0 \\ V_{31} & V_{32} & V_{33} \end{pmatrix}. \tag{A3}$$

A complete set of $\mathcal{H}_2$ eigenvectors is given by

\[
\begin{pmatrix} 0 \\ \phi \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix} \begin{pmatrix} | \phi \rangle \\ 0 \end{pmatrix}, \begin{pmatrix} | \phi \rangle \\ 0 \end{pmatrix} - \begin{pmatrix} \phi \rangle \end{pmatrix}, \tag{A4}
\]

where $| \phi \rangle$ and $| \psi \rangle$ constitute a complete set of $H_2 (H_2 = T - V_{12})$ partially bound and scattering eigenvectors. These may be taken as the asymptotic parts $\psi^{( \pm )}$ of $\mathcal{H}$ scattering eigenvectors $\psi^{( \pm )}$ which satisfy

$$\psi^{( \pm )} = \phi^{( \pm )} + Q^{( \pm )} (E \mathcal{L}^2) \psi^{( \pm )}. \tag{A5}$$

Choosing $| \phi \rangle = | \phi \rangle$, $| \psi \rangle = | \psi \rangle$ in (A4) generates
from (A5) the scattering solutions
\[ \psi_{\pm 0} = \frac{1}{2} (\psi_{0}^\pm + \psi_{0}^\mp) h (\psi_{g}^\pm - \psi_{g}^\mp) = \begin{pmatrix} |\phi_1^\pm \rangle \\ 0 \\ -|\phi_2^\pm \rangle \end{pmatrix} \]
respectively. If there are any \(|\phi_2\rangle\), then choosing
\[ \hat{\phi} = \begin{pmatrix} 0 \\ |\phi_2\rangle \\ 0 \end{pmatrix} \]
in (A5) generates \(\psi_{\pm 1,3}\) discussed previously, and choosing
\[ \hat{\phi} = \frac{1}{2} \begin{pmatrix} |\phi_2\rangle \\ 0 \\ -|\phi_2\rangle \end{pmatrix} \]
generates another physical scattering solution corresponding to \(|\phi_2^\pm\rangle\) which is a homogeneous solution of (1.5). We can, of course, keep one of these as the physical representative and replace the second by a difference (generating a new spurious wavelike \(H\)-eigensolution). If any \(|\phi_2\rangle\) exist, then choosing
\[ \hat{\phi} = \begin{pmatrix} 0 \\ |\phi_2\rangle \\ 0 \end{pmatrix} \]
generates another new spurious wavelike \(H\)-eigensolution
\[ \psi^\pm = \begin{pmatrix} |\phi_2\rangle \\ 0 \\ -|\phi_2\rangle \end{pmatrix} \]
which is a homogeneous solution of (1.5). The discussion of the spectral theory and functional calculus for ACQM Hamiltonians of Ref. 5 must be slightly modified for this case. In particular, if \(H\) in (A1) is scalar spectral, then the newly discovered wavelike eigensolutions must be included in the basis.

**APPENDIX B**

We investigate here the componentwise interpretational features of the scattering eigenvectors \(\psi^\pm\) of \(H\) first for a connected choice of \(V\). Making a formal expansion of the solution of \(\psi^\pm = \phi^\pm + G^\pm(E)\psi^\pm\) yields
\[ |\psi^\pm\rangle = |\phi^\pm\rangle + \sum_{n=0}^{\infty} (G^\pm(E)\psi^\pm)|\phi^\mp\rangle, \tag{B1} \]
using the component labeling notation of Appendix A. The appearance of \(G^\pm(E)\) allows \(|\psi^\pm\rangle\) to support channel \(j\) clustering [i.e., \(|i k\rangle\) bound states where \(|i j k\rangle = |1 2 3\rangle\)]. The key feature of the connectivity assumption is that it guarantees we cannot resum the second term in (B1) to obtain a contribution of the form \(G^\pm(E)\psi^\pm|\phi^\mp\rangle\) where \(k \neq j\). Here we assume this means that \(|\psi_j^\pm\rangle\) cannot support channel \(k\) clustering.

Another approach uses the differential form of the channel space Schrödinger equation. We simply look at the form of \(H\) in each asymptotic tube and check which components of \(\psi\) can support the corresponding bound states, e.g., in the 2-tube
\[ \mathcal{U}_B = \begin{pmatrix} H_1 & V_1 & 0 \\ 0 & H_2 & V_2 \\ V_1 & 0 & H_3 \end{pmatrix} \sim \begin{pmatrix} T & 0 & 0 \\ 0 & H_2 & V_2 \\ V_2 & 0 & T \end{pmatrix}. \tag{B2} \]
Thus \((\mathcal{U}_B - E)|\psi\rangle = 0\) in the 2-tube becomes
\[ T|\psi_1\rangle = E|\psi_1\rangle, \]
\[ T|\psi_1\rangle + V_2|\psi_2\rangle = E|\psi_2\rangle, \]
\[ H_2|\psi_2\rangle + V_2|\psi_3\rangle = E|\psi_3\rangle, \tag{B3} \]
so \(|\psi_1\rangle\) and thus \(|\psi_2\rangle\) cannot support channel 2-clustering (unlike \(|\psi_3\rangle\)). Both these techniques carry over to the \(N\)-particle case.

Application of both approaches to the example of Appendix A suggests how the interpretational property breaks down. If
\[ \hat{\phi} = \begin{pmatrix} 0 \\ |\phi_2\rangle \\ 0 \end{pmatrix} \]
then
\[ \psi^\pm = \begin{pmatrix} \sum_{n>0} (G(V^3G)^n(g(V^2)|\phi_2\rangle \\ |\phi_2\rangle \\ \sum_{n>1} (G(V^3G)^n-1g(V^2)|\phi_2\rangle \end{pmatrix}, \tag{B4} \]
demonstrating that any post collision 2-channel bound pair part of the wavefunction is distributed between \(|\psi_1^\pm\rangle\) and \(|\psi_2^\pm\rangle\). Accordingly, we can resum the expressions for these components to obtain a contribution \(G_{\psi}^\pm \cdots\). This behavior is obvious from the differential form of the \(H\) eigenvector equation and the structure of \(\mathcal{U}_B\).

**APPENDIX C**

A proof of the biorthogonality of the scattering eigenvectors and duals of \(H\) is given here using biorthogonality of the corresponding inhomogeneous terms in their integral equations [eigenvectors and duals of \(\mathcal{U}_B\)]. As mentioned in the text, this property is directly verifiable where the dual eigenvector has equal components. However, a proof covering all cases is given here. Accordingly, we implement a general notation where \(\tilde{\psi}^{f=\xi}\) denote any scattering eigenvector and corresponding dual of \(H\) associated with energy eigenvalue \(E_j\). The corresponding inhomogeneous terms are denoted by \(\tilde{\psi}^{f=\xi}\) (the \(\pm\) here can be dropped for \(\tilde{\psi}^{f=\xi}\)). Our aim is thus to prove that
\[ \langle \xi^{f=\xi}, \tilde{\psi}^{f=\xi} \rangle = \delta_{fK}, \tag{C1} \]
which should be interpreted as
\[ \langle \xi^{f=\xi}, \int dK a_K \psi^{f=\xi} \rangle = a_f \tag{C2} \]
for suitable \(a_K\). Here \(\int dK\) denotes sum/integration over the state labels and \(\delta_{fK}\) is the corresponding Kronecker/Dirac delta function. The following restricted spectral representation result for \(\mathcal{U}_B\), derived from the Plemelj relations, is required here:
\[ G = (E) \int dK a_K \psi_K^+(t) \]
\[ = \int dK a_K \left( \mp i \alpha(E-E_K) + \frac{\partial}{E-E_K} \right) \psi_K^+(t). \]  
(C3)

Here \( \partial \) represents the Cauchy principal value integral. A corresponding representation for \( G (E) \) comes from the standard theory since \( H_0 \) is self-adjoint.

As a preliminary to proving (C2), we consider
\[ \langle \xi, \bar{K} | \bar{\eta} [G(E)] | \bar{J} \rangle = \int dJ a_J \left[ \pm i \alpha \langle \xi, \bar{J} | \bar{K} \rangle \psi_J^+(E_K - E_J) \right. 
\[ + \left. \left( \frac{\partial}{E-E_K} \right) \psi_J^+ \right] \]
\[ = - \int dJ a_J \langle \xi, \bar{J} | \bar{K} \rangle \bar{\psi}_J^+ \bar{G} \phi^+ (E_J) \bar{\psi}_J^+. \]  
(C4)

Thus finally,
\[ \langle \xi, \bar{K} | \bar{J} \rangle = \left[ 1 + \bar{K} G (E_K) \right] \int dJ a_J \bar{\psi}_J^+ \]
\[ = \int dJ a_J \langle \xi, \bar{J} | \bar{K} \rangle \bar{\psi}_J^+ \bar{G} \phi^+ (E_J) \bar{\psi}_J^+. \]  
(C5)

as required. We have used (2.6), (C4), (2.1), and (2.2).

**APPENDIX D**

We first give an example demonstrating how breakdown of the componentwise interpretational property implies that
\[ Q^{-1}(t) = \bar{Q}^{-1} \]  
(D1)

We take the Hamiltonian of Appendix A and suppose that (13) bound states exist. The outgoing 2-channel bound state components in \( \phi_{\pm(1,3)} \) were shown to be distributed between the 1 and 3 components. Consequently, if
\[ \xi(t) \langle 0, \phi_2(0) | e^{-iHt} | 0 \rangle \]  
then
\[ 0 \sim \langle \xi(t) | \phi_{\pm(1,3)} (0) \rangle \]
\[ = \langle \xi(t) | \bar{Q}^{-1} (t) \phi_{\pm(1,3)} (0) \rangle \]
\[ = 0 \]  
\[ \text{as } t \rightarrow \infty. \]  
(D2)

Specifically, one can show in this case that
\[ \lim_{t \rightarrow \infty} Q^{-1}(t) = (1 - \sum_k \phi_k \bar{\phi}_k) \bar{Q}^{-1}. \]  
(D3)

For general 3-particle, 3-channel \( H \), if any outgoing \( i \) channel bound state flux is missing from the \( i \) component of \( \phi_{\pm(1,3)} (0) \), then \( \lim_{t \rightarrow \infty} \langle \xi(t), \phi_{\pm(1,3)} (t) \rangle \) will be less than \( \bar{S}_{\pm(1,3)}. \)

**APPENDIX E**

There are many relations satisfied by the super-operators of Sec. 5 analogous to standard scattering theory identities. Some of these are presented here. Suppose that
\[ H_0 \mathcal{A} = E_0 \mathcal{A}, \]  
so that \( \mathcal{L}_0 \mathcal{A} = (E - E_0) \mathcal{A} \). Then clearly
\[ \mathcal{Q}(E') = \mathcal{Q}(E) \mathcal{A}, \]  
(E1)
so
\[ \mathcal{Q}(E') = \mathcal{Q}(E) \mathcal{A} \mathcal{Q}(E'), \]  
(E2)

\[ \mathcal{Q}(E') = \mathcal{Q}(E) \mathcal{A} \mathcal{Q}(E'), \]  
(E3)

On the other hand if \( \mathcal{A} \) satisfies
\[ \mathcal{L}_0 \mathcal{A} = w \mathcal{A}, \]  
(E4)

\[ \mathcal{Q}(E') = \mathcal{Q}(E) \mathcal{A} \mathcal{Q}(E'), \]  
(E5)

where \( \mathcal{Q}(E') = \lim_{t \rightarrow \infty} \mathcal{Q}(E, iE') \) and \( \mathcal{Q}(E) \) satisfies
\[ \mathcal{Q}(E) = 1 + \mathcal{Q}(E') \mathcal{Q}(E), \]  
(E6)

where \( \mathcal{Q}(E) = (E - E')^{-1} \) so
\[ \mathcal{Q}(E) = \mathcal{Q}(E_0) + \mathcal{Q}(E_0) \mathcal{Q}(E) = \mathcal{Q}(E_0) + \mathcal{Q}(E) \mathcal{Q}(E_0). \]  
(E7)

Thus
\[ \mathcal{Q}(E) = \int \mathcal{Q}(E, E') d\mathcal{Q}(E,E'). \]  
(E8)

The frequency dependent transition super-operator of (5.17) may also be defined by
\[ \mathcal{L}(z) = z \mathcal{Q}(z), \]  
(E9)

so \( \mathcal{Q}(z) = \mathcal{Q}(z) \mathcal{Q}(z) \) and \( \mathcal{L}(z) \mathcal{Q}(z) = \mathcal{L}(z) \mathcal{Q}(z) \). Besides (5.17), \( \mathcal{L}(z) \) also satisfies
\[ \mathcal{L}(z) = z \mathcal{L}(z) \mathcal{Q}(z). \]  
(E10)

**APPENDIX F**

For the 3-particle system where no (1,2) bound states exist, we consider the following 2x2 choices of \( \mathcal{H} \). Firstly, if
\[ \mathcal{H} = (H_V + V_1 V_2) H_2 + V_2 \]  
(F1)

and
\[ G(z) = (z - H)^{-1} \]  
then
\[ |\psi(n), \rangle = G(E_n) V_2 |\psi(n)\rangle, \]  
\( k = 1,2 \),
\[ |\psi(\alpha), \rangle = G(\tilde{E} |\psi(\alpha), \rangle, \]  
\( k = 1,2 \), \( \alpha = (1,2), (2,3) \) and (1). (F2)

Further choosing \( \theta^j = \zeta^j \) so \( \psi_{\alpha 2} = \psi_{\alpha 2} \) (Ref. 5) and setting
\[ (E - H_2) \delta \tilde{z} = 0, \]  
\( t \tilde{z} \), one obtains
\[ \psi_{\alpha 2} = \alpha_k \psi_{\alpha 2} + G_2 \tilde{z} \tilde{t} \psi_{\alpha 2} \]  
(F3)

where \( \{ k, \tilde{k} \} = \{ 1,2 \} \).

Secondly, if
\[ \mathcal{H} = (T + V_1 + V_3) V_2 + T + V_2 \]  
(F4)
then
\[ |\psi(n_k)\rangle = G_0(E_k)|V_k + \delta_{k,1} V_3\rangle |\psi(n)\rangle, \quad k = 1, 2, \]
\[ |\psi_\pm\rangle = G_0\biggl(\biggl( t^{\pm}_{\frac{1}{2}} G_0 V_2 \biggr) |\phi_0\rangle + \biggl( t^{-}_{\frac{1}{2}} G_0 V_3 \biggr) |\phi_0\rangle \biggr) \]
and
\[ \psi_\pm = \epsilon^{\pm}|\phi_0\rangle + G_0\left( \begin{array}{c} t^{\pm}_{\frac{1}{2}} \epsilon |\phi_0\rangle \\ t^{-}_{\frac{1}{2}} \epsilon |\phi_0\rangle \end{array} \right) \]
\[ = \epsilon^{\pm}|\phi_0\rangle + G_0\left( \begin{array}{c} t^{\pm}_{\frac{1}{2}} \epsilon |\phi_0\rangle \\ t^{-}_{\frac{1}{2}} \epsilon |\phi_0\rangle \end{array} \right) \]
\[ + G_0\left( \begin{array}{c} t^{\pm}_{\frac{1}{2}} \epsilon |\phi_0\rangle \\ t^{-}_{\frac{1}{2}} \epsilon |\phi_0\rangle \end{array} \right) \]
\[ \times \psi_\pm = \psi_\pm. \]

From (F2) and (F5) we see that for a canonical choice of \( \theta^\prime \), the spurious wave-like eigenvectors span
\[ \zeta = \{ \psi; \Sigma_{-1} \} |\psi_0\rangle = 0 \]. Thus, with the usual technical assumptions, both these Faddeev-like \( \mathcal{H} \) are scalar spectral. Furthermore, the partial interpretational property is satisfied for both and the scattering equations with kernel \( G_0 \) have unique solutions.

Finally, we consider the BKLT-type choice
\[ \mathcal{H} = \left( \begin{array}{cc} H_1 & V_1 + V_3 \\ V_2 + V_3 & H_2 \end{array} \right) \]
(F7)
In addition to scattering solutions analogous to those described above, others may exist which are associated with the decomposition
\[ \mathcal{H} = \mathcal{H}_3 + \mathcal{V}^3 \]
(F8)
where
\[ \mathcal{H}_3 = \left( \begin{array}{cc} T & V_3 \\ V_2 & T \end{array} \right), \quad \mathcal{V}^3 = \left( \begin{array}{cc} V_1 & V_2 \\ V_2 & V_1 \end{array} \right) \]

A complete set of \( \mathcal{H}_3 \) eigenvectors is given by
\[ \left\{ \begin{array}{c} (\phi) \\ (\phi) \end{array} \right\}, \quad \left\{ \begin{array}{c} (\phi) \\ (-\phi) \end{array} \right\}, \]
(F9)
where \( \left\{ (\phi); (\phi) \right\} = \left\{ (\phi), (\phi) \right\} \) constitute complete sets of \( \mathcal{H}_3 \) scattering and partially bound eigenvectors. These may be taken as the asymptotic part \( \epsilon^{\pm} \) of \( \mathcal{H} \) scattering eigenvectors which satisfy
\[ \psi_\pm = \psi^{\pm}_{0} + G_0(E)\mathcal{V}_3^2 \psi_\pm \]
(F10)
This generates scattering solutions
\[ \frac{1}{2} (\psi^{\pm}_{20} + \psi^{\pm}_{23}), \quad \psi^{\pm} = \left( \begin{array}{c} (\phi) \\ -\epsilon (\phi) \end{array} \right), \]
\[ \psi^{\pm} = \psi^{\pm}_{20} - \psi^{\pm}_{23} = \left( \begin{array}{c} (\phi) \\ \epsilon (\phi) \end{array} \right), \]
respectively. Clearly
\[ \psi_\pm = \left( \begin{array}{c} (\phi) \\ -\epsilon (\phi) \end{array} \right) \]
are homogeneous solutions of (1.5). The partial interpretational property is not destroyed by the existence of such solutions since they do not mix with the outgoing parts of other scattering solutions. This is verified by taking a Neumann expansion for the latter and observing that it is not possible to resum any subset of terms to obtain a contribution \( \mathcal{G}_2 \)...
where \( \mathcal{G}_2(z) = (z - \mathcal{H}_3)^{-1} \). The structure of this Hamiltonian is discussed in more detail in Ref. 30.

Remark: Suppose now that (1 2) bound states do exist and consider the \( \mathcal{H}_3 \) eigenvectors \( \psi^{\pm}_{012} \) for the above choices of \( \mathcal{H} \). For (F1) we may choose the position of the asymptotic part in either (of the 2) components, for (F4) only in component 1, and for (F7) only distributed equally in both components.