# Existence and uniqueness of bound-state eigenvectors for some channel coupling Hamiltonians

J. W. Evans

*Ames Laboratory*[a] *and Department of Chemistry, Iowa State University, Ames, Iowa 50011*

For the three-particle, two-cluster, $2 \times 2$ channel coupling Hamiltonians used, e.g., in $H_2^+$ and He bound-state calculations, we demonstrate that typically there exist unique eigenvectors for all bound states. This result also holds, with some technical assumptions on the potentials, for the corresponding $3 \times 3$ case provided there are no spurious eigenvectors with bound-state eigenvalues. The proofs use the analogous results for the corresponding Faddeev-type Hamiltonians together with spurious multiplier relationships.

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## I. INTRODUCTION

Inherent difficulties with the standard Lippmann–Schwinger equation approach to many-body scattering theory[1] have lead to the development of a variety of alternative approaches. These are often based on decomposition of the wave function or $T$-matrices into components associated with various clusterings (arrangement channels) of the particles.[2] The "arrangement channel quantum mechanics" approach[3] for a system of $N$ nonrelativistic particles is characterized by a non-Hermitian Hamiltonian H with components $H_{\alpha\beta}$ labeled by some subset of the $N$ particle clusterings $\alpha, \beta, \cdots$. These satisfy[4]

$$\sum_{\alpha} H_{\alpha\beta} = H \quad \text{for all } \beta, \tag{1}$$

where $H$ is the $N$ particle Hilbert space Hamiltonian. From Eq. (1), any eigenvector $\psi$ of H with components $|\psi_\alpha\rangle$ and eigenvalue $\lambda$ is either (a) *physical* satisfying $\sum_\alpha |\psi_\alpha\rangle = |\psi\rangle \neq 0$ and $\lambda = E$, where $H |\psi\rangle = E |\psi\rangle$ or (b) *spurious* satisfying $\sum_\alpha |\psi_\alpha\rangle = 0$.

Despite a recent analysis of the structure of general H,[5] there are still many unresolved questions. For example, if there exists a physical eigenvector of H for each one of $H$ and if the spurious eigenvectors span $\{\psi: \sum_\alpha |\psi_\alpha\rangle = 0\}$, then H is scalar spectral (its eigenvectors and their biorthogonal duals provide a spectral resolution of the identity). However, at present, the only nontrivial cases for which this has been proved are some three-particle Faddeev-like choices $H_F$.[6,7] Should H contain the appropriate physics, then clearly the existence of a "representation" where the wave function naturally decomposes into arrangement channel components is extremely useful.[4] The first application outside of scattering theory involved molecular bound-state calculations,[8] despite the lack of a proof of existence of these solutions for the Baer–Kouri–Levin–Tobocman $H_B$ used. Dramatic early successes with simple wave function component approximations suggested existence of the solutions considered and also a rigorous basis for atoms/molecules-in-molecules pictures. These results are supported by more recent finite-element method calculations.[9] The significance of a rigorous

proof of bound-state existence and uniqueness should be clear from the above discussion and is given here for three-particle, two-cluster, $2 \times 2$ and $3 \times 3$ $H_B$ using this property for the corresponding $H_F$.

## II. BOUND-STATE EIGENVECTOR EXISTENCE AND UNIQUENESS

For a system of three distinguishable particles labeled $i = 1, 2, 3$, we denote the two cluster channels $i = (i)(j k)$, where $\{i, j, k\} = \{1, 2, 3\}$. Let $T$ be the kinetic energy (with center-of-mass part removed) and $V_i = V_{jk}$ the potential internal to channel $i$, so $H_i = T + V_i$. We assume the particles act through pairwise potentials, so $H = H_i + V^i$ for all $i$, where $V^i = V_j + V_k$.

Consider first the $2 \times 2$ channel coupling Hamiltonians

$$H_B = \begin{pmatrix} H_1 & V^2 \\ V^1 & H_2 \end{pmatrix}, \quad H_F = \begin{pmatrix} H_1 + V_3 & V_1 + V_3 \\ V_2 & H_2 \end{pmatrix} \tag{2}$$

that are related through the identity

$$(\lambda - H_B) = (\lambda - H_F)(1 + M(\lambda)), \tag{3}$$

where the "spurious multiplier" $M(\lambda) = G_0(\lambda)(H_F - H_B)$ and $G_0(\lambda) = (\lambda - T)^{-1}$. An "integral" form of Eq. (3) can be obtained by multiplying from the left by $G_0(\lambda) = (\lambda - H_0)^{-1}$, where $(H_0)_{ij} = \delta_{ij} H_i$. If $|\psi\rangle$ is a bound state of $H$ with eigenvalues $E < 0$, then the corresponding $H_F$ eigenvector is given by[7]

$$\psi_F = \begin{pmatrix} G_0(E)(V_1 + V_3)|\psi\rangle \\ G_0(E)V_2|\psi\rangle \end{pmatrix}. \tag{4}$$

From Eq. (3) and the summation condition (a) for physical eigenvectors, any corresponding $H_B$ eigenvector $\psi_B$ must satisfy

$$(1 + M(E))\psi_B = \psi_F. \tag{5}$$

If $E > 0$, then it is readily verified that the expressions of Eqs. (4) and (5) still hold with $G_0(E) = P(E - T)^{-1}$, where $P$ represents the Cauchy principal value integral. Equations (4) and (5) motivate the following result:

**Theorem 1:** Suppose that the eigenvalue $E$ of a bound state $|\psi\rangle$ of $H$ is not in the spectrum of $\hat{H}_3 = T - V_3$. Then if $\hat{G}_3(\lambda) = (\lambda - \hat{H}_3)^{-1}$,

$$\psi_B = \begin{pmatrix} \hat{G}_3(E)(V_1 + V_3)|\psi\rangle \\ |\psi\rangle - \hat{G}_3(E)(V_1 + V_3)|\psi\rangle \end{pmatrix} \tag{6}$$

is the corresponding $H_B$ eigenvector. If $E$ is in the spectrum of $\hat{H}_3$ but does *not* correspond to the threshold energy of some $\hat{H}_3$ partially bound state or the complete breakup, then Eq. (6) still holds with $\hat{G}_3(E) = P(E - \hat{H}_3)^{-1}$.

*Proof*: The simplest proof of Eq. (6) is via direct substitution into the $H_B$ eigenvalue equation. For motivational purposes, we remark that this form of $\psi_B$ can be obtained from Eq. (5) by noting that, formally,

$$(1 + M(E))^{-1} = \begin{pmatrix} (1 + G_0(E)V_3)^{-1} & 0 \\ 1 - (1 + G_0(E)V_3)^{-1} & 1 \end{pmatrix}$$
$$= \begin{pmatrix} \hat{G}_3(E)(E - T) & 0 \\ 1 - \hat{G}_3(E)(E - T) & 1 \end{pmatrix} \qquad (7)$$

and substituting from Eq. (4) for $\psi_F$. ∎

Starting with a modified choice of $H_F$, where $V_3$ now appears on the second row, one similarly obtains

$$\psi_B = \begin{pmatrix} |\psi\rangle - \hat{G}_3(E)(V_2 + V_3)|\psi\rangle \\ \hat{G}_3(E)(V_2 + V_3)|\psi\rangle \end{pmatrix}. \qquad (8)$$

The consistency of Eqs. (6) and (8) is readily verified. Suppose that particles 1 and 2 are identical so that $|\psi\rangle$ is either gerade $|\psi^+\rangle$ or ungerade $|\psi^-\rangle$. Let $|\psi_{Bi}^{\pm}\rangle$, $i = 1, 2$ denote the channel components of the corresponding $\psi_B^{\pm}$ and let $P_{12}$ be the operator which interchanges particles 1 and 2; so $|\psi^{\pm}\rangle = \pm P_{12}|\psi^{\pm}\rangle$. Then using the expression for $|\psi_{B1}^{\pm}\rangle$ from Eq. (6) and $|\psi_{B2}^{\pm}\rangle$ from Eq. (8), one recovers the previously observed result[8]

$$|\psi_{B1}^{\pm}\rangle = \pm P_{12}|\psi_{B2}^{\pm}\rangle. \qquad (9)$$

We remark that the $\psi_F(\psi_B)$ are strictly only eigenvectors if their components lie in the three-particle Hilbert space [$T$-$(\hat{H}_{3-})$ boundedness of the $V_i$ is sufficient[6]]. Then the results of Ref. 7 show that since the physical $H_F$ and $H_B$ (weak) eigenvectors include all scattering solutions and their spurious (weak) eigenvectors span $\{\psi: \Sigma_i |\psi_i\rangle = 0\}$, these Hamiltonians are scalar spectral. If the components of any $\psi_F(\psi_B)$ be outside the three-particle Hilbert space, then the corresponding $E$ is in the residual (rather than point) spectrum of $H_F(H_B)$.[5]

The Hamiltonian $H_B$ was first used for $H + e$ scattering[10] and since for $H_2^+$, He, $H^-$ bound-state calculations.[8] A natural assignment of particles 1, 2, and 3 is made so that no (1 2) pair bound states exist. The analysis above applies where all degrees of freedom are retained, as well as to the Born–Oppenheimer (BO) case, where the nuclear kinetic energies are ignored. Except for the BO $H_2^+$ case, an infinite number of $\hat{H}_3$ partially bound states exist.

We now consider $3 \times 3$ choices of $H_F$ and $H_B$ corresponding to the above system where the existence of bound-state solutions is of considerable theoretical and possible practical interest. Here we have

$$H_B' = \begin{bmatrix} H_1 & 0 & V^3 \\ V^1 & H_2 & 0 \\ 0 & V^2 & H_3 \end{bmatrix}, \quad H_F' = \begin{bmatrix} H_1 & V_1 & V_1 \\ V_2 & H_2 & V_2 \\ V_3 & V_3 & H_3 \end{bmatrix} \qquad (10)$$

that are related through the identity

$$(\lambda - H_B') = (\lambda - H_F')(1 + M'(\lambda)), \qquad (11)$$

where the "spurious multiplier" $M'(\lambda) = G_0(\lambda)(H_F' - H_B')$. The familiar integral form of Eq. (11)[11] can be obtained by

multiplying from the left by $G_0'(\lambda) = (\lambda - H_0')^{-1}$, where $(H_0')_{ij} = \delta_{ij}H_i$. For a bound state $|\psi\rangle$ with $E < 0$, the corresponding unique $H_F'$ eigenvector is given by $(\psi_F')_k = G_0(E)V_k|\psi\rangle$ for $k = 1, 2, 3$.[6] From Eq. (11) and the summation condition (a), any corresponding $H_B$ eigenvector $\psi_B'$ must satisfy

$$(1 + M'(E))\psi_B' = \psi_F'. \qquad (12)$$

If $E > 0$, the expression for $\psi_F'$ and Eq. (12) still hold with $G_0(E) = P(E - T)^{-1}$ (cf. above). Equation (12) motivates the following result:

**Theorem 2:** Let $E \neq 0$ be the eigenvalue of some bound state $|\psi\rangle$ of $H$. Suppose that $V_i$ satisfy the conditions of Hunziker's theorem[12] and guarantee that $M'(E)$ is bounded. (We assume $T$-boundedness for the latter.) Then either there exists a unique eigenvector $\psi_B'$ of $H_B'$ satisyfing Eq. (12) or $H_B'$ has a spurious eigenvector with eigenvalue $E$. In the latter case (nonunique), $\psi_B'$ exist only if certain biorthogonality conditions are (accidentally) met.

*Proof*: A simple calculation shows that $(M'(\lambda))^2$ is *connected*.[2] Consequently, since $M'(\lambda)$ involves only the free Green's function and given the assumptions on $V_i$, Hunziker's theorem may be applied to prove that $(M'(\lambda))^2$ is *compact*.[12] Then from Fredholm theory[13] and noting that $(1 - M'(E))\psi_F'$ is normalizable, it follows that either

$$(1 - (M'(E))^2)\psi_B' = (1 - M'(E))\psi_F' \qquad (13)$$

has a unique solution $\psi_B'$, which also satisfies Eq. (12), or

$$(1 - (M'(E))^2)\psi = 0 \qquad (14)$$

has a nontrivial solution. In the former case, to show that $\psi_B'$ in Eq. (13) satisfies Eq. (12), one simply notes that

$$(1 - (M'(E))^2)\{(1 + M'(E))\psi_B' - \psi_F'\} = 0. \qquad (15)$$

Let $P(\lambda, M)$ denote the M-invariant projection operator onto the eigenvectors of the operator M with eigenvalue $\lambda$. Then a simple calculation, e.g., using a Dunford contour integral representation for the P's,[14] shows that

$$P(\pm 1, M'(E)) = \tfrac{1}{2}(1 \pm M'(E))P(1, (M'(E))^2), \qquad (16)$$

which is bounded, since $M'(E)$ is bounded. Thus, if $\psi$ satisfies Eq. (14), then either $(1 + M'(E))\psi = 0$ or $(1 - M'(E))\psi = 0$. Suppose first that the former is satisfied for *some* solution of Eq. (14). This is just the familiar condition for $\psi$ to be a spurious $H_B'$ eigenvector with eigenvalue $E$.[11] Second, suppose that the latter is satisfied for *all* solutions of Eq. (14). If $\zeta'$ denotes a three-component dual-channel space vector, then from Eq. (16) it is clear that all solutions of $\zeta'(1 - (M'(E))^2) = 0'$ satisfy $\zeta'(1 - M'(E)) = 0'$. Thus, from Fredholm theory, Eq. (13) still has (nonunique) solutions $\psi_B'$. Furthermore, the choice of $\psi_B'$ biorthogonal to all the above $\zeta'$ is the unique solution of Eq. (12).

Finally, we note that if spurious eigenvectors exist, then the corresponding solutions of $\zeta'(1 + M'(E)) = 0'$ must be biorthogonal to $\psi_F'$ for there to exist a solution $\psi_B'$ of Eq. (13). ∎

The possibility that physical bound states can be replaced by spurious solutions has been anticipated from gen-

eral spectral theoretic arguments. These show that the point spectrum of $H$ is contained in the union of the point and residual spectra of H (Ref. 5), from which this replacement strictly follows only if the eigenvalue of a "missing" bound state is physically nondegenerate and not contained in the residual spectrum of H. An explicit example of this replacement phenomenon has been given in Ref. 15. Of course, a similar analysis to that given above follows for the other channel-coupling choice of $3 \times 3$ $H'_B$.[3]

Finally, we remark that if a true three-body potential $V_{123}$ is included diagonally in the Hamiltonians of Eq. (2), then the analysis goes through the minor modifications. For those of Eq. (10), the same is true provided the analog of Hunziker's theorem with $G_0(\lambda)$ replaced by $G_{123}(\lambda) = (\lambda - T - V_{123})^{-1}$ is valid, and the $V_i$ are $T + V_{123}$ bounded. A treatment regarding spurious multipliers as intertwining operators for pairs of channel space Hamiltonians, extending the analysis presented here, is given in Ref. 16.

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1162     J. Math. Phys., Vol. 24, No. 5, May 1983

J. W. Evans     1162