Conservation of connectivity of model-space effective interactions
under a class of similarity transformation

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Abstract

Effective interaction operators usually act on a restricted model space and give the same energies
(for Hamiltonian) and matrix elements (for transition operators etc.) as those of the original oper-
ators between the corresponding true eigenstates. Various types of effective operators are possible.
Those well defined effective operators have been shown being related to each other by similarity
transformation. Some of the effective operators have been shown to have connected-diagram ex-
pansions. It is shown in this paper that under a class of very general similarity transformations,
the connectivity is conserved. The similarity transformation between hermitian and non-hermitian
Rayleigh-Schrödinger perturbative effective operators is one of such transformation and hence the
connectivity can be deducted from each other.
I. INTRODUCTION

The full Hilbert space time-independent Hamiltonian $H$ can be transformed into an effective Hamiltonian $H_{\text{eff}}$, which acts on a restricted model space and gives the desirable exact eigenvalues. Correspondingly, effective transition operator $O_{\text{eff}}$ is introduced to give the same matrix elements while acting between the model space eigenstates as the original transition operator $O$ acting between the corresponding true eigenstates. The explicit forms of $H_{\text{eff}}$ and $O_{\text{eff}}$ are generally much more complicated than those of the original Hamiltonian $H$ and operator $O$, which act on the infinite-dimensional Hilbert space. Nonetheless, they are important and convenient ab initio computation tools for a variety of problems. Another general application of them is to give theoretical justification to phenomenological Hamiltonian and transition operator, such as those used in $f^N$ energy level and transition intensity calculations.

$H_{\text{eff}}$ and $O_{\text{eff}}$ have been widely explored with both perturbative methods (Brillouin-Wigner scheme, Rayleigh-Schrödinger and time-dependent scheme) and non-perturbative methods, such as iterative schemes and multi-reference open-shell coupled cluster theories. The results were initially single reference theory and have been generalized with many efforts to multi-reference cases for both model space and Fock space. Well defined effective Hamiltonians and operators for model space are related to the original operators by a similarity transformation. Similarity transformation play very important rules in the derivation of effective Hamiltonian and is assumed to take certain exponential (normal) forms in coupled-cluster methods, hence the connectivity of effective operators follows trivially. In perturbative methods, the projected transformation, i.e., the wave operator, is defined by order by order expansions. Various effective operators can then be defined with the wave operator and are related to each other by a class of similarity transformation. In this paper, the connectivity is proved to be conserved under such transformation. Therefore if one of those effective operators has been proved to be connected, then the connectivity of all the others follows.
II. FORMULATION OF THE PROBLEM AND LEMMAS

Following Lindgren\[2, 17, 19\] the effective multi-reference perturbative Hamiltonian for
\[ H = H_0 + V, \]
which produces a set of exact eigenvalues, is
\[ H^{(0)}_{\text{eff}} = PH\Omega P, \tag{1} \]
where \( P \) is the model space projector, \( \Omega = 1 + \chi \) is the wave operator, which produces exact
eigenstates while acting on the model function (eigenfunction of \( H^{(0)}_{\text{eff}} \)), and \( \chi \) has nonzero
matrix elements between the space \( Q \) and \( P \) only, where \( Q \) is the orthogonal space of \( P \).
The superscripts \((0)\) is used to distinguish this effective Hamiltonian from others. Such
superscripts is consistent with that of Suzuki \textit{et al.}\[8\], which will be used throughout this
paper.

The effective Hamiltonian \( H^{(0)}_{\text{eff}} \) is not hermitian and therefore has different and non-
orthonormal bra eigenfunctions \( b \langle \Phi^\alpha_0 \mid \) and ket eigenfunctions \( \mid \Phi^\beta_0 \rangle_k \), which can be bi-
orthonormalized and are related to exact eigenstates of \( H \) with wave operator, i.e.,
\[ b \langle \Phi^\alpha_0 \mid H_{\text{eff}} \mid \Phi^\beta_0 \rangle_k = E_\alpha \delta_{\alpha\beta}, \tag{2} \]
\[ b \langle \Phi^\alpha_0 \mid \Phi^\beta_0 \rangle_k = \delta_{\alpha\beta}, \tag{3} \]
\[ \langle \Phi^\beta \rangle = \Omega \mid \Phi^\beta_0 \rangle_k \tag{4} \]
\[ \langle \Phi^\beta \rangle = b \langle \Phi^\alpha_0 \mid (\Omega^+\Omega)^{-1}\Omega^+. \tag{5} \]
The nonhermitian effective operator \( O_{\text{eff}} \) of operator \( O \) for this biorthonormal bases is
\[ O_{\text{eff}} = (\Omega^+\Omega)^{-1}\Omega^+O\Omega, \tag{6} \]
which has been proved to have connected diagrammatic expansion.\[23\] The model space
projector can be written with the biorthonormal as
\[ P = \sum_\alpha \mid \Phi^\alpha_0 \rangle_k b \langle \Phi^\alpha_0 \mid. \tag{7} \]

The hermitian effective Hamiltonian and associated hermitian operator \[1, 7, 18\] are
\[ H^{(-1/2)}_{\text{eff}} = (\Omega^+\Omega)^{1/2}H^{(0)}_{\text{eff}}(\Omega^+\Omega)^{-1/2} \]
\[ = H_0 + (\Omega^+\Omega)^{1/2}V\Omega, \tag{8} \]
\[ O^{(-1/2)}_{\text{eff}} = (\Omega^+\Omega)^{-1/2}\Omega^+O\Omega(\Omega^+\Omega)^{-1/2} \]
\[ = (\Omega^+\Omega)^{1/2}O^{(0)}_{\text{eff}}(\Omega^+\Omega)^{-1/2}, \tag{9} \]
where the second equality in (8) holds only for strictly degenerate model space.

It can be seen that the hermitian effective Hamiltonian and operator are related to the nonhermitian ones by a similarity transformation. We will show that the relations between the effective Hamiltonian and operator and the original Hamiltonian and operator are also similarity transformations (followed by a projection to model space, which can be avoided). Define a transformation operator $T_n$ (arbitrary real $n$) as

$$T_n = (1 + \chi - \chi^*)(1 + \chi^* \chi + \chi \chi^*)^n.$$  

(10)

As $\chi$ has only matrix elements between $Q$ and $P$, it can be shown that

$$\chi^2 = \chi^* \chi^2 = 0,$$

(11)

and the $T_n^{-1}$ can be derived with these properties as

$$T_n^{-1} = (1 + \chi^* \chi + \chi \chi^*)^{-n-1}(1 - \chi + \chi^*).$$

(12)

It can be seen that $T_{-1/2}$ is a hermitian transformation. The similarity transformations of Hamiltonian, effective operator and eigenstates generated by $T_n$ are

$$\tilde{H}_n = T_n^{-1} H T_n,$$

(13)

$$\tilde{O}_n = T_n^{-1} O T_n,$$

(14)

$$|\Phi^\alpha\rangle = T_n |\Phi^\alpha_n\rangle_b,$$

(15)

$$\langle \Phi^\beta | = b \langle \Phi^\beta_n | T_n^{-1},$$

(16)

where $\Phi^\alpha$’s and $\Phi^\alpha_n$’s are eigenstates for $H$ and $\tilde{H}_n$ respectively. The decoupling condition

$$Q \tilde{H}_n P = 0,$$

(17)

is required to diagonalize the transformed Hamiltonian in model space. It can be shown that it is satisfied as follows:

$$Q \tilde{H}_n P = Q(1 + \chi \chi^*)^{-n-1}(1 - \chi)H(1 + \chi)P(1 + \chi^* \chi)^n$$

(18)

$$= Q(1 + \chi \chi^*)^{-n-1}(1 - \chi)(\sum E_\alpha |\Phi_\alpha\rangle \langle \phi^0_\alpha | P(1 + \chi^* \chi)^n$$

(19)

$$= Q(1 + \chi \chi^*)^{-n-1}(1 - \chi)(1 + \chi)PH_{\text{eff}}^{(0)}(1 + \chi^* \chi)^n$$

(20)

$$= 0.$$

(21)
Furthermore,

\[ P \tilde{H}_n Q = (Q \tilde{H}_{-(n+1)} P)^+ = 0. \]  

(22)

As there is no matrix element of \( \tilde{H}_n \) between model space and the orthogonal space, the diagonalization can be done in model space to give exact eigenvalues and model functions.

The effective Hamiltonian for the model space can be simplified as

\[ H_{\text{eff}}^{(n)} = P \tilde{H}_n P \]  

(23)

\[ = (P + \chi^+ \chi)^{-n-1} (P + \chi^+)H(P + \chi)(P + \chi^+ \chi)^n \]  

(24)

\[ = (P + \chi^+ \chi)^{-n-1} (P + \chi^+) \langle \sum_{\alpha} (P + \chi) | \Phi_{\alpha} \rangle k b \langle \Phi_{\alpha} | 0 E_{\alpha} \rangle (P + \chi^+ \chi)^n \]  

(25)

\[ = (P + \chi^+ \chi)^{-n-1} (P + \chi^+) \tilde{H}_{\text{eff}}^{(0)} (P + \chi^+ \chi)^n \]  

(26)

\[ = (P + \chi^+ \chi)^{-n} H(P + \chi)(P + \chi^+ \chi)^n. \]  

(27)

It can be shown that both \( T_n^{-1} | \Phi_{\alpha} \rangle \) and \( \langle \Phi_{\alpha} | T_n \) are in model space, which are the ket and bra model functions respectively. Therefore the effective operator for model space can be derived by projecting \( \tilde{O}_n \) to model space, i.e.,

\[ O_{\text{eff}}^{(n)} = P \tilde{O}_n P \]  

(28)

\[ = (P + \chi^+ \chi)^{-n-1} (P + \chi^+)O(P + \chi)(P + \chi^+ \chi)^n. \]

Such results have been derived by Suzuki and Okamoto in other ways. They showed that the effective Hamiltonian is related to the origin Hamiltonian by a similarity transformation. However, the similarity transformation is not suitable for the effective operator. Here a similarity transformation for both Hamiltonians and operators have been shown. This is what we have been expected, as Hamiltonian is only a special operator which need be decoupled. Hereafter we do not distinguish between them and the “operator” refers to both.

Various effective operators \( \tilde{O}_n \) are related to the original operator by similarity transformation, and therefore are related to each other by similarity transformation, i.e.,

\[ \tilde{O}_{n+a} = (1 + \chi^+ \chi + \chi \chi^+)^{-a} \tilde{O}_n (1 + \chi^+ \chi + \chi \chi^+)^a, \]  

(29)

\[ O_{\text{eff}}^{(n+a)} = (P + \chi^+ \chi)^{-a} O_{\text{eff}}^{(n)} (P + \chi^+ \chi)^a. \]  

(30)

Such property between operators are very important, since commutation relations, which are closely related to symmetries, are conserved under similarity transformation.
It is well known that the similarity transformation generated by an exponential function of a connected operator (referred as cluster function) preserves the connectivity, which has been the bases of coupled cluster methods, i.e.:

If \( S \) and \( O \) are connected, then \( \exp(-S)O \exp(S) \) is connected.

The proof of this is straightforward by using the famous Campbell-Baker-Hausdorff formulas.

We will show that the similarity transformation between various perturbative effective operators generated by \( (P + \chi^+\chi)^a \), or \( (\Omega^+\Omega)^a \), also preserves the connectivity, i.e.:

**Theorem:** \( (\Omega^+\Omega)^aO(\Omega^+\Omega)^{-a} \) is connected if \( O \) is connected, where \( \Omega \) is perturbative wave operator for complete multi-reference model space. The completeness means that model space contains all bases which can be formed by distribution the valence electrons among the valence shells.

The following lemmas are used to prove this theorem

**Lemma 1.** The RS perturbative expansion of the wave operator \( \Omega \) can be written in a exponential form, i.e.,

\[
\Omega = \{ \exp(S) \},
\]

where the curly brackets mean that the creation and annihilation operators within them are rearranged into normal form with respect to a closed-shell state. This notation for normal form will be used throughout this paper. In the case of quasi-degenerate complete model space, \( S \) is a sum of connected diagrams.

**Lemma 2.** \( \{ \exp(S_1) \} \{ \exp(S_2) \} = \{ \exp(S_{S_1S_2}) \} \), where \( S_1 \), \( S_2 \) and \( S_{S_1S_2} \) are all connected. \( S_{S_1S_2} \) is the connected part of \( \{ \exp(S_1) \} \{ \exp(S_2) \} \).

**Lemma 3.** \( xO - Ox = O^{(1)} + (1 - \delta)xO^{(1)} + \delta O^{(1)}x \), where \( x = \{ \exp(S) \} - 1 \), \( S \), \( O \) and \( O^{(1)} \) are connected and in normal form, and \( \delta \) is an arbitrary real number. The order of \( O^{(1)} \) is higher than \( O \) by at least one, where the order is the smallest number of \( V \) of all the terms of the operator concerned.

**Lemma 4.** Define \( \alpha^{(m)(n)}_i \) (integer \( n \) and \( i, n = 1, 2, \ldots, \infty, 0 \leq i \leq n \)) recursively as

\[
\alpha^{(0)(n)}_i = \begin{pmatrix} a & -a \\ n-i & i \end{pmatrix},
\]

\[
\alpha^{(k)(n)}_i = \sum_{j=0}^{i} [\alpha^{(k-1)(n+1)}_j + \alpha^{(k-1)(n)}_j],
\]

6
where $k = 1, 2, \cdots$. The following equality holds for arbitrary positive integer $m$ and $n$:

$$\sum_{i=0}^{n} \alpha_{i}^{(m)(n)} = 0. \quad (34)$$

In addition to applying the theorem to show the connectivity of various MBPT effective Hamiltonians and transition operators, the theorem and lemmas can also be used to show the connectivity of various effective Hamiltonian in Coupled-Cluster (CC) theories\[4, 20, 21, 22\]. In those theories various similarity transformations, generated by

$$T = \{ \exp \hat{S} \} \quad (35)$$

to the right and $T^{-1}$ (generally $\neq \{ \exp(-\hat{S}) \}$ to the left, have been used to transform original Hamiltonian operator $H$ or CCSD (CC Singleton and doubleton excited contribution) Hamiltonian operator $\exp(-T_1 - T_2)H\exp(T_1 + T_2)$ into Coupled-Cluster effective Hamiltonian which have certain zero components convenient for calculation of eigenvalues and eigenvectors. From the theorem and Lemma 2 it is straightforward to show that all such transformations preserve connectivity. Moreover, if necessary, more general similarity transform generated by $T^a$ ($a$ an arbitrary number) can be used in CC methods.

III. PROOF OF THE THEOREM AND THE LEMMAS

Lemma 1 has been proved by Lindgren by using factorization theorem and mathematical induction\[2, 17\], and Lemma 2 has been proved in another paper\[23\]. We shall prove the theorem to be true firstly by using these lemmas and then prove lemma 3 and lemma 4 afterwards.

A. Proof of the theorem

Denoting $x = \Omega^+\Omega - 1$ and using the definition of $\alpha_{i}^{(0)(n)}$ in lemma 4, we have

$$(\Omega^+\Omega)^a O(\Omega^+\Omega)^{-a} = O + \sum_{n=1}^{\infty} \sum_{i=0}^{n} \alpha_{i}^{(0)(n)} x^{n-i} O x^{i}$$

$$= \sum_{n=1}^{\infty} \sum_{i=0}^{n} \beta_{i}^{(0)(n)} x^{n-1-i} (xO - O x) x^{i}, \quad (36)$$

where

$$\beta_{i}^{(m)(n)} = \sum_{j=0}^{i} \alpha_{j}^{(m)(n)}, \quad (i = 0, 1, \cdots, n), \quad (37)$$
and the condition $\beta_n^{(0)(n)} = 0$, which follows from lemma 4, has been used in deriving equality (36). It can be seen from lemma 1 and lemma 2 that the $x$ in (36) can be written as

$$x = \{\exp(S)\} - 1,$$

(38)

where $S$ is the connected part of $\exp(S_1)\exp(S_2)$ that contain only valence creation and annihilation operators. Applying the $\delta = 0$ case of lemma 3 to (36), we get

$$(\Omega^+\Omega)^aO(\Omega^+\Omega)^{-a} = O + \beta_0^{(0)(1)} O^{(1)} + \sum_{n=1}^{\infty} \sum_{i=0}^{\infty} (\beta_i^{(0)(n+1)} + \beta_i^{(0)(n)}) x^{n-i} O^{(1)} x^i$$

(39)

$$= O + \alpha_0^{(0)(1)} O^{(1)} + \sum_{n=1}^{\infty} \sum_{i=0}^{\infty} \alpha_i^{(1)(n)} x^{n-i} O^{(1)} x^i.$$

(40)

As shown by lemma 4 that $\sum_{i=0}^{n} \alpha_i^{(1)(n)} = 0$. We can simply repeat the above procedure to arbitrary $m$ and get

$$(\Omega^+\Omega)^aO(\Omega^+\Omega)^{-a} = O + \sum_{l=0}^{m-1} b_l^{(1)(l)} O^{(l)} + \sum_{n=1}^{\infty} \sum_{i=0}^{\infty} \alpha_i^{(m)(n)} x^{n-i} O^{(m)} x^i.$$

(41)

We conclude by mathematic induction that Eq. (41) holds for arbitrary $m > 0$. As $O^{(m)}$ is connected and its order increases by at least 1 as $m$ increases by 1, we have proved that to arbitrary large but finite order, the expansion of $(1 + x)^a O(1 + x)^{-a}$ is connected.

**B. Proof of lemma 3**

A special case of the lemma 4 of [23] is

$$\{\exp(S)\} O = \{\exp(S) O^L\}$$

$$= \{\exp(S) O\} + \{\exp(S) O_1^L\}$$

(42) (43)

where $O^L$ is the connected part of $\{\exp(S)\} O$, and $O_1^L = O_1^L - O$ is the connected part of $(\{\exp(S)\} - 1) O$, whose order is higher than $O$ by at least one.

Denoting $x = \{\exp(S)\} - 1$, we have

$$x O = \{x O\} + \{(1 + x) O_1^L\}.$$

(44)
Similarly, it can be proved that
\[ Ox = \{Ox\} + \{O^R_1(1 + x)\}, \]
(45)
where \( O^R_1 \) is the connected part of \( Ox \), whose order is also higher than \( O \) by at least 1.

The lemma 5 of [23], which has been proved, is
\[ \{\exp(S)O\} = \{\exp(S)\}O^t, \]
(46)
where \( S, O \) and \( O^t \) are all connected, and the order of \( O^t \) is the same as \( O \).

The following equation can be derived using the latest three equations
\[ xO - Ox = \{(1 + x)(O^L_1 - O^R_1)\} \]
\[ = (1 + x)O^{(1)}, \]
(47)
where \( O^{(1)} \) is connected and the order is no less than \( O^L_1 - O^R_1 \).

The case \( \delta \neq 0 \) can also be proved with some mathematical manipulation. Note that \( O^{(1)} \) depends on the value of \( \delta \).

C. Proof of Lemma 4

The case \( m = 0 \) of Eq. [24] can be proved directly by the binomial expansion of \((1 + x)^a(1 + x)^{-a}\).

For \( m = 1 \), we have
\[ \alpha^{(1)(n)}_i = \sum_{i_1=0}^{i} [\alpha^{(0)(n+1)}_{i_1} + \alpha^{(0)(n)}_{i_1}] \]
\[ = \sum_{i_1=0}^{i} \left[ \begin{pmatrix} a \\ n + 1 - i_1 \end{pmatrix} \begin{pmatrix} -a \\ i_1 \end{pmatrix} + \begin{pmatrix} a \\ n - i_1 \end{pmatrix} \begin{pmatrix} -a \\ i_1 \end{pmatrix} \right] \]
\[ = \sum_{i_1=0}^{i} \begin{pmatrix} a \\ n - i_1 \end{pmatrix} \begin{pmatrix} -a \\ i_1 \end{pmatrix} \begin{pmatrix} 1 + a - (n + 1 - j) \\ n + 1 - j \end{pmatrix} \]
\[ = \sum_{i_1=0}^{i} \begin{pmatrix} 1 + a \\ n + 1 - i_1 \end{pmatrix} \begin{pmatrix} -a \\ i_1 \end{pmatrix}. \]
(48)

Suppose, for a given \( k \), that the following equation holds:
\[ \alpha^{(k)(n)}_i = \sum_{i_1=0}^{i} \sum_{i_2=0}^{i_k-1} \sum_{i_k=0}^{i} \begin{pmatrix} a + k \\ n + k - i_k \end{pmatrix} \begin{pmatrix} -a \\ i_k \end{pmatrix}. \]
(49)

The recursive relation tells us that
\[
\alpha_j^{(k+1)(n)} = \sum_{i=0}^{j} \left( \alpha_i^{(k)(n+1)} + \alpha_i^{(k)(n)} \right)
\]

\[
= \sum_{i=0}^{j} \sum_{i_1=0}^{i} \cdots \sum_{i_k=0}^{i_k-1} \left( \frac{a+k}{n+k-i_k} \right) \left( -a \right) \left( \frac{a+k+1-(n+1+k-i_k)}{n+1+k-i_k} \right) + 1
\]

\[
= \sum_{i=0}^{j} \sum_{i_1=0}^{i} \cdots \sum_{i_k=0}^{i_k-1} \left( \frac{a+k+1}{n+k+1-i_k} \right) \left( -a \right) \left( \frac{a+k+1-(n+1+k-i_k)}{n+1+k-i_k} \right) + 1
\]

By mathematical induction, we conclude that Eq. 49 holds for all \(k\). Then Eq. 34 reduces to the following equation:

\[
\sum_{i=0}^{n} \alpha_i^{(m)(n)} = \sum_{i=0}^{n} \sum_{i_1=0}^{i} \cdots \sum_{i_m=0}^{i_m-1} \left( \frac{a+m}{n+m-i_m} \right) \left( -a \right) \left( \frac{(n+m-i_m)!}{m!(n-i_m)!} \right)
\]

\[
= \sum_{i_m=0}^{n} \left[ \left( \frac{a+m}{n+m-i_m} \right) \left( -a \right) \sum_{i_{m-1}=i_m}^{n} \cdots \sum_{i_1=i_2=\cdots=i_1=1}^{n} 1 \right].
\]

It is straightforward to prove by mathematical induction that

\[
\sum_{i_m=0}^{n} \cdots \sum_{i_1=i_2=\cdots=i_1=1}^{n} 1 = \frac{(n+m-i_m)!}{m!(n-i_m)!}.
\]

Substituting the corresponding summations in Eq. 51 with this result, we get

\[
\sum_{i=0}^{n} \alpha_i^{(m)(n)} = \sum_{i_m=0}^{n} \left( \frac{a+m}{n+m-i_m} \right) \left( -a \right) \left( \frac{(n+m-i_m)!}{m!(n-i_m)!} \right)
\]

\[
= \sum_{i_m=0}^{n} \left( \frac{a+m}{m} \right) \left( \frac{a}{n-i_m} \right) \left( -a \right) \left( \frac{(n+m-i_m)!}{m!(n-i_m)!} \right)
\]

\[
= \left( \frac{a+m}{m} \right) \delta_{n0}.
\]

IV. CONCLUSION

It has been shown that the perturbative effective Hamiltonian and operator are related to the original Hamiltonian and operator respectively by the same similarity transformation, which includes the hermitian special case. Such transformation conserves the commutation relations and hence most symmetry properties. Various effective Hamiltonians and effective
operators respectively are related to each other by a similarity transformation generated by \(\exp \{S\}^a\), where \(S\) is connected, \(a\) is an arbitrary real number, and curved bracket means normal form. An effective Hamiltonian or operator with connected-diagram expansion will be transformed into a new operator with connected-diagram expansion, consequently the connectivity can be deduced from each other. In particular, The hermitian effective Hamiltonian and operator are related to the simplest non-hermitian effective Hamiltonian and operator respectively by such a transformation, and therefore are connected from the fact that the later effective Hamiltonian and operator has been proved to be connected. [23] This rigorous mathematic proof saves one from understanding the complicated demonstration by recursive insertion of energy diagrams. [1].

[9] Various examples are reviewed in Ref. [3].