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## Formal Relation among Various Hermitian and non-Hermitian Effective Interactions

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A general definition of the model-space effective interaction is given. All the effective interactions proposed so far, mainly the  $E$ -independent effective hamiltonians derived in a time-independent way are classified systematically.

### 1. Introduction

Nuclear many-body theory has been intensively studied for many years and reached a high level of understanding, but there still are some unresolved fundamental problems.

One of the leading approaches is to introduce an effective interaction and reduce the full many-body problem to a certain model-space problem. There have been many review works concerning the effective interaction theory, for example, Ref. 1.

The principle of determining the effective interaction is that it should have the property of decoupling between the model space and the excluded space as discussed by Lee and one of the authors (K.S.).<sup>2</sup> The property of decoupling is necessary for the effective interaction, but it does not give the condition of determining uniquely the effective interaction. Therefore many kinds of the effective interactions are possible.<sup>5</sup> Very recently Holt, Kuo and Brown<sup>6</sup> published a paper to study the various versions of hermitian effective interaction.

The purpose of the present paper is to give a general definition of the effective

interaction and show that all the effective interactions in time-independent approach proposed so far can be classified systematically.

## 2. Unified description of effective interaction

We start with a general definition of an effective hamiltonian. Let us write the Schrödinger equation for a hamiltonian  $H$  defined in a full Hilbert space,

$$H|\Phi_k\rangle = E_k|\Phi_k\rangle, \quad (1)$$

where  $|\Phi_k\rangle$  is supposed to be orthonormal to each other,  $\langle\Phi_k|\Phi_{k'}\rangle = \delta_{kk'}$ .

We introduce a model space that consists of some reference states. We denote the projection operators onto the model space and its complement by  $P$  and  $Q$ , respectively. We consider an eigenvalue equation for a hamiltonian  $\mathcal{H}$  and an overlap (or metric)  $\chi$  defined in the  $P$  space,

$$\mathcal{H}|\xi_k\rangle = E_k\chi|\xi_k\rangle, \quad (k = 1, 2, \dots, d), \quad (2)$$

where  $d$  is the dimension of the  $P$  space. If  $d$  eigenvalues  $\{E_k\}$  agree with the eigenvalues of the original hamiltonian  $H$ , we call  $\mathcal{H}$  the effective hamiltonian. If we separate the hamiltonian into the unperturbed hamiltonian  $H_0$ , which has the property  $H_0 = PH_0P + QH_0Q$  and the perturbation (interaction),  $V$ , we call  $V_{eff} = \mathcal{H} - PH_0P$  the effective interaction.

We introduce an operator  $\omega$  that acts as a mapping between the  $P$  and  $Q$  spaces.<sup>7</sup> The operator  $\omega$  has the property,  $\omega = Q\omega P$ . With the operator  $\omega$  we define an operator  $X(n)$  given by <sup>a</sup>

$$X(n) = (1 + \omega - \omega^\dagger)(1 + \omega^\dagger\omega + \omega\omega^\dagger)^n, \quad (3)$$

where  $n$  is an integer or a half integer. The inverse of  $X(n)$  is given by

$$X^{-1}(n) = (1 + \omega^\dagger\omega + \omega\omega^\dagger)^{-n-1}(1 + \omega^\dagger - \omega). \quad (4)$$

We note that the transformation  $X(n)$  contains a special case of  $X(n = 0)$  that is essentially equivalent to the transformation introduced by Navrátil, Geyer and Kuo.<sup>8</sup> We refer to some important properties of  $X(n)$  and  $X^{-1}(n)$ :

$$X(n)P = (P + \omega)(P + \omega^\dagger\omega)^n, \quad (5)$$

$$QX^{-1}(n) = (Q + \omega\omega^\dagger)^{n-1}(Q - \omega) \quad (6)$$

and

$$QX^{-1}(m)X(n)P = 0. \quad (7)$$

We consider a transformation of  $H$  defined as

$$\overline{H}(m, n) = X^{-1}(m)HX(n), \quad (8)$$

<sup>a</sup>The definition of  $X(n)$  is different from that given in the previous works.<sup>3,5</sup> The present definition is more general than the previous one, but the effective interactions to be derived are the same.

and we also define an overlap operator

$$\begin{aligned}\chi(m, n) &= PX^{-1}(m)X(n)P \\ &= (P + \omega^\dagger\omega)^{n-m}.\end{aligned}\quad (9)$$

We now can prove the fact that if  $\overline{H}(m, n)$  satisfies the following equation of decoupling

$$Q\overline{H}(m, n)P = 0, \quad (10)$$

which is explicitly written as<sup>7</sup>

$$QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0, \quad (11)$$

the operator  $P\overline{H}(m, n)P$  and  $\chi(m, n)$  can be an effective hamiltonian and a corresponding overlap, respectively.

We write the  $P$ -space effective hamiltonian for a set of  $(m, n)$  as

$$\begin{aligned}\mathcal{H}(m, n) &= P\overline{H}(m, n)P \\ &= (P + \omega^\dagger\omega)^{-m-1}(P + \omega^\dagger)H(P + \omega)(P + \omega^\dagger\omega)^n.\end{aligned}\quad (12)$$

The  $\mathcal{H}(m, n)$  can also be expressed as

$$\mathcal{H}(m, n) = (P + \omega^\dagger\omega)^{-m}H(P + \omega)(P + \omega^\dagger\omega)^n. \quad (13)$$

In the derivation of the above expression, we have used the relation written as

$$\omega^\dagger H(P + \omega) = \omega^\dagger\omega H(P + \omega) \quad (14)$$

or equivalently

$$(P + \omega^\dagger)H(P + \omega) = (P + \omega^\dagger\omega)H(P + \omega) \quad (15)$$

which is obtained by multiplying the l.h.s. of Eq. (11) by  $\omega^\dagger$ .

### 3. Classification of effective hamiltonians

Among various effective hamiltonians we will discuss the detail of three kinds of the effective hamiltonians, namely,  $\mathcal{H}(0, 0)$ ,  $\mathcal{H}(0, -1)$  and  $\mathcal{H}(-1/2, -1/2)$ .

(1)  $m = n = 0$

The effective hamiltonian  $\mathcal{H}(0, 0)$  is given by

$$\mathcal{H}(0, 0) = PH(P + \omega), \quad (16)$$

and the corresponding overlap is  $\chi(0, 0) = P$ . The  $\omega$  is related with the Møller wave operator,  $\Omega$ , as  $\Omega = P + \omega$ . The effective hamiltonian  $\mathcal{H}(0, 0)$  is written as

$$\mathcal{H}(0, 0) = \mathcal{H}_B = PH\Omega. \quad (17)$$

This form has been used as the standard effective hamiltonian which was studied by Bloch and Horowitz.<sup>9</sup> The structure of  $\mathcal{H}(0, 0)$  would be the simplest, but it is non-hermitian.

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(2)  $m = 0, n = -1$

The  $\mathcal{H}(0, -1)$  is given explicitly by

$$\mathcal{H}(0, -1) = PH(P + \omega)(P + \omega^\dagger \omega)^{-1}. \quad (18)$$

The corresponding overlap is

$$\chi(0, -1) = (P + \omega^\dagger \omega)^{-1}. \quad (19)$$

The  $\mathcal{H}(0, -1)$  given in Eq. (18) is apparently non-hermitian, but it is actually hermitian. This is obvious from the expression of  $\mathcal{H}(m, n)$  in Eq. (12). The  $\mathcal{H}(0, -1)$  is also written in a manifestly hermitian form as

$$\mathcal{H}(0, -1) = (P + \omega^\dagger \omega)^{-1}(P + \omega^\dagger)H(P + \omega)(P + \omega^\dagger \omega)^{-1}. \quad (20)$$

This effective hamiltonian agrees with Kato's effective hamiltonian<sup>17</sup> defined originally as

$$\mathcal{H}_K = P\bar{P}H\bar{P}P \quad (21)$$

with the overlap  $\chi_K = P\bar{P}P$ , where  $\bar{P} = \sum_{k=1}^d |\Phi_k\rangle\langle\Phi_k|$ . In terms of  $\omega$  we can prove<sup>4</sup> that  $\bar{P}$  is written as

$$\bar{P} = (P + \omega)(P + \omega^\dagger \omega)^{-1}(P + \omega^\dagger). \quad (22)$$

Substituting  $\bar{P}$  in the above expression into Eq. (21), we readily see that  $\mathcal{H}_K$  is equivalent to  $\mathcal{H}(0, -1)$ . Furthermore we also see, from Eq. (22), that  $\chi_K$  agrees with  $\chi(0, -1)$  in Eq. (19).

(3)  $m = n = -1/2$

Using Eq. (12),  $\mathcal{H}(-1/2, -1/2)$  is expressed as

$$\mathcal{H}(-1/2, -1/2) = (P + \omega^\dagger \omega)^{-1/2}(P + \omega^\dagger)H(P + \omega)(P + \omega^\dagger \omega)^{-1/2}, \quad (23)$$

and from Eq. (13) we also have

$$\mathcal{H}(-1/2, -1/2) = (P + \omega^\dagger \omega)^{1/2}H(P + \omega)(P + \omega^\dagger \omega)^{-1/2}. \quad (24)$$

The above expression does not look manifestly hermitian, but two expressions are equivalent and  $\mathcal{H}(-1/2, -1/2)$  is really hermitian. The corresponding overlap is  $\chi(-1/2, -1/2) = P$ .

Historically several definitions of the hermitian effective hamiltonians have been proposed. Among them we refer to the following three hermitian effective hamiltonians, i.e.,

$$\mathcal{H}_{\bar{P}} = (P\bar{P}P)^{-1/2}P\bar{P}H\bar{P}P(P\bar{P}P)^{-1/2}, \quad (25)$$

$$\mathcal{H}_\Omega = (\Omega^\dagger \Omega)^{1/2}PH\Omega(\Omega^\dagger \Omega)^{-1/2}, \quad (26)$$

$$\mathcal{H}_G = Pe^{-G}He^G P. \quad (27)$$

The exponent  $G$  in Eq. (27) is related with  $\omega$  as<sup>10,15,16</sup>

$$\begin{aligned} G &= \operatorname{arctanh}(\omega - \omega^\dagger), \quad (G^\dagger = -G) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \{\omega(\omega^\dagger \omega)^n - \text{h.c.}\}. \end{aligned} \quad (28)$$

We can prove that all of  $\mathcal{H}_{\overline{P}}$ ,  $\mathcal{H}_{\Omega}$  and  $\mathcal{H}_G$  are equivalent to  $\mathcal{H}(-1/2, -1/2)$  as follows: Using Eq. (22) for  $\overline{P}$ , we can easily show that  $\mathcal{H}_{\overline{P}}$  and  $\mathcal{H}_{\Omega}$  are equivalent to the expressions of  $\mathcal{H}(-1/2, -1/2)$  in Eq. (23) and Eq. (24), respectively. The  $\mathcal{H}_G$  is of a canonical form, that is,  $\mathcal{H}_G$  is derived by means of a unitary transformation of the original hamiltonian  $H$ . We note here that  $e^G$  with  $G$  given in Eq. (28) becomes<sup>10</sup>

$$e^G = (1 + \omega - \omega^\dagger)(1 + \omega^\dagger\omega + \omega\omega^\dagger)^{-1/2} \quad (29)$$

which is just equivalent to the transformation  $X(-1/2)$ , i.e.,

$$X(-1/2) = e^G. \quad (30)$$

The  $\mathcal{H}_G$  is then written as

$$\mathcal{H}_G = PX^{-1}(-1/2)HX(-1/2)P. \quad (31)$$

From the above expression the equivalence of  $\mathcal{H}_G$  to  $\mathcal{H}(-1/2, -1/2)$  is obvious. The definition of  $\mathcal{H}_{\overline{P}}$  is of des Cloizeaux<sup>11</sup> and  $\mathcal{H}_{\Omega}$  was originally given by Okubo.<sup>7</sup> The structure of  $\mathcal{H}_{\Omega}$  was extensively studied by Brandow.<sup>12,13</sup> The canonical form  $\mathcal{H}_G$  is often referred to as the Van Vleck form.<sup>14</sup>

#### 4. Family of hermitian effective interactions

We re-start with the Schrödinger equation in a more concrete expression

$$(H_0 + V)|\Phi_k\rangle = E_k|\Phi_k\rangle, \quad (k = 1, 2, \dots, d). \quad (32)$$

The state vector  $|\Phi_k\rangle$  is decomposed as

$$\begin{aligned} |\Phi_k\rangle &= P|\Phi_k\rangle + Q|\Phi_k\rangle = |\phi_k\rangle + Q|\Phi_k\rangle \\ &= (P + \omega)|\phi_k\rangle, \quad (|\phi_k\rangle = P|\Phi_k\rangle). \end{aligned} \quad (33)$$

If we write the corresponding model-space Schrödinger equation as

$$P(H_0 + V_{LS})P|\phi_k\rangle = E_k|\phi_k\rangle, \quad (34)$$

the non-hermitian effective interaction  $V_{LS}$  is expressed as

$$PV_{LS}P = Pe^{-\omega}(H_0 + V)e^{\omega}P - PH_0P. \quad (35)$$

We note that

$$PH\Omega P = P(H_0 + V_{LS})P. \quad (36)$$

The state vectors  $|\phi_k\rangle$  are, in general, not mutually orthogonal, since they are merely projections (onto  $P$  space) of the orthogonal state vectors  $|\Phi_k\rangle$ . If we introduce the bi-orthogonal state,  $|\tilde{\phi}_k\rangle$ , corresponding to the model-space state  $|\phi_k\rangle$  as  $\langle\tilde{\phi}_k|\phi_{k'}\rangle = \delta_{kk'}$ , then the formal expression for  $\omega$  is given by

$$\omega = \sum_{k=1}^d Q|\Phi_k\rangle\langle\tilde{\phi}_k|P. \quad (37)$$

Recently, Holt, Kuo and Brown<sup>6</sup> have used the  $Z$  transformation method to study the various versions of hermitian effective interactions in order to reorient, or to suitably stretch,<sup>19</sup> the vectors  $|\phi_k\rangle$  such that they become orthonormal to each other.

$$\begin{aligned} Z|\phi_k\rangle &= |v_k\rangle, \quad (Z = PZP); \\ \langle v_k|v_{k'}\rangle &= \delta_{kk'}; \quad (k, k' = 1, 2, \dots, d). \end{aligned} \quad (38)$$

Using the fact that the eigenvectors  $|\Phi_k\rangle$  are orthonormal to each other we can derive

$$\begin{aligned} \delta_{kk'} &= \langle \Phi_k|\Phi_{k'}\rangle = \langle \phi_k|P + \omega^\dagger\omega|\phi_{k'}\rangle \\ &= \langle v_k|(Z^{-1})^\dagger(P + \omega^\dagger\omega)Z^{-1}|v_{k'}\rangle. \end{aligned} \quad (39)$$

Then we have

$$P + \omega^\dagger\omega = Z^\dagger Z. \quad (40)$$

The bi-orthogonal state  $|\tilde{\phi}_k\rangle$  is related to  $|v_k\rangle$  as

$$|\tilde{\phi}_k\rangle = Z^\dagger Z|\phi_k\rangle = Z^\dagger|v_k\rangle. \quad (41)$$

One can easily check that  $\langle \tilde{\phi}_k|\phi_{k'}\rangle = \langle \phi_k|Z^\dagger Z|\phi_{k'}\rangle = \langle v_k|v_{k'}\rangle = \delta_{kk'}$ . A formal expression for  $\omega$  in Eq. (37) is re-written as

$$\omega = \sum_{k=1}^d Q|\Phi_k\rangle\langle v_k|Z. \quad (42)$$

Using Eq. (38) the model-space eigenvalue equation (34) is transformed into

$$Z(H_0 + V_{LS})Z^{-1} = \sum_{k=1}^d E_k|v_k\rangle\langle v_k|. \quad (43)$$

Since  $E_k$  is real and the vectors  $|v_k\rangle$  are orthogonal to each other,  $Z(H_0 + V_{LS})Z^{-1}$  must be hermitian. Then the hermitian effective interaction,  $V_{herm}$ , is written as

$$\begin{aligned} V_{herm} &= Z(H_0 + V_{LS})Z^{-1} - PH_0P \\ &= Ze^{-\omega}(H_0 + V)e^{\omega}Z^{-1} - PH_0P. \end{aligned} \quad (44)$$

One must first obtain the  $Z$  transformation in order to calculate  $V_{herm}$ . There are certainly many ways to construct  $Z$ , and this fact generates a family of hermitian effective interactions, all originating from the non-hermitian  $V_{LS}$ .<sup>6</sup>

One can construct  $Z$  using the Schmidt orthogonalization procedure, and there are some ways in using the procedure.<sup>6</sup> Holt, Kuo and Brown showed some well-known hermitization transformation.<sup>6</sup>

(1) Okubo form

$$Z = P(1 + \omega^\dagger\omega)^{1/2}P, \quad (45)$$

$$\begin{aligned} V_{okb} &= P(1 + \omega^\dagger\omega)^{1/2}P(H_0 + V_{LS})P(1 + \omega^\dagger\omega)^{-1/2}P \\ &\quad - PH_0P. \end{aligned} \quad (46)$$

(2) Andreozzi form<sup>20</sup>

$$Z = L^T, \quad (47)$$

$$V_{andr} = PL^T P(H_0 + V_{LS})P(L^{-1})^T P - PH_0 P, \quad (48)$$

where we put  $Z^\dagger Z = LL^T$  for Eq. (40), and  $L$  is a lower triangle Cholesky matrix and  $L^T$  being its transpose.

(3) Suzuki-Okamoto form

$$Z = Pe^{-G}e^\omega P, \quad (49)$$

$$V_{suzu} = Pe^{-G}(H_0 + V)e^G P - PH_0 P. \quad (50)$$

One can easily check the choices (45), (47) and (49) satisfy the property (40).

We now can understand systematically the formal relation among various effective hamiltonians as shown in Fig.1.

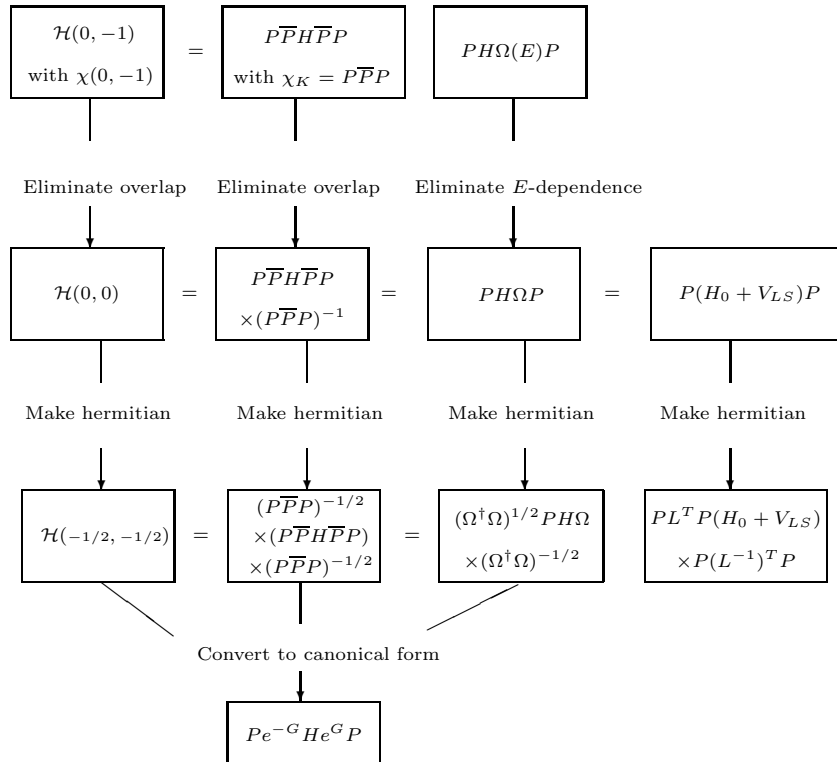


Fig. 1. Formal relation among various effective hamiltonians in time-independent approach

## 5. Summary

We have given the general definition of the  $P$ -space effective hamiltonian or interaction, mainly the  $E$ -independent effective hamiltonians derived in a time-independent way. We have discussed the relation among hermitian and non-hermitian effective hamiltonians.

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