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Effective Operators in Time-Independent Approach

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An effective operator $\Theta_{\rm eff}$ is defined so that it operates in a restricted model space and gives the same matrix element as that of the original operator Θ between the corresponding true eigenstates. The $\Theta_{\rm eff}$ is determined dependently on the model-space eigenstates, and therefore various types of $\Theta_{\rm eff}$ are possible. General solutions for $\Theta_{\rm eff}$ are derived in the time-independent and algebraic approach. These $\Theta_{\rm eff}$ contain the usual non-Hermitian and Hermitian effective operators as special cases. The explicit expansion form for $\Theta_{\rm eff}$ is given by extending the $\hat{Q}$-box formalism of Kuo et al. developed in the derivation of the effective interaction to the problem of constructing the effective operator.

§ 1. Introduction

In nuclear, atomic, molecular and solid state physics, it is usually necessary to recast the problems in an entire Hilbert space in the form of the problems in a restricted model space.[1)~6)] Effective Hamiltonians (or interactions) and effective operators are introduced in order to systematically take into account contributions from the complement of the model space to physical quantities evaluated in the model space. Much work has been made on these problems both as regards formal theories and numerical calculations in actual systems. The general structure of these theories, however, has not been fully discussed in contrast to actual calculations within limited order of approximations.

General theory of effective Hamiltonian has been developed by several authors in energy-independent and energy-dependent approaches both for degenerate and non-degenerate (quasidegenerate) unperturbed systems.[7)~11)] In the time-independent approach the construction of the Hermitian effective Hamiltonian has been established and its relation with the non-Hermitian effective Hamiltonian has been discussed.[12)~14)] Mutual relations among various effective interactions have been clarified and effective interactions have been classified in a unified manner in the time-independent approach.[9),10)]

The resulting effective Hamiltonians have been shown to be expressed in terms of the $\hat{Q}$-box in the framework of the folded-diagram theory by Kuo et al.[15)] The $\hat{Q}$-box has been introduced as the partial summation of the non-folded diagrams. The energy derivatives of the $\hat{Q}$-box generate the folded diagrams. The inclusion of the folded diagrams removes the energy dependence of effective interaction. The $\hat{Q}$-box formalism was originally introduced for degenerate unperturbed systems and recently generalized to non-degenerate systems.[16)]

Very recently Navratil, Geyer and Kuo[17)] have proposed energy-independent Hermitian and non-Hermitian effective operators by utilizing a double similarity transformation method[18)] for the construction of effective Hamiltonians. Furthermore Hurtubise and Freed[11),19)~21)] have given a general method for deriving the effective Hamiltonians and operators by introducing mapping operators between the model-space eigenstates and the corresponding true eigenstates. Their approach is different from the method given by the present authors[9] on the basis of the similarity-transformation theory. It will be of interest to see the formal relation between two approaches.

The aim of the present paper is twofold. The one is to discuss the formal structure of effective operators by defining a general effective operator which contains various types of the effective operators defined so far. The other is to give an expansion formula for the effective operator in terms of the $\hat{\Theta}$-box. The $\hat{\Theta}$-box is the building block introduced for constructing effective operators and it is an analogue to the $\hat{Q}$-box in the effective interaction theory. We want to show that every effective operator can be expanded into a series of the $\hat{\Theta}$- and $\hat{Q}$-boxes.

The organization of this paper is as follows. In § 2 we define general effective operators and derive their operator forms. The relation between the Hermitian and non-Hermitian effective operators is discussed in § 3. In § 4 general expansion formulae for the effective operators are given both for the degenerate and non-degenerate unperturbed systems. Concluding remarks are given in § 5.

§ 2. Derivation of general effective operator

We first review a general theory of effective interaction in the time-independent approach. We consider an operator ω which satisfies[22]

$$\omega = Q\omega P\,, \tag{2·1}$$

where P and Q are projection operators onto the model space and its complement, respectively. With ω we introduce an operator X_n defined by[9]

$$X_n = (1+\omega)(1+\omega^\dagger\omega+\omega\omega^\dagger)^n\,, \tag{2·2}$$

where n is an integer or a half integer. The inverse of X_n is given by

$$X_n^{-1} = (1+\omega^\dagger\omega+\omega\omega^\dagger)^{-n}(1-\omega)\,. \tag{2·3}$$

For the derivation of Eq. (2·3) we have used the fact that $\omega^2=0$ which comes from Eq. (2·1).

We next define a transformed Hamiltonian

$$\tilde{H}_n = X_n^{-1}HX_n \tag{2·4}$$

and require the decoupling condition

$$Q\tilde{H}_nP=0\,. \tag{2·5}$$

We easily see that the above equation is satisfied if ω is a solution to

$$\begin{aligned} QX_0^{-1}HX_0P &= QHP + QHQ\omega - \omega PHP - \omega PHQ\omega \\ &= 0\,. \end{aligned} \tag{2·6}$$

A general effective Hamiltonian is given by

$$H_{\rm eff}^{(n)}=P\tilde{H}_nP$$
$$=(P+\omega^\dagger\omega)^{-n}H(P+\omega)(P+\omega^\dagger\omega)^n \tag{2·7}$$

which has been derived in Ref. 9). The model-space eigenvalue equation is then

$$H_{\rm eff}^{(n)}|\phi_k^{(n)}\rangle=E_k|\phi_k^{(n)}\rangle\,. \tag{2·8}$$

Since $\tilde{H}_n$ is a transformed Hamiltonian as in Eq. (2·4) and satisfies the decoupling condition in Eq. (2·5), we readily see that the eigenvalue E_k agrees with one of the eigenvalues of the original Hamiltonian H. The true eigenstate $|\Phi_k^{(n)}\rangle$ corresponding to the model-space eigenstate $|\phi_k^{(n)}\rangle$ is given by

$$|\Phi_k^{(n)}\rangle=X_n|\phi_k^{(n)}\rangle$$
$$=(P+\omega)(P+\omega^\dagger\omega)^n|\phi_k^{(n)}\rangle\,. \tag{2·9}$$

The biorthogonal state of $|\Phi_k^{(n)}\rangle$ becomes

$$\langle\tilde{\Phi}_k^{(n)}|=\langle\tilde{\phi}_k^{(n)}|X_n^{-1}$$
$$=\langle\tilde{\phi}_k^{(n)}|(P+\omega^\dagger\omega)^{-n-1}(P+\omega^\dagger)\,, \tag{2·10}$$

where $\langle\tilde{\phi}_k^{(n)}|$ is the biorthogonal state of $|\phi_k^{(n)}\rangle$, satisfying $\langle\tilde{\phi}_i^{(n)}|\phi_j^{(n)}\rangle=\delta_{ij}$.

We here note that the general effective Hamiltonian $H_{\rm eff}^{(n)}$ includes the cases: When $n=0$, we have

$$H_{\rm eff}^{(0)}=PH(P+\omega)\,, \tag{2·11}$$

which is the well-known standard non-Hermitian effective Hamiltonian. When $n=-1/2$, we have[9)]

$$H_{\rm eff}^{(-1/2)}=(P+\omega^\dagger\omega)^{1/2}H(P+\omega)(P+\omega^\dagger\omega)^{-1/2}\,, \tag{2·12}$$

which is the Hermitian effective interaction, although it does not look manifestly Hermitian.

Recently Hurtubise and Freed[11),19)~21)] have proposed a general theory of effective interactions and operators by introducing a transformation by mapping operators between the model-space eigenstates and the corresponding true eigenstates. Their approach is different from our approach based on the similarity transformation and the decoupling condition as in Eqs. (2·4) and (2·6). However, we can show that their mapping operators have some solutions written in terms of ω and two approaches lead to the same solutions for the effective Hamiltonians. The detail of this problem will be discussed in the Appendix.

We now define a general effective operator in the bra-ket representation as

$$\Theta_{\rm eff}^{(n)}=\sum_{i,j}|\phi_i^{(n)}\rangle\langle\tilde{\Phi}_i^{(n)}|\Theta|\Phi_j^{(n)}\rangle\langle\tilde{\phi}_j^{(n)}|\,, \tag{2·13}$$

where Θ is a general time-independent and Hermitian operator. From the above definition we obtain the relation

$$\langle\tilde{\phi}_i^{(n)}|\Theta_{\rm eff}^{(n)}|\phi_j^{(n)}\rangle=\langle\tilde{\Phi}_i^{(n)}|\Theta|\Phi_j^{(n)}\rangle\,. \tag{2·14}$$

The above equation gives a formula for converting the matrix element in the entire space to that in the model space.

The effective operator $\Theta_{\rm eff}^{(n)}$ can be written in an operator form as

$$\Theta_{\rm eff}^{(n)}=(P+\omega^{\dagger}\omega)^{-n-1}(P+\omega^{\dagger})\Theta(P+\omega)(P+\omega^{\dagger}\omega)^{n}\,, \tag{2·15}$$

where we have used the relations in Eqs. (2·9) and (2·10), and

$$\sum_k|\phi_k^{(n)}\rangle\langle\tilde{\phi}_k^{(n)}|=P\,. \tag{2·16}$$

We here note that the relation in Eq. (2·14) holds independently of the normalization of $|\phi_k^{(n)}\rangle$ and $|\Phi_k^{(n)}\rangle$ as long as these two states are related as in Eq. (2·9). We, however, want to know the matrix element between the normalized true eigenstates. In order that $|\Phi_k^{(n)}\rangle$ be unity normalized, in this case $\langle\tilde{\Phi}_k^{(n)}|$ is identical to $\langle\Phi_k^{(n)}|$, the model-space state $|\phi_k^{(n)}\rangle$ should be normalized according to

$$\langle\phi_k^{(n)}|(P+\omega^{\dagger}\omega)^{2n+1}|\phi_k^{(n)}\rangle=1\,, \tag{2·17}$$

which is derived from Eq. (2·9). If all the true eigenstates $|\Phi_k^{(n)}\rangle$ with different n's are unity normalized, they should be the same, that is, we may write as $|\Phi_k^{(n)}\rangle=|\Phi_k\rangle$, because they are all the eigenstates of H with the eigenvalue E_k. We here do not consider the degeneracy of the eigenvalues of the original Hamiltonian H. Even though H has some degenerate eigenvalues, we can construct the eigenstates $|\Phi_k^{(n)}\rangle$ with different n's so as to be the same. We finally obtain an expression of the matrix element of Θ between the true eigenstates $|\Phi_i\rangle$ and $|\Phi_j\rangle$ as

$$\langle\Phi_i|\Theta|\Phi_j\rangle=\langle\tilde{\phi}_i^{(n)}|\Theta_{\rm eff}^{(n)}|\phi_j^{(n)}\rangle\,. \tag{2·18}$$

We here note that the above equality holds only if the P-space eigenstate $|\phi_j^{(n)}\rangle$ is normalized so as to satisfy the condition in Eq. (2·17).

We can derive another expression that is independent of the normalization of the P-space eigenstates $|\phi_k^{(n)}\rangle$ as

$$\begin{aligned}\langle\Phi_i|\Theta|\Phi_j\rangle&={\rm sign}(\langle\tilde{\Phi}_i^{(n)}|\Theta|\Phi_j^{(n)}\rangle)\sqrt{\langle\tilde{\Phi}_i^{(n)}|\Theta|\Phi_j^{(n)}\rangle\langle\tilde{\Phi}_j^{(n)}|\Theta|\Phi_i^{(n)}\rangle}\\&={\rm sign}(\langle\tilde{\phi}_i^{(n)}|\Theta_{\rm eff}^{(n)}|\phi_j^{(n)}\rangle)\sqrt{\langle\tilde{\phi}_i^{(n)}|\Theta_{\rm eff}^{(n)}|\phi_j^{(n)}\rangle\langle\tilde{\phi}_j^{(n)}|\Theta_{\rm eff}^{(n)}|\phi_i^{(n)}\rangle}\,.\end{aligned} \tag{2·19}$$

For the derivation of the above equation, we have used the fact that the states $|\Phi_k^{(n)}\rangle$ and $\langle\tilde{\Phi}_k^{(n)}|$ differ from $|\Phi_k\rangle$ and $\langle\tilde{\Phi}_k|$, respectively, only in normalization.

The general form of $\Theta_{\rm eff}^{(n)}$ includes two important cases: When $n=0$ and $n=-1/2$, we have respectively

$$\Theta_{\rm eff}^{(0)}=(P+\omega^{\dagger}\omega)^{-1}(P+\omega^{\dagger})\Theta(P+\omega) \tag{2·20}$$

and

$$\Theta_{\rm eff}^{(-1/2)}=(P+\omega^{\dagger}\omega)^{-1/2}(P+\omega^{\dagger})\Theta(P+\omega)(P+\omega^{\dagger}\omega)^{-1/2}\,. \tag{2·21}$$

The $\Theta_{\rm eff}^{(0)}$ is just the same as the effective operator derived, in a different way, by Navratil, Geyer and Kuo.[17] This effective operator is associated with the usual non-Hermitian effective interaction which is denoted by $H_{\rm eff}^{(0)}$ as in Eq. (2·11).

Another effective operator $\Theta_{\rm eff}^{(-1/2)}$ is the Hermitian form which has already been derived by several authors.[1),11),23),24)]

For practical purposes the Hermitian form $\Theta_{\rm eff}^{(-1/2)}$ would be more useful than the others, because when $n=-1/2$, Eq. (2·17) becomes $\langle\phi_k^{(-1/2)}|\phi_k^{(-1/2)}\rangle=1$ and therefore we do not have to require a special normalization condition. In this case the biorthogonal state $|\tilde{\phi}_k^{(-1/2)}\rangle$ is the same as $|\phi_k^{(-1/2)}\rangle$ and we have

$$\langle\Phi_i|\Theta|\Phi_j\rangle=\langle\phi_i^{(-1/2)}|\Theta_{\rm eff}^{(-1/2)}|\phi_j^{(-1/2)}\rangle\,. \tag{2·22}$$

However, in practice, the task of constructing the Hermitian effective interaction is often much more difficult than the non-Hermitian form, although the study of the Hermitian effective interaction theory has been under progress.[25)] On the other hand, the non-Hermitian form $\Theta_{\rm eff}^{(0)}$ seems to have the simplest structure. In any case we can choose an effective operator among $\Theta_{\rm eff}^{(n)}$ in Eq. (2·15) considering actual situations of the system.

§ 3. Relation between non-Hermitian and Hermitian effective operators

It will be convenient if we could find a way of converting the non-Hermitian form to the Hermitian form and vice versa. For this purpose we introduce basis states according to[14)]

$$\omega^\dagger\omega|\alpha_i\rangle=\mu_i^2|\alpha_i\rangle\,. \tag{3·1}$$

Note that $\omega^\dagger\omega$ is a P-space operator which is Hermitian and has positive-or-zero eigenvalues. The states $|\alpha_i\rangle$ are orthogonal to each other, i.e., $\langle\alpha_i|\alpha_j\rangle=\delta_{ij}$. Since ω acts as a transformation of a P-space state to a Q-space state as shown in Eq. (2·1) we can show that

$$\omega|\alpha_i\rangle=\mu_i|\nu_i\rangle\,, \tag{3·2}$$

where $|\nu_i\rangle$ is a Q-space state that is the image of $|\alpha_i\rangle$ generated by the mapping operator ω.

With the basis $|\alpha_i\rangle$, we have a representation of $\Theta_{\rm eff}^{(0)}$ as

$$\langle\alpha_i|\Theta_{\rm eff}^{(0)}|\alpha_j\rangle=\frac{(\langle\alpha_i|+\mu_i\langle\nu_i|)\Theta(|\alpha_j\rangle+\mu_j|\nu_j\rangle)}{(1+\mu_i^2)}\,. \tag{3·3}$$

In a similar manner we have for $\Theta_{\rm eff}^{(-1/2)}$

$$\langle\alpha_i|\Theta_{\rm eff}^{(-1/2)}|\alpha_j\rangle=\frac{(\langle\alpha_i|+\mu_i\langle\nu_i|)\Theta(|\alpha_j\rangle+\mu_j|\nu_j\rangle)}{\sqrt{1+\mu_i^2}\sqrt{1+\mu_j^2}}\,. \tag{3·4}$$

We easily see that the matrix element of the Hermitian effective operator can be written in terms of the non-Hermitian one as

$$\langle k|\Theta_{\rm eff}^{(-1/2)}|l\rangle=\sum_{i,j}\frac{\sqrt{1+\mu_i^2}}{\sqrt{1+\mu_j^2}}\langle\alpha_i|\Theta_{\rm eff}^{(0)}|\alpha_j\rangle\langle k|\alpha_i\rangle\langle\alpha_j|l\rangle\,, \tag{3·5}$$

where $|k\rangle$ and $|l\rangle$ are arbitrary basis states. The above equation gives a relation converting the non-Hermitian form to the Hermitian form. Therefore, we may say that the transformation of the non-Hermitian form to the Hermitian form is reduced to the calculation of $\omega^\dagger\omega$.

§ 4. Perturbative and non-perturbative expressions of effective operators

We now discuss how to calculate the effective operator $\Theta_{\rm eff}^{(n)}$. As seen from the expression of $\Theta_{\rm eff}^{(n)}$ in Eq. (2·15), the procedure of calculating the effective operator is reduced to the calculation of ω which obeys Eq. (2·6).

We here want to derive a general expression of the effective operator, assuming that the unperturbed Hamiltonian, denoted by H_0, is non-degenerate in the P space, i.e.,

$$H=H_0+V\,, \tag{4·1}$$

where V is the perturbation and

$$PH_0P=\sum_{k=1}^{d}\varepsilon_k P_k\,, \tag{4·2}$$

where d is the dimension of the P space and

$$P_k=|k\rangle\langle k|\,. \tag{4·3}$$

The effective interaction theory for a system with non-degenerate unperturbed energies ε_k has been developed in time-independent and time-dependent ways. We here follow the time-independent approach. In this approach the standard non-Hermitian effective interaction, denoted by R, is given by

$$R=PVP+PVQ\omega\,. \tag{4·4}$$

With R the operator ω in Eq. (2·6) is solved as[10)]

$$\omega=\sum_{n=1}^{\infty}\sum_{k_1\cdots k_n}\frac{(-1)^{n+1}}{(\varepsilon_{k_1}-QHQ)\cdots(\varepsilon_{k_n}-QHQ)}QVP_{k_1}\prod_{m=2}^{n}RP_{k_m}\,, \tag{4·5}$$

where, for $n=1$, we define

$$\prod_{m=2}^{n=1}RP_{k_m}=P\,. \tag{4·6}$$

In the degenerate case that $\varepsilon_\alpha=\varepsilon_0$, the solution ω becomes

$$\omega=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(\varepsilon_0-QHQ)^n}QVPR^{n-1}\,. \tag{4·7}$$

We factorize $\Theta_{\rm eff}^{(n)}$ as

$$\Theta_{\rm eff}^{(n)}=(P+\omega^\dagger\omega)^{-n-1}\hat{\Theta}(P+\omega^\dagger\omega)^n \tag{4·8}$$

with

$$\hat{\Theta}=(P+\omega^\dagger)\Theta(P+\omega)\,. \tag{4·9}$$

The procedure of the calculation of $\Theta_{\text{eff}}^{(n)}$ is divided into two parts, the calculations of $\hat{\Theta}$ and $\omega^{\dagger}\omega$. Using the solution of ω in Eq. (4·5), $\hat{\Theta}$ is given by

$$\hat{\Theta}=\hat{\Theta}_{PP}+(\hat{\Theta}_{PQ}+\text{h.c.})+\hat{\Theta}_{QQ}\,, \tag{4·10}$$

where

$$\hat{\Theta}_{PP}=P\hat{\Theta}P\,, \tag{4·11}$$

$$\begin{aligned}\hat{\Theta}_{PQ}&=P\hat{\Theta}\omega P\\&=\sum_{n=1}^{\infty}\sum_{k_1,\cdots,k_n}\hat{\Theta}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n})P_{k_1}\{\prod_{m=2}^{n}RP_{k_m}\}\end{aligned} \tag{4·12}$$

with

$$\hat{\Theta}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n})=P\Theta Q\frac{(-1)^{n+1}}{(\varepsilon_{k_1}-QHQ)\cdots(\varepsilon_{k_n}-QHQ)}QVP \tag{4·13}$$

and

$$\begin{aligned}\hat{\Theta}_{QQ}&=P\omega^{\dagger}\Theta\omega P\\&=\sum_{n=1}^{\infty}\sum_{k_1,\cdots,k_n}\sum_{n'=1}^{\infty}\sum_{l_1,\cdots,l_{n'}}\{\prod_{m=2}^{n}(P_{k_m}R^{\dagger})\}P_{k_1}\\&\quad\times\hat{\Theta}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n};\varepsilon_{l_1},\cdots,\varepsilon_{l_{n'}})P_{l_1}\{\prod_{m'=2}^{n'}RP_{l_{m'}}\}\end{aligned} \tag{4·14}$$

with

$$\begin{aligned}&\hat{\Theta}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n};\varepsilon_{l_1},\cdots,\varepsilon_{l_{n'}})\\&\quad=PVQ\frac{(-1)^{n}}{(\varepsilon_{k_1}-QHQ)\cdots(\varepsilon_{k_n}-QHQ)}Q\Theta Q\\&\quad\times\frac{(-1)^{n'}}{(\varepsilon_{l_1}-QHQ)\cdots(\varepsilon_{l_{n'}}-QHQ)}QVP\,.\end{aligned} \tag{4·15}$$

If the unperturbed energies ε_k are all degenerate, Θ_{PQ} and Θ_{QQ} become

$$\Theta_{PQ}=\sum_{n=0}^{\infty}\hat{\Theta}_n R^n \tag{4·16}$$

with

$$\begin{aligned}\hat{\Theta}_n&=P\Theta Q\frac{(-1)^n}{(\varepsilon_0-QHQ)^{n+1}}QVP\\&=\frac{1}{n!}\frac{d^n\hat{\Theta}(\varepsilon)}{d\varepsilon^n}\Big|_{\varepsilon=\varepsilon_0}\end{aligned} \tag{4·17}$$

and

$$\hat{\Theta}_{QQ}=\sum_{n,m=0}^{\infty}(R^{\dagger})^n\hat{\Theta}_{nm}R^m \tag{4·18}$$

with

$$\hat{\Theta}_{nm}=PVQ\frac{(-1)^n}{(\varepsilon_0-QHQ)^{n+1}}Q\Theta Q\frac{(-1)^m}{(\varepsilon_0-QHQ)^{m+1}}QVP$$
$$=\frac{1}{n!m!}\frac{\partial^n}{\partial\varepsilon_1{}^n}\frac{\partial^m}{\partial\varepsilon_2{}^m}\hat{\Theta}(\varepsilon_1;\varepsilon_2)|_{\varepsilon_1=\varepsilon_0,\varepsilon_2=\varepsilon_0}\,. \tag{4·19}$$

In Eqs. (4·16) and (4·18) we have used the notations for $n=0$ and $m=0$ that $\hat{\Theta}_0=\hat{\Theta}(\varepsilon_0)$ and $\hat{\Theta}_{00}=\hat{\Theta}(\varepsilon_0;\varepsilon_0)$.

In the degenerate case, as seen in Eqs. (4·17) and (4·19), the terms $\hat{\Theta}_{PQ}$ and $\hat{\Theta}_{QQ}$ can be generated by the energy derivatives of two kinds of the elements $\hat{\Theta}(\varepsilon)$ and $\hat{\Theta}(\varepsilon_1;\varepsilon_2)$ which are written explicitly as

$$\hat{\Theta}(\varepsilon)=P\Theta Q\frac{1}{\varepsilon-QHQ}QVP \tag{4·20}$$

and

$$\hat{\Theta}(\varepsilon_1;\varepsilon_2)=PVQ\frac{1}{(\varepsilon_1-QHQ)}Q\hat{\Theta}Q\frac{1}{(\varepsilon_2-QHQ)}QVP\,. \tag{4·21}$$

In the non-degenerate case, we can show that $\hat{\Theta}_{PQ}$ and $\hat{\Theta}_{QQ}$ can also be generated from $\hat{\Theta}(\varepsilon)$ and $\hat{\Theta}(\varepsilon_1;\varepsilon_2)$ by using the partial fraction method.[16] For example, if we use an identity

$$\frac{1}{(\varepsilon_k-QHQ)(\varepsilon_l-QHQ)}=\left(\frac{1}{\varepsilon_k-QHQ}-\frac{1}{\varepsilon_l-QHQ}\right)/(\varepsilon_l-\varepsilon_k)\,, \tag{4·22}$$

we can easily derive a relation

$$\hat{\Theta}(\varepsilon_k,\varepsilon_l)=\frac{1}{\varepsilon_k-\varepsilon_l}\{\hat{\Theta}(\varepsilon_k)-\hat{\Theta}(\varepsilon_l)\}\,. \tag{4·23}$$

In the same way, we also have a relation

$$\hat{\Theta}(\varepsilon_k,\varepsilon_l;\varepsilon_m,\varepsilon_n)=\frac{1}{(\varepsilon_k-\varepsilon_l)}\frac{1}{(\varepsilon_m-\varepsilon_n)}$$
$$\times\{\hat{\Theta}(\varepsilon_k;\varepsilon_m)-\hat{\Theta}(\varepsilon_k;\varepsilon_n)-\hat{\Theta}(\varepsilon_l;\varepsilon_m)+\hat{\Theta}(\varepsilon_l;\varepsilon_n)\}\,. \tag{4·24}$$

In general, it can be proved that $\hat{\Theta}(\varepsilon_k,\cdots,\varepsilon_n)$ and $\hat{\Theta}(\varepsilon_k,\cdots,\varepsilon_l;\varepsilon_m,\cdots,\varepsilon_n)$ can be expressed in terms of two kinds of the operators $\hat{\Theta}(\varepsilon)$ and $\hat{\Theta}(\varepsilon_1;\varepsilon_2)$.

Another part of constructing $\hat{\Theta}_{\rm eff}^{(n)}$ is the calculation of $\omega^\dagger\omega$. With the solution ω in Eq. (4·5), $\omega^\dagger\omega$ becomes

$$\omega^\dagger\omega=-\sum_{n=1}^{\infty}\sum_{k_1,\cdots,k_n}\sum_{n'=1}^{\infty}\sum_{l_1,\cdots,l_{n'}}\{\prod_{m=2}^{n}P_{k_m}R^\dagger\}P_{k_1}$$
$$\times\hat{Q}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n},\varepsilon_{l_1},\cdots,\varepsilon_{l_{n'}})P_{l_1}\{\prod_{m'=2}^{n'}RP_{l_{m'}}\}\,, \tag{4·25}$$

where $\hat{Q}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n},\varepsilon_{l_1},\cdots,\varepsilon_{l_{n'}})$ is the multi-energy $\hat{Q}$-box defined by

$$\hat{Q}(\varepsilon_{k_1},\cdots,\varepsilon_{k_n},\varepsilon_{l_1},\cdots,\varepsilon_{l_{n'}})=PVQ\frac{(-1)^{n+n'+1}}{(\varepsilon_{k_1}-QHQ)\cdots(\varepsilon_{k_n}-QHQ)}$$

$$\times \frac{1}{(\varepsilon_{l_1} - QHQ)\cdots(\varepsilon_{l_{n'}} - QHQ)} QVP . \tag{4·26}$$

It has been shown[16),26)] that the multi-energy $\hat{Q}$-box can also be expressed in terms of the differential quotients and/or the derivatives of the single-energy $\hat{Q}$-box, namely, $\hat{Q}(\varepsilon)$.

In the degenerate case, $\omega^\dagger \omega$ is simplified to

$$\omega^\dagger \omega = -\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} (R^\dagger)^{n-1} \hat{Q}_{n+m-1} R^{m-1} , \tag{4·27}$$

where $\hat{Q}_{n+m-1}$ is the energy derivative of $\hat{Q}(\varepsilon)$ defined generally by

$$\hat{Q}_k = (-1)^k PVQ\left(\frac{1}{\varepsilon_0 - QHQ}\right)^{k+1} QVP$$

$$= \frac{1}{k!} \frac{d^k \hat{Q}(\varepsilon)}{d\varepsilon^k}\bigg|_{\varepsilon=\varepsilon_0} \tag{4·28}$$

with

$$\hat{Q}(\varepsilon) = PVP + PVQ\frac{1}{\varepsilon - QHQ} QVP . \tag{4·29}$$

We have given some general formulae for constructing the effective operator in terms of the non-Hermitian effective interaction R. The structure of R has been well known for both systems with degenerate and non-degenerate unperturbed energies. In the degenerate case, R is expanded into[3),6),15)]

$$R = F_0 + F_1 + F_2 + F_3 + \cdots , \tag{4·30}$$

$$F_0 = \hat{Q} , \tag{4·31}$$

$$F_1 = \hat{Q}_1 \hat{Q} , \tag{4·32}$$

$$F_2 = \hat{Q}_2 \hat{Q}\hat{Q} + \hat{Q}_1 \hat{Q}_1 \hat{Q} , \tag{4·33}$$

$$F_3 = \hat{Q}_3 \hat{Q}\hat{Q}\hat{Q} + \hat{Q}_2 \hat{Q}_1 \hat{Q}\hat{Q} + \hat{Q}_1 \hat{Q}_2 \hat{Q}\hat{Q} + \hat{Q}_1 \hat{Q}_1 \hat{Q}_1 \hat{Q} + \hat{Q}_2 \hat{Q}\hat{Q}_1 \hat{Q} . \tag{4·34}$$

Here, for simplicity, we have dropped the energy variables in $\hat{Q}(\varepsilon)$.

If we substitute the above expansion formula for R into $\omega^\dagger \omega$ in Eq. (4·27), we have

$$\omega^\dagger \omega = -\{\hat{Q}_1 + (\hat{Q}_2 \hat{Q} + \text{h.c.})$$

$$+ (\hat{Q}_3 \hat{Q}\hat{Q} + \text{h.c.}) + (\hat{Q}_2 \hat{Q}_1 \hat{Q} + \text{h.c.}) + \hat{Q}\hat{Q}_3 \hat{Q} + \cdots\} . \tag{4·35}$$

From the expansion formulae of R and $\omega^\dagger \omega$, we readily see that the effective operator can be expanded into a series of the $\hat{Q}$-box, $\hat{\Theta}_n$ in Eq. (4·17) and $\hat{\Theta}_{nm}$ in Eq. (4·19). We here show the final perturbative expansion form of the non-Hermitian effective operator $\Theta_{\text{eff}}^{(0)}$,

$$\Theta_{\text{eff}}^{(0)} = (P + \hat{Q}_1 + \hat{Q}_1 \hat{Q}_1 + \hat{Q}_2 \hat{Q} + \hat{Q}\hat{Q}_2 + \cdots)(\chi_0 + \chi_1 + \chi_2 + \cdots) , \tag{4·36}$$

where

$$\chi_0 = P\Theta P + (\hat{\Theta}_0 + \text{h.c.}) + \hat{\Theta}_{00}\,, \tag{4·37}$$

$$\chi_1 = (\hat{\Theta}_1\hat{Q} + \text{h.c.}) + (\hat{\Theta}_{01}\hat{Q} + \text{h.c.})\,, \tag{4·38}$$

$$\chi_2 = (\hat{\Theta}_1\hat{Q}_1\hat{Q} + \text{h.c.}) + (\hat{\Theta}_2\hat{Q}\hat{Q} + \text{h.c.}) + (\hat{\Theta}_{02}\hat{Q}\hat{Q} + \text{h.c.}) + \hat{Q}\hat{\Theta}_{11}\hat{Q}\,. \tag{4·39}$$

The above results can easily be generalized to the non-degenerate case. The result is

$$\Theta_{\text{eff}}^{(0)} = [P + \sum_{k,l} P_k\hat{Q}(\varepsilon_k, \varepsilon_l)P_l + \sum_{k,l,m} P_k\hat{Q}(\varepsilon_k, \varepsilon_l)P_l\hat{Q}(\varepsilon_l, \varepsilon_m)P_m$$
$$+ \{\sum_{k,l,m} P_k\hat{Q}(\varepsilon_k, \varepsilon_l, \varepsilon_m)P_l\hat{Q}(\varepsilon_m)P_m + \text{h.c.}\} + \cdots]$$
$$\times(\chi_0 + \chi_1 + \chi_2 + \cdots)\,, \tag{4·40}$$

where

$$\chi_0 = P\Theta P + \sum_k \{\hat{\Theta}(\varepsilon_k)P_k + \text{h.c.}\} + \sum_{k,l} P_k\hat{\Theta}(\varepsilon_k; \varepsilon_l)P_l\,, \tag{4·41}$$

$$\chi_1 = \sum_{k,l} \{\hat{\Theta}(\varepsilon_k, \varepsilon_l)P_k\hat{Q}(\varepsilon_l)P_l + \text{h.c.}\} + \sum_{k,l,m} \{P_k\hat{\Theta}(\varepsilon_k; \varepsilon_l, \varepsilon_m)P_l\hat{Q}(\varepsilon_m)P_m + \text{h.c.}\}\,. \tag{4·42}$$

We next discuss a non-perturbative way of constructing the effective operator. We consider the eigenvalue equation of the effective Hamiltonian as

$$(PH_0P + R)|\phi_k\rangle = E_k|\phi_k\rangle\,. \tag{4·43}$$

The state $|\phi_k\rangle$ is the same as $|\phi_k^{(n=0)}\rangle$ in Eq. (2·8). With E_k and $|\phi_k\rangle$ the solution for the operator ω in Eq. (2·6) can be written as[22]

$$\omega = \sum_k \frac{1}{E_k - QHQ} QVP|\phi_k\rangle\langle\tilde{\phi}_k|\,. \tag{4·44}$$

With the solution for ω, $\omega^\dagger\omega$ becomes

$$\omega^\dagger\omega = \sum_{k,l} |\tilde{\phi}_k\rangle\langle\phi_k|PVQ\frac{1}{E_k - QHQ}\frac{1}{E_l - QHQ}QVP|\phi_l\rangle\langle\tilde{\phi}_l|$$
$$= -\sum_{k,l} |\tilde{\phi}_k\rangle\langle\phi_k|\frac{\hat{Q}(E_k) - \hat{Q}(E_l)}{E_k - E_l}|\phi_l\rangle\langle\tilde{\phi}_l|\,, \tag{4·45}$$

where we have used Eq. (4·22), and for $E_k = E_l$ the differential quotient should be replaced by the derivative $d\hat{Q}(E)/dE|_{E=E_k}$.

Using Eq. (4·44), the operator $\hat{\Theta}$ in Eq. (4·9) is expressed as

$$\hat{\Theta} = P\Theta P + \{\sum_k \hat{\Theta}(E_k)|\phi_k\rangle\langle\tilde{\phi}_k| + \text{h.c.}\}$$
$$+ \sum_{k,k'} |\tilde{\phi}_k\rangle\langle\phi_k|\hat{\Theta}(E_k; E_{k'})|\phi_{k'}\rangle\langle\tilde{\phi}_{k'}|\,. \tag{4·46}$$

If we use the eigenstates $\{|\alpha_i\rangle\}$ of $\omega^\dagger\omega$ in Eq. (3·1), the matrix element of $\Theta_{\text{eff}}^{(n)}$ between arbitrary states $|l\rangle$ and $|m\rangle$ is finally given by

$$\langle m|\Theta_{\text{eff}}^{(n)}|l\rangle = \sum_{i,j} \langle m|\alpha_i\rangle\langle\alpha_j|l\rangle\frac{(1+\mu_j^2)^n}{(1+\mu_i^2)^{n+1}}\{\langle\alpha_i|\Theta|\alpha_j\rangle + \sum_k \langle\alpha_i|\hat{\Theta}(E_k)|\phi_k\rangle\langle\tilde{\phi}_k|\alpha_j\rangle$$

$$+\sum_k\langle a_i|\tilde{\phi}_k\rangle\langle\phi_k|\hat{\Theta}(E_k)|a_j\rangle+\sum_{k,k'}\langle a_i|\tilde{\phi}_k\rangle\langle\phi_k|\hat{\Theta}(E_k;E_{k'})|\phi_{k'}\rangle\langle\tilde{\phi}_{k'}|a_j\rangle\}, \tag{4·47}$$

where μ_i^2 and μ_j^2 are the eigenvalues of $\omega^\dagger\omega$ as given in Eq. (3·1). The above non-perturbative formula will be simple and useful, but its applicability depends on the accuracy of the effective interaction R. If R is accurate, the effective operator is also accurate.

§ 5. Concluding remarks

We have derived a general solution for the effective operator. This solution contains, as special cases, the effective operators given by Navratil, Geyer and Kuo[17] and by Hurtubise and Freed.[11] When we want to express the effective operator in the state-independent operator form, the problem of the normalization of the model-space states takes place unless the effective operator is not given through unitary transformation. However, we have shown that this normalization problem can be resolved by taking geometric mean of the effective operator over the model-space states and their biorthogonal states as shown in Eq. (2·19).

We have given a general expansion formula for the effective operator in terms of the $\hat{\Theta}$-box and the usual $\hat{Q}$-box. The $\hat{\Theta}$ expresses a certain set of diagrams that contain the vertex of the original operator Θ. The general diagram rule of the $\hat{\Theta}$-box expansion, however, has not yet been clarified and it will be an interesting open problem. For the Hermitian effective operator the diagrammatical representation of the first few perturbation terms has been given by Stout and Kuo,[24] and Hurtubise and Freed.[21]

We have also derived the non-perturbative solution for the effective operator as in Eq. (4·47). In this expression the construction of the effective operator has been reduced to the calculation of the $\hat{\Theta}$-boxes at the energy variables equal to the true eigenvalues of the Hamiltonian.

In this study we have shown that the effective operator, in the perturbative or non-perturbative forms, can be calculated by using the operators, $\hat{\Theta}(\varepsilon_k)$, $\hat{\Theta}(\varepsilon_k;\varepsilon_l)$ and the usual $\hat{Q}$-box $\hat{Q}(\varepsilon)$. All the terms appeared in the expression of the effective operators can be generated from the derivatives or the differential quotients of these three basic elements with respect to the energy variables.

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Appendix A
—— *Relation of the Present Approach with the Hurtubise and Freed Formulation* ——

Recently Hurtubise and Freed[11),19)~21)] have made a general formulation of effective Hamiltonians and operators. They introduced two mapping operators k and l such that the effective Hamiltonian can be given by

$$\bar{H}_{\rm eff}=lHk\,. \tag{A·1}$$

In the bra-ket representation their mapping operators are written as[11)]

$$k=\sum_{m=1}^{d}|\Phi_m\rangle\langle\tilde{\phi}_m| \tag{A·2}$$

and

$$l=\sum_{m=1}^{d}|\phi_m\rangle\langle\Phi_m|\,, \tag{A·3}$$

where $|\Phi_m\rangle$ is the true eigenstate of H. The state $|\phi_m\rangle$ is the model-space eigenstate of $\bar{H}_{\rm eff}$ and $\langle\tilde{\phi}_m|$ is the biorthogonal state of $|\phi_m\rangle$.

The operator l is not the inverse of k in the entire Hilbert space. Therefore, their theory is different from our approach that is based on the similarity-transformation theory. The mapping operators k and l are determined dependently on the choice of the model-space eigenstates $|\phi_m\rangle$. It will be of interest to solve k and l that are associated with the model-space eigenstates $\{|\phi_m{}^{(n)}\rangle\}$ in Eq. (2·8). In this case we can prove that k and l are given with the index n as

$$k^{(n)}=(P+\omega)(P+\omega^\dagger\omega)^n \tag{A·4}$$

and

$$l^{(n)}=(P+\omega^\dagger\omega)^{-n-1}(P+\omega^\dagger)\,. \tag{A·5}$$

We easily see that $k^{(n)}$ and $l^{(n)}$ satisfy

$$l^{(n)}k^{(n)}=P \tag{A·6}$$

and

$$k^{(n)}l^{(n)}=\bar{P}\,, \tag{A·7}$$

where

$$\bar{P}=\sum_{m=1}^{d}|\Phi_m\rangle\langle\Phi_m|=(P+\omega)(P+\omega^\dagger\omega)^{-1}(P+\omega^\dagger)\,. \tag{A·8}$$

Equations (A·6) and (A·7) are the important conditions imposed on the solutions for k and l as in Ref. 11). The relation in Eq. (A·8) has been derived in Ref. 9). We easily see, for special cases, that $k^{(n)}$ for $n=0$ and $n=-1/2$ are identical to $\hat{K}_B$ and $\hat{K}_C$ in their notations, respectively.

The effective Hamiltonian is now given by

$$\bar{H}_{\rm eff}^{(n)}=l^{(n)}Hk^{(n)}=(P+\omega^\dagger\omega)^{-n-1}(P+\omega^\dagger)H(P+\omega)(P+\omega^\dagger\omega)^n\,. \tag{A·9}$$

The above form looks apparently different from $H_{\rm eff}^{(n)}$ in Eq. (2·7). However, if we use the fact that $\bar{P}$ and H are commutable, we can prove that $\bar{H}_{\rm eff}^{(n)}$ in Eq. (A·9) is identical to $H_{\rm eff}^{(n)}$. Their approach is different from our similarity-transformation theory, but two approaches lead to some of the same solutions for the effective Hamiltonians.

We note that their mapping operators k and l have a certain set of the solutions that are expressed in terms of the mapping operator ω. Since the formal solution for

ω has been known as in Eqs. (4·5) and (4·7) for both the non-degenerate and degenerate unperturbed systems, the mapping operators $k^{(n)}$ and $l^{(n)}$ can also be constructed in the framework of the $\hat{Q}$-box theory.

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