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Degenerate Perturbation Theory in Quantum Mechanics

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The relations are discussed among a number of different formulations of perturbation theory for an effective Hamiltonian of a general quantum system. Although the definitions and the formulations are apparently different, it is shown that the effective Hamiltonians, which have appeared in the history of time-independent approaches, can be written simply in a unified form. Expansion formulae are given explicitly for both the non-Hermitian and Hermitian effective Hamiltonians, and a discussion is given on a method for summing up the expansion series and obtaining a convergent result.

§ 1. Introduction

There have been a number of formulations of degenerate perturbation theory in quantum mechanics. These formulations present various expansion formulae for an effective Hamiltonian or an effective interaction. A comprehensive review of the recent developments on this subject may be seen in Kuo's lecture.[1] The effective Hamiltonian is introduced as an operator which acts within a model space (zero-order eigenspace) and yields the same eigenvalues as those of the original Hamiltonian. Such requirements for the effective Hamiltonian are not sufficient for determining it uniquely. This is the reason why many definitions or expressions of the effective Hamiltonian are possible. In the present study, we confine ourselves to discussing only time-independent formulations.

The interrelations among various degenerate-perturbation approaches were discussed formerly by Klein[2] and Brandow,[3] and the formal equivalence among some formulations was proved. In particular, they discussed the relation among a variety of expressions of the Hermitian effective Hamiltonian. However, the formal equivalence among different expressions of the Hermitian form is not always obvious, although an indirect proof of the equivalence has been given.[2)~4)] One of the aims of the present study is to discuss this problem of the equivalence among many different expressions of the effective Hamiltonian.

Another subject to be discussed is the convergence problem. For the non-Hermitian effective interaction, an iteration method has been proposed which always brings about a convergent result by Lee and one of the authors (K.S.).[5] On the other hand, no method has yet been known for calculating a convergent Hermitian effective interaction. In the present study, a method will be outlined by which the non-Hermitian effective interaction is converted to an equivalent hermitized form and thus the convergent Hermitian effective interaction can be obtained.

In § 2, two effective Hamiltonians, one of which is non-Hermitian and the other is Hermitian, are introduced by means of the similarity-transformation method for the effective Hamiltonian. In § 3, the relations among different expressions of the effective Hamiltonian are discussed. In § 4, expansion formulae for both of the non-Hermitian and Hermitian effective interactions are given in an explicit form. In § 5, a method is given

for summing up the series in the perturbation expansion and obtaining a convergent result for the effective interaction. In § 6, some conclusions obtained in the present study are given.

§ 2. Similarity transformation and effective interaction

2.1. *Effective interaction by means of similarity transformation*

We introduce the projection operators P and Q which project a state onto the model space and its complement, respectively. The model space and its complement are referred to as the P and Q spaces, respectively.

We consider a quantum system with the Hamiltonian

$$H=H_0+V\,, \tag{2·1}$$

where H_0 is an unperturbed Hamiltonian and V is a perturbation. The model space is defined as a zero-order eigenspace of H_0 so that we have

$$[H_0, P]=[H_0, Q]=0\,. \tag{2·2}$$

The aim now is to construct an operator V^{eff} such that it acts only inside the P space and the effective Hamiltonian PH_0P+V^{eff} has eigenvalues which agree with those of the full Hamiltonian H. This approach to the quantum mechanical eigenvalue problem is often referred to as *partitioning technique* which was mainly due to Feshbach[6] and Löwdin.[7]

A general equation for constructing V^{eff} can be derived by applying the similarity transformation theory.[1),5)] We consider a transformed Hamiltonian

$$\mathcal{H}=X^{-1}HX\,. \tag{2·3}$$

If the operator X is a solution to the decoupling equation

$$Q\mathcal{H}P=Q(X^{-1}HX)P=0\,, \tag{2·4}$$

the P-space operator $P\mathcal{H}P$ can be an effective Hamiltonian and V^{eff} is obtained as

$$V^{\text{eff}}=P(X^{-1}HX)P-PH_0P\,. \tag{2·5}$$

A different choice of X leads us to a different effective interaction. We here consider two types of the similarity transformations.

2.2. *Non-Hermitian effective interaction*

We define a transformation X as

$$X=e^{\omega}\,, \tag{2·6}$$

where ω is an operator which satisfies

$$\omega=Q\omega P\,, \tag{2·7}$$

$$P\omega=\omega Q=0\,, \tag{2·8}$$

$$\omega^2=\omega^3=\cdots=0\,. \tag{2·9}$$

From Eq. (2·9), we have

$$e^{\omega}=1+\omega \tag{2·10}$$

and the decoupling equation (2·4) becomes

$$Q(e^{-\omega}He^{\omega})P=QVP+QHQ\omega-\omega PHP-\omega PVQ\omega=0\,. \tag{2·11}$$

The transformation X in Eq. (2·6) is not unitary so that the effective interaction is non-Hermitian. The effective Hamiltonian and the effective interaction, which are denoted respectively by $\mathcal{H}_{\rm NH}$ and R, are given by

$$\begin{aligned}\mathcal{H}_{\rm NH}&=P(e^{-\omega}He^{\omega})P\\&=PHP+PVQ\omega\,,\end{aligned} \tag{2·12}$$

$$R=PVP+PVQ\omega\,. \tag{2·13}$$

The decoupling equation (2·11) was given formerly by Ōkubo[8] in the investigation of the Tamm-Dancoff theory. The same equation was also derived by Poves and Zuker[9] and was used to reformulate the degenerate perturbation theory. An equation used by Schucan and Weidenmüller[10] for the discussion of the convergence problem is proved to be essentially equivalent to Eq.(2·11). Lee and one of the authors (K.S.)[5] proposed an iteration method for solving Eq. (2·11) in a non-perturbative way.

2.3. *Hermitian effective interaction*

Another choice of the transformation X is

$$X=e^{G}\,, \tag{2·14}$$

where G is an anti-Hermitian operator satisfying

$$G^{\dagger}=-G \tag{2·15}$$

from which we see that X is a unitary operator.

The decoupling equation (2·4) is now written as

$$Q(e^{-G}He^{G})P=0\,. \tag{2·16}$$

The solution G to the above equation is ambiguous. For the unique determination of G we require

$$PGP=QGQ=0 \tag{2·17}$$

which are the usual restrictive conditions.[2),3)]

This approach of the unitary transformation has long history since Van Vleck[11] suggested first. After his work this approach was followed by Jordahl,[12] Kemble,[13] Primas[14] and Kvasnička.[15] The historical review of this approach can be seen in the papers of Klein[2] and Brandow.[3]

The decoupling equation (2·16) is quite complicated in structure. Many authors tried to solve it perturbatively and first several terms were obtained in the perturbation expansion of the effective interaction.[11)~15)] A general perturbative solution for G was given in Klein's paper.[2]

The exact and non-perturbative solution for G was given in terms of the operator ω

as

$$G=\operatorname{arctanh}(\omega-\omega^{\dagger})$$
$$=\sum_{n=0}^{\infty}\frac{(-)^n}{2n+1}\{\omega(\omega^{\dagger}\omega)^n-\text{h.c.}\}. \tag{2·18}$$

The above solution was obtained by Shavitt and Redmon,[33] Westhaus[34] and one of the authors (K.S.).[16] This relation between G and ω is essential in discussing the formal relation between the Hermitian and non-Hermitian effective interactions.

Since X is unitary, the effective Hamiltonian $\mathcal{H}_{\text{H}}$ and the effective interaction W become Hermitian. With the solution G in Eq. (2·18), $\mathcal{H}_{\text{H}}$ and W are given by

$$\mathcal{H}_{\text{H}}=P(e^{-G}He^{G})P\,, \tag{2·19}$$

$$W=\mathcal{H}_{\text{H}}-PH_0P$$
$$=PVP+\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}F(m,n)\{(\omega^{\dagger}\omega)^mPVQ\omega(\omega^{\dagger}\omega)^n+\text{h.c.}\}, \tag{2·20}$$

where $F(m, n)$ is a coefficient defined through the expansion formula

$$\frac{\sqrt{1+x}}{\sqrt{1+x}+\sqrt{1+y}}=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}F(m,n)x^my^n\,. \tag{2·21}$$

The proof of the relation (2·20) and an explicit form of the coefficient $F(m, n)$ have been given in Refs. 16) and 33). In terms of the non-Hermitian effective interaction R, W is expressed as[16]

$$W=\frac{1}{2}(R+R^{\dagger})+\sum_{\substack{m\geqq 0,\ n\geqq 0\\(m+n\neq 0)}}F(m,n)(\omega^{\dagger}\omega)^m(R-R^{\dagger})(\omega^{\dagger}\omega)^n\,. \tag{2·22}$$

This expression may be convenient to see how the non-Hermiticity $R-R^{\dagger}$ contributes to the Hermitian effective interaction W.

§ 3. Various effective Hamiltonians and relations among them

There have been a number of different definitions of the effective Hamiltonian or the effective interaction. The relations among them have already been discussed by Klein[2] and Brandow.[3] Some important investigations have been made on the formal relations among various different expressions. However, it seems that obscurity still remains in the proof of the equivalence among them.

Suppose that as the perturbation is turned on, the zero-order eigenstates $\{|\phi_k\rangle\}$in the P space evolve into orthogonal eigenstates $\{|\Phi_k\rangle\}$. In the unitary-transformation method, the state $|\phi_k\rangle$ is an eigenstate of $\mathcal{H}_{\text{H}}$ in Eq. (2·19), and $|\Phi_k\rangle$ is a transformed state $e^{G}|\phi_k\rangle$. We define a projection operator

$$\bar{P}=\sum_{k=1}^{d}|\Phi_k\rangle\langle\Phi_k|, \tag{3·1}$$

where d is the dimension of the P space. The operator $\bar{P}$ can be written in terms of ω as

$$\bar{P}=(P+\omega)(P+\omega^{\dagger}\omega)^{-1}(P+\omega^{\dagger}). \tag{3·2}$$

In the derivation of the above relation, we have used

$$P=\sum_{k=1}^{d}|\phi_k\rangle\langle\phi_k| \tag{3·3}$$

and

$$e^{G}=(1+\omega-\omega^{\dagger})(1+\omega^{\dagger}\omega+\omega\omega^{\dagger})^{-1/2} \tag{3·4}$$

which has already been proved in Ref. 16).

We next define an operator $\mathcal{Q}$ which satisfies the equation

$$[\mathcal{Q}, H_0]=V\mathcal{Q}-\mathcal{Q}V\mathcal{Q}\,. \tag{3·5}$$

The above equation was given by Lindgren.[17] The operator $\mathcal{Q}$ is the Møller wave operator which is rather familiar in the perturbation theory. Compared with Eq. (2·11) for ω, we readily see that $\mathcal{Q}$ is related to ω as

$$\mathcal{Q}=P+\omega\,. \tag{3·6}$$

It may be worthwhile pointing out that Lindgren's equation (3·5) is essentially equivalent to Eq. (2·11) which is derived with the requirement that the transformed interaction should not have non-zero matrix element between the P- and Q-space state.

The effective Hamiltonian appeared so far in the history of the degenerate perturbation theory can be classified into the following three categories:

(I) Kato's effective Hamiltonian

The effective Hamiltonian of Kato[18] is defined as

$$\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}=PH\bar{P}P\,. \tag{3·7}$$

Using Eq. (3·2), we can express $\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}$ in terms of ω as

$$\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}=PH(P+\omega)(P+\omega^{\dagger}\omega)^{-1}\,. \tag{3·8}$$

It must be noted that Kato's effective Hamiltonian requires the use of a non-diagonal metric (or non-identity overlap) $P\bar{P}P$. The model-space eigenvalue equation becomes

$$\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}|\zeta_k\rangle=E_k\,P\bar{P}P|\zeta_k\rangle. \tag{3·9}$$

The Hamiltonian $\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}$ in Eqs. (3·7) and (3·8) is not manifestly Hermitian, but it is really Hermitian. This property of $\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}$ can be easily verified by means of Eq. (2·11) for ω. Although $\mathcal{H}_{\mathrm{K}}^{(\mathrm{I})}$ is Hermitian, the model-space eigenstates $\{|\zeta_k\rangle\}$ are not orthogonal, because the non-diagonal metric $P\bar{P}P$ appears in the eigenvalue equation (3·9).

(II) Non-Hermitian effective Hamiltonian

Elimination of the non-diagonal metric in Kato's definition leads us to the following non-Hermitian effective Hamiltonian

$$\mathcal{H}_{\mathrm{a}}^{(\mathrm{II})}=PH\bar{P}P(1/P\bar{P}P). \tag{3·10}$$

Another expression of the non-Hermitian form is

$$\mathcal{H}_{\mathrm{b}}^{(\mathrm{II})}=PH\Omega$$
$$=PH_0P+PV\Omega\,. \tag{3·11}$$

This expression of the effective Hamiltonian may be the most familiar definition in the degenerate perturbation theory. As is well known, in the standard perturbation theory which is often referred to as of Bloch-Horowitz,[19] Brillouin-Wigner or Rayleigh-Schrödinger, this definition has been employed. A general theory for the perturbation expansion of Ω and $PV\Omega$ was developed extensively by Bloch[20] and des Cloizeaux.[21] The time-independent folded-diagram approach of Brandow[22] is also based on this definition.

From the relations (3·2) and (3·6), we easily see that all the non-Hermitian effective Hamiltonians $\mathcal{H}_{\mathrm{NH}}$ in Eq. (2·12), $\mathcal{H}_{\mathrm{a}}^{(\mathrm{II})}$ in Eq. (3·10) and $\mathcal{H}_{\mathrm{b}}^{(\mathrm{II})}$ in Eq. (3·11) are formally identical, and they are written as

$$\mathcal{H}_{\mathrm{NH}}=\mathcal{H}_{\mathrm{a}}^{(\mathrm{II})}=\mathcal{H}_{\mathrm{b}}^{(\mathrm{II})}=PH(P+\omega). \tag{3·12}$$

(III) Hermitian effective interaction

Much effort has been made for constructing a Hermitian effective Hamiltonian. A straightforward way would be the unitary-transformation method described in the previous section.

Other definitions of the Hermitian effective Hamiltonian are

$$\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}=(P\bar{P}P)^{-1/2}P\bar{P}H\bar{P}P(P\bar{P}P)^{-1/2} \tag{3·13}$$

and

$$\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}=(\Omega^{\dagger}\Omega)^{1/2}PH\Omega(\Omega^{\dagger}\Omega)^{-1/2}\,. \tag{3·14}$$

The definition of $\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}$ is of des Cloizeaux,[21] and it was called by Brandow[3] the *rationalized Kato-Bloch Hamiltonian.* The definition of $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$ appeared already in the papers of Ōkubo,[8] and Fukuda, Sawada and Taketani.[23] The structure of $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$ was studied extensively by Brandow[3),22] and he showed that two expressions of $\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}$ and $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$ are identical. The $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$ is not manifestly Hermitian but it is really Hermitian which was also proved by Brandow.[3]

A remaining problem has been whether the Hamiltonian $\mathcal{H}_{\mathrm{H}}$ in Eq. (2·19) derived from the unitary-transformation method is identical to $\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}$ (or $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$) or not. Concerning this problem, an indirect proof was given by Klein.[2] He demonstrated that in both cases of $\mathcal{H}_{\mathrm{H}}$ and $\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}$ a set of the orthogonal model-space eigenstates $\{|\phi_k\rangle\}$ in Eq. (3·3) are determined uniquely, as long as the exponent G is subject to the restriction (2·17), so that $\mathcal{H}_{\mathrm{H}}$ and $\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}$ (or $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$) must be the same. Another indirect proof of the equivalence was given by Jørgensen[4] and Brandow.[3]

A direct and simple proof of the equivalence among $\mathcal{H}_{\mathrm{H}}$, $\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}$ and $\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}$ is given by the use of Eqs. (3·2),(3·4) and (3·6). If we write them in terms of ω, they become

$$\mathcal{H}_{\mathrm{H}}=\mathcal{H}_{\mathrm{a}}^{(\mathrm{III})}=\mathcal{H}_{\mathrm{b}}^{(\mathrm{III})}=(P+\omega^{\dagger}\omega)^{1/2}H(P+\omega)(P+\omega^{\dagger}\omega)^{-1/2}\,. \tag{3·15}$$

The equivalence among three different definitions of the Hermitian effective Hamiltonian is now self-evident.

It may be quite interesting to note that every effective Hamiltonian appeared so far in the degenerate perturbation theory can be expressed in a unified way as

$$\mathcal{H}=(P+\omega^{\dagger}\omega)^{m}H(P+\omega)(P+\omega^{\dagger}\omega)^{n}\,. \tag{3·16}$$

In general, for any set of m and n $\mathcal{H}$ can be an effective Hamiltonian in the sense that the model-space eigenvalue problem becomes

$$\mathcal{H}|\xi_k\rangle=E_k(P+\omega^{\dagger}\omega)^{m+n}|\xi_k\rangle \tag{3·17}$$

and the model-space eigenstate $|\xi_k\rangle$ is related to the true eigenstate $|\Phi_k\rangle$ as

$$|\xi_k\rangle=(P+\omega^{\dagger}\omega)^{-n}P|\Phi_k\rangle, \tag{3·18}$$

where we have used a fact that the projected state $P|\Phi_k\rangle$ is an eigenstate of $PH(P+\omega)$.[5] Among various choices of (m, n), two cases of $(m, n)=(0, 0)$ and $(m, n)=(1/2, -1/2)$ have special meanings. The former choice gives probably the simplest structure, and the latter has an advantage of being Hermitian.

§ 4. Expansion formulae for effective interactions

4.1. *Expansion of non-Hermitian effective interaction*

We consider a degenerate system, that is, the energies of the unperturbed Hamiltonian PH_0P are degenerate. We write

$$PH_0P=E_0P\,. \tag{4·1}$$

We define a P-space operator $\hat{Q}$ as

$$\begin{aligned}\hat{Q}&=PVP+PVQ\frac{1}{E_0-QHQ}QVP\\&=PVP+PVQ\frac{1}{e}QVP+PVQ\frac{1}{e}QVQ\frac{1}{e}QVP+\cdots,\end{aligned} \tag{4·2}$$

where

$$e=E_0-QH_0Q\,. \tag{4·3}$$

We further define the energy derivative of $\hat{Q}$ as

$$\begin{aligned}\hat{Q}_n&=\frac{1}{n!}\frac{d^n\hat{Q}}{dE_0{}^n}\\&=(-)^nPVQ\left(\frac{1}{E_0-QHQ}\right)^{n+1}QVP\,.\end{aligned} \tag{4·4}$$

Let us refer to $\hat{Q}$ as the Q-box according to Kuo and his collaborators.[1),24)] The operator $\hat{Q}$ has been used widely as a building block in constructing the effective interaction by many authors.[5),21),22)]

The non-Hermitian effective interaction R in Eq. (2·13) can be expanded in powers of $\{\hat{Q}_n\}$ as

$$R=\sum_{k=1}^{\infty}\sum_{m_1,m_2,\cdots,m_k}f(m_1,m_2,\cdots,m_k)\hat{Q}_{m_1}\hat{Q}_{m_2}\cdots\hat{Q}_{m_k}\,, \tag{4·5}$$

where $f(m_1,\cdots,m_k)$ is a coefficient, and in the summation $m_i(i=1,\cdots,k)$ run over all zero-

or-positive integers. In the above expressions, we have used the notation $\hat{Q}_0=\hat{Q}$.

The coefficient $f(m_1,\cdots,m_k)$ is given explicitly as

$$f(m_1,m_2,\cdots,m_k)=\delta_{m_k,0}\delta_{(m_1+m_2+\cdots+m_k),k-1}\prod_{i=1}^{k-2}\eta(i-\sum_{j=1}^{i}m_{k-j}) \quad \text{for } k\geqq 3,$$

$$f(m_1)=\delta_{m_1,0} \quad \text{for } k=1,$$

$$f(m_1,m_2)=\delta_{m_1,1}\delta_{m_2,0} \quad \text{for } k=2, \tag{4·6}$$

where $\eta(x)$ is the step function defined by

$$\eta(x)=\begin{cases}1 & \text{for } x\geqq 0,\\ 0 & \text{for } x<0.\end{cases} \tag{4·7}$$

The coefficient $f(m_1,\cdots,m_k)$ takes the value zero or one because of the property of $\eta(x)$ in Eq. (4·7).

The expression for $f(m_1,\cdots,m_k)$ in Eq. (4·6) is obtained as follows: From Eqs. (2·11) for ω and (2·13) for R we have an equation

$$R=\sum_{n=0}^{\infty}\hat{Q}_nR^n. \tag{4·8}$$

This equation has already been derived by des Cloizeaux[21] and Brandow.[22] Substituting R in Eq. (4·5) into Eq. (4·8), we obtain a recursion formula

$$f(m[1,k])=\sum_{\{l_i\}}f(m[2,l_1+1])f(m[l_1+2,l_1+l_2+1])\cdots f(m[k-l_{m_1}+1,k]), \tag{4·9}$$

where the summation must be taken over a set of m_1 positive integers $\{l_i\}$ satisfying

$$l_1+l_2+\cdots+l_{m_1}=k-1, \tag{4·10}$$

and we have used an abbreviation

$$f(m[i,j])=f(m_i,m_{i+1},\cdots,m_j). \tag{4·11}$$

On the r.h.s. of Eq. (4·9), the summation is taken over all combinations deviding the set of $k-1$ integers $(m_2,\cdots,m_k)$ into m_1 subsets. The recursion relation (4·9) determines $f(m_1,\cdots,m_k)$ uniquely if we start with $f(m_1)=\delta_{m_1,0}$. The coefficient $f(m_1,\cdots,m_k)$ in Eq. (4·6) can be proved to be just the solution to the recursion relation (4·9).

Two different rules for generating the expansion of R have been known. One is of des Cloizeaux[21] and the other of Lee,[25] and Krenciglowa and Kuo.[26] Both of the rules are proved to be equivalent to that given in an explicit expression in Eq. (4·5) with Eq. (4·6).

4.2. *Expansion of the Hermitian effective interaction*

The perturbation expansion of the Hermitian effective interaction has been studied by many authors in Refs.2),3), 11)~15), 21) and 22). Although first several terms in the perturbation expansion have been given, no explicit and general expansion form in terms of $\{\hat{Q}_n\}$ has yet been known. However, if we use the relation between two exponents G and ω in Eq. (2·18) and write the Hermitian effective interaction as W in Eq. (2·20) or (2·22), the perturbation expansion of W can be obtained easily.

We first note that $\omega^{\dagger}\omega$ in Eq. (2·22) is related to R and $\{\hat{Q}_n\}$ as

$$\omega^{\dagger}\omega=-\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(R^{\dagger})^{m}\hat{Q}_{m+n+1}R^{n}\,. \tag{4·12}$$

This relation is derived from Eqs. (2·11) for ω and (2·13) for R.[16]

Since R has been given explicitly in terms of $\{\hat{Q}_n\}$, it is sufficient for the Q-box expansion of W to show that W is written in terms of only R and $\{\hat{Q}_n\}$. Substituting $\omega^{\dagger}\omega$ in Eq. (4·12) into Eq. (2·22), we have

$$\begin{aligned}W=[\frac{1}{2}R+&\sum_{k\geq 0,l\geq 0(k+l\neq 0)}(-)^{k+l}F(k,l)\sum_{p_1,\cdots,p_k}\sum_{q_1,\cdots,q_k}\sum_{r_1,\cdots,r_l}\\&\times\sum_{s_1,\cdots,s_l}\{\prod_{i=1}^{k}(R^{\dagger})^{p_i}\hat{Q}_{p_i+q_i+1}(R)^{q_i}\}R\\&\times\{\prod_{j=1}^{l}(R^{\dagger})^{r_j}\hat{Q}_{r_j+s_j+1}(R)^{s_j}\}]+\text{h.c.},\end{aligned} \tag{4·13}$$

where the summation with respect to k and l must be taken over zero-or-positive integers except $k=l=0$ and a set of integers $\{p_i\}$, etc. run over zero-or-positive integers.

If we substitute R in Eq. (4·5) into Eq. (4·13), we obtain a more explicit expansion

Table I. Expansion of Hermitian effective interaction. Numbers in the table denote the coefficient $g(m_1,m_2,\cdots,m_k)$ in the expansion $W=\sum g(m_1,\cdots,m_k)Q_{m_1}\cdots Q_{m_k}+\text{h.c.}$ The values of g for all the combinations $(m_1,\cdots,m_k)$ other than those given in the table are zero.

k	$m_1m_2\cdots m_k$	g	k	$m_1m_2\cdots m_k$	g
1	0	1	5	03010	−1/8
				01300	−1/8
2	10	1/2		22000	1/2
				20200	3/8
3	200	1/2		20020	1/8
	110	3/8		20002	1/8
	101	1/8		02200	−1/8
				21100	1/2
4	3000	1/2		21010	3/8
	2100	1/2		21001	1/4
	2010	3/8		20110	5/16
	2001	1/4		20101	3/16
	1200	3/8		20011	3/16
	1020	1/8		12100	3/8
	0210	−1/8		12010	5/16
	1110	5/16		12001	3/16
	1101	3/16		11200	5/16
				10210	1/16
5	40000	1/2		10201	1/16
	31000	1/2		02110	−3/16
	30100	1/2		02101	1/16
	30010	3/8		02011	1/8
	30001	1/4		01210	−1/8
	13000	3/8		11110	35/128
	10300	1/8		11101	5/32
	10030	1/8		11011	9/128

form for W, but this expression is quite complicated to write and it may not be useful for practical purposes. Although we do not give an explicit expansion formula, the structure of W written in terms of $\{\hat{Q}_n\}$ is now clear. The expression (4·13) with Eq. (4·5) provides us with a definite way of calculating the perturbation-expansion terms up to any order in $\{\hat{Q}_n\}$. The expansion of W through fifth order is given in Table I.

§ 5. Convergent solution for effective interaction

5.1. *Iteration method for the calculation of R*

The Q-box expansion form for R has rather simple structure, but order-by-order calculation is often a hard task even when the expansion is convergent. A simple and useful iteration method has been given by Lee and one of the authors (K.S.)[5] as

$$R_n=(1-\hat{Q}_1-\sum_{m=2}^{n-1}\hat{Q}_m\prod_{k=n-m+1}^{n-1}R_k)^{-1}\hat{Q}\,. \tag{5·1}$$

It has been proved that this iteration scheme always yields the convergent solution as n tends to infinity except the case that an accidental degeneracy occurs between the eigenvalues of the model-space Hamiltonian and the other eigenvalues of the original Hamiltonian H.

For the calculation of R by means of Eq. (5·1) we need $\hat{Q}(=\hat{Q}_0)$ and its energy derivative $\hat{Q}_n$. In actual calculation, the energy derivatives $\{\hat{Q}_n\}$ can be calculated numerically if $\hat{Q}$ is given at some different values near the unperturbed energy E_0. Therefore, when we use the iteration scheme (5·1), we need only to calculate the Q-box. This may be a considerable simplification of the calculation. The efficiency of this formalism has already been examined in the calculation of nuclear effective interaction.[27),28)]

5.2. *Non-perturbative calculation of W*

The expansion formula for the Hermitian effective interaction W is very complicated in structure as has been shown in Eq. (4·13). No iteration scheme has yet been found for the calculation of W. However, once R is known, W can be obtained through

$$\langle\alpha_i|W|\alpha_j\rangle=(\sqrt{1+\mu_i{}^2}\langle\alpha_i|R|\alpha_j\rangle+\sqrt{1+\mu_j{}^2}\langle\alpha_i|R^\dagger|\alpha_j\rangle)\{1/(\sqrt{1+\mu_i{}^2}+\sqrt{1+\mu_j{}^2})\}, \tag{5·2}$$

where $|\alpha_i\rangle$ and $\mu_i{}^2$ are the eigenstate and the eigenvalue of $\omega^\dagger\omega$, respectively, i.e.,

$$\omega^\dagger\omega|\alpha_i\rangle=\mu_i{}^2|\alpha_i\rangle. \tag{5·3}$$

The expression of W in Eq. (5·2) has been given by one of the authors (K.S.).[16)]

In order to calculate W according to Eq. (5·2), we must calculate $\omega^\dagger\omega$ and solve the eigenvalue equation (5·3). The operator $\omega^\dagger\omega$ is given as a series-expansion form in Eq. (4·12). This series for $\omega^\dagger\omega$ can be summed up and we may write

$$\omega^\dagger\omega=-\sum_i|\tilde{\phi}_i\rangle\langle\phi_i|\hat{Q}_1(E_i)|\phi_i\rangle\langle\tilde{\phi}_i|-\sum_{i\neq j}|\tilde{\phi}_i\rangle\langle\phi_i|\phi_j\rangle\langle\tilde{\phi}_j|, \tag{5·4}$$

where $|\phi_i\rangle$ is the eigenstate satisfying

$$(PH_0P+R)|\phi_i\rangle=E_i|\phi_i\rangle \tag{5·5}$$

and $\langle\tilde{\phi}_i|$ is the biorthogonal state of $|\phi_i\rangle$ which satisfies $\langle\phi_i|\tilde{\phi}_j\rangle=\delta_{ij}$. The $\hat{Q}_1(E_i)$ is the energy derivative of the Q-box at the energy E_i in Eq. (5·5). The proof of Eq. (5·4) is given as follows: Note that the true eigenstate $|\Phi_k\rangle$ of H is given by

$$\begin{aligned}|\Phi_k\rangle &= e^{\omega}|\phi_k\rangle \\ &= |\phi_k\rangle+\omega|\phi_k\rangle \end{aligned} \tag{5·6}$$

which may be clear from the similarity-transformation theory described in § 2. The eigenstates $\{|\Phi_k\rangle\}$ are orthogonal although they are not normalized. Therefore, we have for the overlap of two different eigenstates

$$\begin{aligned}\langle\Phi_i|\Phi_j\rangle &= \langle\phi_i|\phi_j\rangle+\langle\phi_i|\omega^{\dagger}\omega|\phi_j\rangle \\ &= 0 \qquad \text{for } i\neq j\end{aligned} \tag{5·7}$$

where we have used the fact that $\langle\phi_i|\omega|\phi_j\rangle=\langle\phi_i|\omega^{\dagger}|\phi_j\rangle=0$ which comes from the properties of ω in Eq. (2·8). The solution ω to the decoupling equation (2·11) is given in terms of E_i, $|\phi_i\rangle$ and $\langle\tilde{\phi}_i|$ as[5]

$$\omega=\sum_i \frac{1}{E_i-QHQ}QVP|\phi_i\rangle\langle\tilde{\phi}_i| \tag{5·8}$$

from which we have

$$\begin{aligned}\langle\phi_i|\omega^{\dagger}\omega|\phi_i\rangle &= \langle\phi_i|PVQ\left(\frac{1}{E_i-QHQ}\right)^2 QVP|\phi_i\rangle \\ &= -\langle\phi_i|\hat{Q}_1(E_i)|\phi_i\rangle.\end{aligned} \tag{5·9}$$

From two equations (5·7) and (5·9) we obtain a unified expression of $\omega^{\dagger}\omega$ in Eq. (5·4).

We now may say that once the Q-box is given, there is no difficulty any more in calculating the Hermitian effective interaction W. The procedures of calculating W are summarized as follows: (1) Calculate R by means of the iterative equation (5·1). (2) Solve the eigenvalue problem for R in Eq. (5·5) and determine the eigenvalues $\{E_i\}$ and the eigenstates $\{|\phi_i\rangle\}$. (3) Calculate the operator $\omega^{\dagger}\omega$ according to Eq. (5·4). (4) Solve the eigenvalue problem for $\omega^{\dagger}\omega$ in Eq. (5·3) and determine the basis $\{|a_i\rangle\}$ and the eigenvalues $\{\mu_i^2\}$. (5) Finally, W is obtained from Eq. (5·2).

It must be noticed that the main part of the procedures is to calculate the Q-box in constructing both of the non-Hermitian and Hermitian effective interactions. The remaining part is to calculate only the operators or vectors which are defined within the P space. The latter part of the calculation is usually a very easy task, because the P space is introduced as a rather small-dimensional subspace.

For the construction of the Hermitian effective interaction W according to Eqs. (5·2) ~(5·5), we need to know the exact eigenvalue E_i of the full Hamiltonian H. Therefore, if our aim of constructing the effective interaction is only to solve the eigenvalues $\{E_i\}$, the Hermitian form W is not necessary. However, the Hermitian effective interaction may have an important role in the description of many-body system. The Hermitian-effective-interaction theory was applied to the derivation of the nuclear effective interaction in Ref.29).

§ 6. Concluding remarks

We have discussed the formal relations among various definitions of the time-independent and energy-independent effective interaction. We have seen that if we represent the effective Hamiltonians in terms of the operator ω defined in § 2, they are all written in a simple and unified form as has been given in Eq. (3·16). We now may say that there is no obscurity in the interrelations among a number of different expressions of the effective Hamiltonian appeared in the history of degenerate perturbation theory.

We have also discussed the problem of constructing a convergent effective interaction. The expansion formulae for both of the non-Hermitian and Hermitian forms have been given in terms of so-called Q-box. We have shown that the procedures of calculating effective interaction are separated into two parts. One is the calculation of the Q-box itself and the other is the summation of the power series of the Q-boxes. In the diagrammatical representation in many-body problem, the former procedure corresponds to the summation of the non-folded diagrams, and the latter is the summation of the folded diagrams.[22),24)] An important conclusion is that the latter part of the procedures, the summation of folded diagrams, can be completed without any approximation.

We have seen that the essential part of the procedures of constructing the effective interaction is to calculate the Q-box for both of the non-Hermitian and Hermitian forms. As for the calculation of the Q-box, an approach of the linked-diagram expansion has been developed by Brandow,[22)] and Kuo and his collaborators.[24),30)] The multiple-scattering approach has also been developed for the purpose of summing up the terms in the Q-box to infinite order by Andō, Bandō, Nagata, Krenciglowa and Adhikari.[31)] The approach of the self-consistent coupled equation of Kirson[32)] may also be considered to be another method of summing up the diagrams in the Q-box to infinite order.

Finally, we may say that in a formal point of view, the structure of degenerate perturbation theory is fairly well understood. The theory formulated in the present study will be applicable to various branches of quantum systems such as atoms, molecules, nuclei and nucleon-pion system.

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