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Convergent Theory for Effective Interaction in Nuclei*)

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A general equation is derived for constructing the effective interaction on the basis of the similarity transformation theory. It is proved that the equation is equivalent to Bloch's equation for the degenerate perturbation theory and, therefore, the present approach is also equivalent to the energy independent Rayleigh-Schrödinger theory. Some iteration methods are proposed to solve the equation, and the convergence conditions for the iteration procedures are discussed. Two iteration methods—self-energy insertion and vertex renormalization—are obtained to reach the true eigenvalues of the full Hamiltonian even when there are some intruder states. It is proved that the self-energy insertion procedure produces the eigenvalues of eigenstates which have large overlap with the model space. On the other hand, the vertex renormalization procedure gives the eigenvalues nearest to the unperturbed starting energy.

§ 1. Introduction

One of the most fundamental problems in the nuclear theory is the derivation of the effective interaction between nucleons in nuclei. There have been many theoretical studies on this subject, which are summarized in several articles,[1)~4)] since Kuo and Brown's pioneering work[5)] in applying Brueckner's reaction matrix theory[6)] to finite nuclei. The folded diagram theory[1),7),8)] has been developed as a powerful perturbation method for the derivation of the effective interaction.

One of the characteristics of the nuclear many-body problem is that the free nucleon-nucleon force may have a strong repulsive core at short distance. For this reason, straightforward application of the perturbation theory to the nuclear many-body problem cannot be successful. Usual treatment of the short-range correlation is to introduce Brueckner's reaction matrix (G matrix).[5),6)] Usually one believes that one can use this G matrix as a starting interaction in the perturbation calculation of the effective interaction. Many numerical calculations, based on the G matrix, have been made, especially for nuclei with a few valence nucleons outside the core, e.g., ^{18}O and ^{18}F (see Refs. 2), 4)).

The most outstanding problem in the perturbation approach is the convergence of the perturbation expansion for the effective interaction. The result obtained by

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Barrett and Kirson[2),9)] questioned the validity of order by order calculation of the effective interaction. Further, the study of Schucan and Weidenmüller[10)] pointed out that the presence of the intruder state in the midst of low lying shell-model states is the essential source of the divergence of the perturbation expansion. Because such an intruder state appears quite often in the nuclear spectra, it throws suspicion on the development of the nuclear many-body theory. These intruder states are usually low lying collective states. The collectivity pushes the intruder state near to the low lying model-space states and this intruder state causes the divergence of the perturbation expansion.

The problem of the divergence has been discussed by many authors. One of the approaches is to use the Padé approximant which approximates the divergent series by the ratio of two polynomials.[11)~13)] In this approach, it has been found that a rather high order of Padé approximant is necessary to obtain an accurate result for the effective interaction. The high order Padé approximant requires the calculation of high order terms in the perturbation expansion. This situation of the Padé approximant method seems not to make any improvement over the difficulty with the divergence of the perturbation expansion.

Another approach is that a new model space which includes intruder states is introduced and the effective interaction is calculated perturbatively in this enlarged model space.[11)] In this approach, some experimental knowledge of the intruder state is necessary to perform a sensible calculation. In the nucleus with two valence nucleons such as ^{18}O or ^{18}F, the intruder states have been established to be $4p$-$2h$ deformed states. Actually, there are a huge number of states with $4p$-$2h$ configuration, but the intruder state is a collective linear combination of these $4p$-$2h$ configurations. How to construct the intruder states from the $4p$-$2h$ configurations may, however, be technically difficult and ambiguous. This situation seems to cause another complication.

There are also other studies which aim at overcoming the divergence of the perturbation expansion, e.g., the partial resummation method based on the folded diagram theory,[14)] the self-consistent coupled equation based on RPA,[15)] the Hartree-Fock basis expansion method,[16)] $\exp(S)$ method,[17)] the generalized vertex method based on the multiple scattering equation,[18)] the unitary transformation method,[19)] etc. All of these "nonperturbed" approaches may be understood as the method of the partial resummation of the perturbation expansion series. In general, a different partial summation leads to a different solution for the effective interaction, whenever the perturbation expansion is divergent.

The effective interaction depends on the set of eigenvalues to be produced. If the perturbation series is divergent, the resummation of the series has to be made with care so as to preserve the equation of motion. Our main interest is to investigate the situation of the resummation procedure. In this paper, we shall propose convergent resummation procedure for the effective interaction in the framework of the time independent Rayleigh-Schrödinger perturbation theory.

In § 2, a general equation is derived for the effective interaction by the use of the similarity transformation theory in the eigenvalue problem. We see that the equation is understood as a generalization of Bloch's equation[20] for the degenerate perturbation theory. In § 3, some iteration procedures are proposed to solve the equation and the convergence conditions for the iterative solutions are discussed. A new solution is derived which is convergent even when the intruder states are present. In § 4, a summary of the findings of this paper is given.

§ 2. Similarity transformation and Rayleigh-Schrödinger theory

We consider a many-body system which is described by the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \tag{2·1}$$

with the Hamiltonian

$$H = H_0 + V\,, \tag{2·2}$$

where H_0 is the unperturbed Hamiltonian and V is the residual interaction.

The fundamental assumption in solving low lying states of the many-body system is that the main components of these states can be constructed from configurations of a few active particles and holes occupying a few active orbits. The set of states with the configurations of active orbits is called model space which is referred to as the P space. The complement of the P space is called the Q space. We define projection operators P and Q which project states onto the P and Q spaces, respectively. The operators P and Q are introduced as the eigenprojectors of H_0 and satisfy the relations

$$\begin{aligned} &[H_0, P] = [H_0, Q] = 0\,, \\ &QH_0P = PH_0Q = 0\,. \end{aligned} \tag{2·3}$$

The aim now is to construct an effective Hamiltonian H_{eff} which acts only inside the P space and satisfies the condition that any eigenvalue of H_{eff} should be one of the exact eigenvalues of the full Hamiltonian H. A general equation for determining H_{eff} can be derived by the use of the similarity transformation theory. We consider a similarity transformation of the Hamiltonian H

$$\mathcal{H} = X^{-1}HX\,, \tag{2·4}$$

where X is a transformation operator which is defined in the entire Hilbert space and has its inverse X^{-1}.

The transformed Hamiltonian $\mathcal{H}$ is decomposed into four terms

$$\mathcal{H} = P\mathcal{H}P + P\mathcal{H}Q + Q\mathcal{H}P + Q\mathcal{H}Q\,. \tag{2·5}$$

The condition that $P\mathcal{H}P$ be the P-space effective Hamiltonian is

$$Q\mathcal{H}P=Q(X^{-1}HX)P=0\,. \tag{2·6}$$

Then the effective Hamiltonian H_{eff} is given by

$$H_{\text{eff}}=P\mathcal{H}P=P(X^{-1}HX)P\,. \tag{2·7}$$

Equation (2·6) provides the necessary and sufficient condition for the determination of H_{eff}. We can prove this statement by following the similarity transformation theory in the eigenvalue problem. We here note that if X is a solution to Eq. (2·6), H_{eff} in Eq. (2·7) satisfies

$$H_{\text{eff}}|\phi\rangle=\mathcal{H}|\phi\rangle \tag{2·8}$$

for any state $|\phi\rangle$ in the P space. Therefore, the eigenvalue of H_{eff} becomes also the eigenvalue of $\mathcal{H}$. This means that the eigenvalue of H_{eff} agrees with one of the eigenvalues of the Hamiltonian H, because the similarity transformation does not change the eigenvalues.

Different choice of X leads us to a different many-body theory. The unitary transformation method[19] or the $\exp(S)$ theory[17] corresponds to a certain choice of X and the fundamental equation for the effective interaction in each theory can be derived from the general equation (2·6).

We here consider a similarity transformation

$$X=e^{\omega}, \tag{2·9}$$

$$\mathcal{H}=e^{-\omega}He^{\omega}, \tag{2·10}$$

where ω is an operator which has the properties

$$\omega=Q\omega P\,, \tag{2·11}$$

$$P\omega P=Q\omega Q=P\omega Q=0\,. \tag{2·12}$$

The ω is introduced as an operator which acts as a transformation of a P-space state to a Q-space state. From Eq. (2·11), we have another property of ω

$$\omega^2=\omega^3=\cdots=0. \tag{2·13}$$

These properties of ω simplify extremely the calculation of the transformation of H in Eq. (2·10). We have from Eq. (2·13)

$$X=e^{\omega}=1+\omega, \tag{2·14}$$

and the four terms in Eq. (2·5) are given by

$$P\mathcal{H}P=PHP+PVQ\omega, \tag{2·15}$$

$$P\mathcal{H}Q=PVQ\,, \tag{2·16}$$

$$Q\mathcal{H}Q=QHQ-\omega PVQ\,, \tag{2·17}$$

$$Q\mathcal{H}P=QVP+QHQ\omega-\omega PHP-\omega PVQ\omega, \tag{2·18}$$

where we have used the relation (2·3) for H_0.

From Eqs. (2·6) and (2·18), we have an equation for ω

$$QVP+QHQ\omega-\omega PHP-\omega PVQ\omega=0\,. \tag{2·19}$$

This is our fundamental equation for determining H_{eff}. If we have a solution ω to Eq. (2·19), we obtain H_{eff} by substituting ω into Eq. (2·15). We define P-space effective interaction by subtracting the unperturbed energy PH_0P from H_{eff}

$$\begin{aligned} R&=H_{\text{eff}}-PH_0P \\ &=PVP+PVQ\omega\,. \end{aligned} \tag{2·20}$$

The P-space eigenvalue problem is then written as

$$H_{\text{eff}}|\phi_\mu\rangle=(PH_0P+R)\,|\phi_\mu\rangle=E_\mu|\phi_\mu\rangle\,. \tag{2·21}$$

The eigenvalue E_μ agrees with one of the eigenvalues of H, as long as ω is a solution to Eq. (2·19). In terms of E_μ and $|\phi_\mu\rangle$, Eq. (2·19) can be solved formally as

$$\omega=\sum_{\mu=1}^{d}\omega(E_\mu)\,|\phi_\mu\rangle\langle\tilde{\phi}_\mu| \tag{2·22}$$

with

$$\omega(E_\mu)=\frac{1}{E_\mu-QHQ}QVP\,, \tag{2·23}$$

where $\langle\tilde{\phi}_\mu|$ is the biorthogonal state corresponding to $|\phi_\mu\rangle$ and d is the dimension of the P space. The effective interaction is then given by

$$R=PVP+\sum_{\mu=1}^{d}PVQ\frac{1}{E_\mu-QHQ}QVP|\phi_\mu\rangle\langle\tilde{\phi}_\mu|\,. \tag{2·24}$$

The true eigenstate of H corresponding to the P-space eigenstate $|\phi_\mu\rangle$ is given by

$$\begin{aligned} |\Psi_\mu\rangle&=e^{\omega}|\phi_\mu\rangle \\ &=|\phi_\mu\rangle+\omega(E_\mu)\,|\phi_\mu\rangle. \end{aligned} \tag{2·25}$$

The term $\omega(E_\mu)\,|\phi_\mu\rangle$ represents the Q-space component in the true eigenstate of H. The eigenstate $|\Psi_\mu\rangle$ in Eq. (2·25) is Feshbach's formal solution and the

effective interaction R in Eq. (2·24) is the Bloch-Horowitz energy dependent solution.

It may be of interest mathematically to note that the transformation of H in Eq. (2·10) defines the Q-space "effective" Hamiltonian $Q\mathcal{H}Q$ in Eq. (2·17) in the sense that

$$\langle\phi_q|Q\mathcal{H}Q=\langle\phi_q|(QHQ-\omega PVQ)=E_q\langle\phi_q|, \tag{2·26}$$

where $\langle\phi_q|$ is an eigenstate in the dual Q space and E_q is one of the exact eigenvalues of H.

The energy independent Rayleigh-Schrödinger (R.S.) theory for the effective interaction can be reformulated on the basis of the similarity transformation in Eq. (2·10). This reformulation may be useful for the understanding of the full structure of the R.S. theory. The usual wave operator used in the R.S. theory is

$$\Omega=P+\omega. \tag{2·27}$$

In terms of Ω, Eq. (2·19) for ω becomes a simple form

$$QH\Omega-Q\Omega PH\Omega=0. \tag{2·28}$$

We now consider a degenerate case that the unperturbed energies of the P-space states are degenerate, i.e.,

$$PH_0P=E_0P. \tag{2·29}$$

In this degenerate case, Eq. (2·28) for Ω is written as

$$\Omega=P+\frac{1}{e}QV\Omega-\frac{Q}{e}\Omega PV\Omega, \tag{2·30}$$

where e is the energy denominator defined by

$$e=E_0-QH_0Q. \tag{2·31}$$

Equation (2·30) is just Bloch's equation.[20] Some equivalent equations have also been derived by Schucan and Weidenmüller[10] and by Lindgren[21] from different approaches. Bloch proved that the R.S. expansion can be generated from Eq. (2·30). The R.S. expansion, which is the order by order expansion in powers of the interaction V, can be derived as follows: We expand Ω as

$$\begin{aligned}\Omega&=P+\Omega^{(1)}+\Omega^{(2)}+\cdots\\&=\sum_{k=0}^{\infty}\Omega^{(k)},\end{aligned} \tag{2·32}$$

where $\Omega^{(0)}=P$ and $\Omega^{(n)}$ for $n\geqq 1$ contains all terms of n-th order in V. From

Eq. (2·30), we obtain an equation for $\Omega^{(n)}$

$$\Omega^{(n)}=\frac{Q}{e}V\Omega^{(n-1)}-\frac{Q}{e}\sum_{k=0}^{n-1}\Omega^{(k)}PV\Omega^{(n-k-1)}. \tag{2·33}$$

The effective interaction R in Eq. (2·20) is now given by $PV\Omega$ and R is expanded as

$$R=\sum_{n=0}^{\infty}R^{(n)} \tag{2·34}$$

with

$$R^{(n)}=PV\Omega^{(n)}, \tag{2·35}$$

where $R^{(n)}$ is $(n+1)$-th order term in V. The solution for $R^{(n)}$ is then given by

$$R^{(n)}=PV\frac{Q}{e}V\Omega^{(n-1)}-\sum_{k=0}^{n-1}PV\frac{Q}{e}\Omega^{(k)}R^{(n-k-1)}. \tag{2·36}$$

If we start with $\Omega^{(0)}=P$ and $R^{(0)}=PVP$, the recurrence procedure in Eqs. (2·33) and (2·36) generates all terms in the R.S. expansion. Equation (2·36), of which general structure has been discussed in Ref. 24), would be fruitful in the study of the linked cluster expansion for the effective interaction.

If the R.S. expansion for R is convergent, we can solve Bloch's equation (2·30) or equivalently Eq. (2·19) for ω perturbatively. However, the system of interest, especially the nuclear many-body system, often has low lying collective states (intruder states) which give rise to the divergence of the perturbation series. As has already discussed by Schucan and Weidenmüller,[10] the R.S. expansion is divergent in almost all of the practical nuclear problems. In the divergent case, the recurrence procedure in Eq. (2·36) becomes unstable and we cannot obtain any reliable solution from the perturbation expansion for R. However, the solution ω or Ω does exist in principle and some other methods are possible to solve Eq. (2·19) or (2·30).

§ 3. Iteration method and convergence condition

Any expansion formula for the effective interaction based on the R.S. theory appears as a solution to the general equation (2·19). However, it should be noted that the equation for ω is nonlinear and the solution ω is not unique. The R.S. perturbation expansion, which is derived from the recurrence procedure in Eq. (2·36), gives us one possible solution to Eq. (2·19). We shall show that the nonlinear equation (2·19) can be solved by the iteration method. It is known to a nonlinear equation that a different iteration procedure (linearization procedure) would lead us to a different solution or a different expansion formula. Several

iteration procedures are possible, but we here discuss two methods which may be important in the application to the practical problem.

(A) *The self-energy insertion procedure*

We consider a linearized iterative equation for the solution ω to Eq. (2·19)

$$\begin{aligned}(E_0-QHQ)\,\omega_n &= QVP-\omega_n(PVP+PVQ\omega_{n-1})\\ &= QVP-\omega_n R_{n-1}\,,\end{aligned} \tag{3·1}$$

where we have used the assumption (2·29) for the unperturbed Hamiltonian H_0. We define R_n as n-th order iterative effective interaction

$$R_n = PVP+PVQ\omega_n\,. \tag{3·2}$$

The solution ω_n to Eq. (3·1) is given by a series expansion

$$\omega_n = -\sum_{m=0}^{\infty}\left(\frac{-1}{E_0-QHQ}\right)^{m+1} QVP\,(R_{n-1})^m. \tag{3·3}$$

The corresponding n-th iterative effective interaction R_n is given by

$$R_n = \hat{Q}+\sum_{m=1}^{\infty}\hat{Q}_m\,(R_{n-1})^m, \tag{3·4}$$

where $\hat{Q}$ is the Q-box interaction[7),14)] defined by

$$\begin{aligned}\hat{Q} &= PVP+PVQ\frac{1}{E_0-QHQ}QVP\\ &= PVP+PV\frac{Q}{e}VP+PV\frac{Q}{e}V\frac{Q}{e}VP+\cdots\,,\end{aligned} \tag{3·5}$$

and $\hat{Q}_m$ is

$$\begin{aligned}\hat{Q}_m &= -PVQ\left(\frac{-1}{E_0-QHQ}\right)^{m+1}QVP\\ &= \frac{1}{m!}\frac{d^m\hat{Q}}{dE_0^m}\,.\end{aligned} \tag{3·6}$$

The solution in Eq. (3·4) is the same as Krenciglowa and Kuo's resummation formula.[14)] In the limiting case that $n\to\infty$, the solution R_∞ agrees with the Des Cloizeaux[22)] and Brandow's formal solution[1)]

$$R_\infty = \hat{Q}+\sum_{m=1}^{\infty}\hat{Q}_m\,(R_\infty)^m. \tag{3·7}$$

As has already discussed by Schucan and Weidenmüller,[10)] the series expansion for R_∞ diverges whenever the intruder state appears in the low lying spectrum to be

produced from the P-space effective interaction. In this divergent case, the recurrence relation for R_n in Eq. (3·4) becomes unstable.

The divergence of the expansion in Eq. (3·7) does not necessarily mean the divergence of the iterative solution ω_n to Eq. (3·1). Actually, the series ω_n in Eq. (3·3) can be summed up and the solution can be expressed in a matrix form as

$$\langle q|\omega_n|\alpha\rangle = \sum_{\beta} \langle q|V|\beta\rangle\langle\beta| \frac{1}{E_0 + R_{n-1} - \varepsilon_q} |\alpha\rangle , \tag{3·8}$$

and the corresponding effective interaction is given by

$$\langle\alpha|R_n|\beta\rangle = \langle\alpha|V|\beta\rangle + \sum_{\gamma,q} \langle\alpha|V|q\rangle\langle q|V|\gamma\rangle\langle\gamma| \frac{1}{E_0 + R_{n-1} - \varepsilon_q} |\beta\rangle , \tag{3·9}$$

where $|q\rangle$ and ε_q are the eigenstate of QHQ and the corresponding eigenvalue respectively, i.e.,

$$QHQ|q\rangle = \varepsilon_q|q\rangle, \tag{3·10}$$

and $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$ are the orthogonal P-space states. Equation (3·9) manifests itself that the iteration procedure in Eq. (3·1) corresponds to the self-energy insertion.

We obtain another expression for the iterative solution ω_n to Eq. (3·1) by introducing the eigenstate of $(n-1)$-th order P-space effective Hamiltonian, i.e.,

$$(PH_0P + R_{n-1})|\phi_\mu^{(n-1)}\rangle = E_\mu^{(n-1)}|\phi_\mu^{(n-1)}\rangle. \tag{3·11}$$

By using $E_\mu^{(n-1)}$ and $|\phi_\mu^{(n-1)}\rangle$, we can solve Eq. (3·1) as

$$\omega_n = \sum_{\mu=1}^{d} \frac{1}{E_\mu^{(n-1)} - QHQ} QVP|\phi_\mu^{(n-1)}\rangle\langle\tilde{\phi}_\mu^{(n-1)}|, \tag{3·12}$$

where $\langle\tilde{\phi}_\mu^{(n-1)}|$ is the biorthogonal state corresponding to $|\phi_\mu^{(n-1)}\rangle$. The effective interaction is now given by

$$\begin{aligned} R_n &= PVP + \sum_{\mu=1}^{d} PVQ \frac{1}{E_\mu^{(n-1)} - QHQ} QVP|\phi_\mu^{(n-1)}\rangle\langle\tilde{\phi}_\mu^{(n-1)}| \\ &= \sum_{\mu=1}^{d} \hat{Q}(E_\mu^{(n-1)})|\phi_\mu^{(n-1)}\rangle\langle\tilde{\phi}^{(n-1)}|, \end{aligned} \tag{3·13}$$

where $\hat{Q}(E_\mu^{(n-1)})$ is defined as the Q-box interaction at $E_0 = E_\mu^{(n-1)}$ in Eq. (3·5). The iterative solution in Eq. (3·13) has been derived by Krenciglowa and Kuo.[11] The solution R_n in Eq. (3·13) is equivalent to the self-consistent solution for the energy dependent Bloch-Horowitz effective interaction in Eq. (2·24).

Let us now discuss the covergence condition for the iteration procedure (A).

Even though there are some intruder states in the sytem, the iterative solution in Eq. (3·9) or (3·13) is generally convergent. The iterative solution converges to a subset of eigensolutions of the full Hamiltonian. The problem is which subset of eigenvalues and eigenstates can be obtained from the iterative equation (3·9) or (3·13). It has already been known from the model calculation that if the solution is convergent, the eigenstates with large P-space overlap are obtained from the P-space eigenvalue problem in Eq. (2·21).[23]

The general convergence condition can be derived from the iterative equation (3·1). Let us define $\delta\omega_n$ as a small deviation of ω_n from the exact solution ω,

$$\delta\omega_n = \omega_n - \omega \,. \tag{3·14}$$

The corresponding deviation δR_n of R_n from the solution R is given by

$$\delta R_n = PVQ(\delta\omega_n) \,. \tag{3·15}$$

From Eq. (3·1), we have the following relation between δR_n and δR_{n-1}:

$$\delta R_n|\phi_\mu\rangle = -\{\omega^\dagger(E_\mu)\,\omega\}\,\delta R_{n-1}|\phi_\mu\rangle \,, \tag{3·16}$$

where $|\phi_\mu\rangle$ is the eigenstate of the P-space effective Hamiltonian in Eq. (2·21) and $\omega(E_\mu)$ is defined in Eq. (2·23). In the derivation of Eq. (3·16), we have neglected the higher order term with respect to the deviations $\delta\omega_n$ and $\delta\omega_{n-1}$. The relation (3·16) can also be derived from the solution R_n in Eq. (3·9). The convergence condition of the iteration means that the norm $\|\delta R_n|\phi_\mu\rangle\|$ must be smaller than $\|\delta R_{n-1}|\phi_\mu\rangle\|$. From Eq. (3·16), the convergence condition becomes

$$\begin{aligned}\|\delta R_n|\phi_\mu\rangle\|^2 &= \langle\phi_\mu|\delta R_{n-1}^\dagger\{\omega^\dagger\omega(E_\mu)\,\omega^\dagger(E_\mu)\,\omega\}\,\delta R_{n-1}|\phi_\mu\rangle \\ &< \|\delta R_{n-1}|\phi_\mu\rangle\|^2 .\end{aligned} \tag{3·17}$$

We here consider the eigenvalue problem

$$F_\mu|\tilde{\xi}\rangle = W_{\mu\xi}|\tilde{\xi}\rangle \tag{3·18}$$

with

$$F_\mu = \omega^\dagger\omega(E_\mu)\,\omega^\dagger(E_\mu)\,\omega \,. \tag{3·19}$$

The F_μ is a P-space operator and Hermitian. We easily see that F_μ satisfies

$$\langle\phi|F_\mu|\phi\rangle \geqq 0 \tag{3·20}$$

for any state $|\phi\rangle$ in the P space. Therefore, the eigenvalue $W_{\mu\xi}$ must be zero or positive and the normalized eigenstates $\{|\tilde{\xi}\rangle\}$ in Eq. (3·18) span the orthogonal set in the P space. The condition (3·17) is now written as

$$\sum_{\xi}|\langle\tilde{\xi}|\delta R_{n-1}|\phi_\mu\rangle|^2 W_{\mu\xi} < \sum_{\xi}|\langle\tilde{\xi}|\delta R_{n-1}|\phi_\mu\rangle|^2 \tag{3·21}$$

which must be satisfied for any small deviation δR_{n-1}. We then obtain the convergence condition

$$W_{\mu\xi}<1. \quad \text{(for any } \mu \text{ and } \xi\text{)} \tag{3·22}$$

If the full Hamiltonian H has the solutions ω and $\omega(E_\mu)$ such that $W_{\mu\xi}$ satisfy the condition (3·22), the iteration procedure in Eq. (3·1) or equivalently in Eqs. (3·9) and (3·13) converges and the effective interaction R can be obtained.

From the condition (3·22), we obtain a necessary condition for the convergence which may be of great interest in the practical application. If the condition (3·22) is satisfied, we have an inequality

$$\langle\phi_\mu|\{\omega^\dagger(E_\mu)\,\omega(E_\mu)\}^2|\phi_\mu\rangle<1\,, \tag{3·23}$$

where we have used the relation between $\omega(E_\mu)$ and ω in Eq. (2·22). We then obtain

$$\rho_Q=|\langle\phi_\mu|\omega^\dagger(E_\mu)\,\omega(E_\mu)\,|\phi_\mu\rangle|<1\,, \tag{3·24}$$

where $|\phi_\mu\rangle$ is a normalized P-space eigenstate. By using the expression of the true eigenstate $|\Psi_\mu\rangle$ of H in Eq. (2·25), we can write the condition (3·24) as

$$\frac{\langle\Psi_\mu|Q|\Psi_\mu\rangle}{\langle\Psi_\mu|\Psi_\mu\rangle}=\frac{\rho_Q}{1+\rho_Q}<1/2\,. \tag{3·25}$$

It is clear from the condition (3·25) that ρ_Q represents a measure of the probability of the Q-space occupation in the true wavefunction $|\Psi_\mu\rangle$. It is concluded that if the iteration procedure in Eq. (3·1) gives a convergent solution for R, the true wavefunction $|\Psi_\mu\rangle$ should have large overlap with the P space.

If the eigenvalues $\{E_\mu\}$ are far away from the eigenvalues $\{\varepsilon_q\}$ of QHQ— in some realistic physical problems this condition is satisfied — the matrix element of ω becomes very small, i.e.,

$$|\langle q|\omega|\phi_\mu\rangle|=|\langle q|V|\phi_\mu\rangle/(E_\mu-\varepsilon_q)\,|\ll 1\,. \tag{3·26}$$

In this case, the matrix element of F_μ in Eq. (3·19) becomes also very small and the condition $W_{\mu\xi}<1$ is satisfied. We then see that if $E_\mu\ll\varepsilon_q$, the iteration in Eq. (3·9) or (3·13) converges and we obtain the true eigenstate $|\Psi_\mu\rangle$ in Eq. (2·25) which has large overlap with the P space.

We see from the convergence condition that when we intend to calculate the low lying states, the model space must be chosen so that it contains the major component of the low lying states to be produced. If there is an intruder state and we choose the usual shell-model states as the P space, the condition $\rho_Q<1$ is not satisfied for this intruder state. In order to obtain the intruder state in the framework of the effective interaction theory based on the iterative self-energy insertion procedure, we need some modification to the P space. However, even if

there are some intruder states, the iteration is generally convergent. This iteration scheme may be efficient for the calculation of the "two-body" effective interaction to be used in the shell-model calculation, because the eigenstates to be obtained are dominated by the model space component.

(B) *Vertex renormalization procedure*

We next consider an iterative equation

$$\{E_0-(QHQ-\omega_{n-1}PVQ)\}\omega_n=QVP-\omega_{n-1}PVP\,. \tag{3·27}$$

In order to clarify the meaning of the iteration procedure, we introduce a renormalized interaction defined by

$$S_{n-1}=(1-\omega_{n-1})V\,. \tag{3·28}$$

The Q-space projection $QS_{n-1}Q$ means the Q-space "effective" interaction, which may be clear from Eqs. (2·17) and (2·26). In terms of S_{n-1}, Eq. (3·27) can be solved as

$$\omega_n=\frac{1}{E_0-QH_0Q-QS_{n-1}Q}QS_{n-1}P \tag{3·29}$$

and

$$R_n=PS_{n-1}P+PS_{n-1}Q\frac{1}{E_0-QH_0Q-QS_{n-1}Q}QS_{n-1}P\,, \tag{3·30}$$

where we have used the properties

$$PS_{n-1}P=PVP\,,$$
$$PS_{n-1}Q=PVQ\,. \tag{3·31}$$

We see from Eq. (3·30) that S_{n-1} serves as a renormalized vertex interaction in this iteration procedure. However, it is worth pointing out that although Eq. (3·30) looks symmetric in the expression, the effective interaction R_n is not Hermitian, because $S_{n-1}^{\dagger}\neq S_{n-1}$. It can be said from the expression for R_n in Eq. (3·30) that the iteration in Eq. (3·27) is, in essence, the vertex renormalization procedure.

If we start with $\omega_0=0$ in Eq. (3·27), the solution R_n can be written in terms of the Q-box interaction and its derivatives. The first few terms are given by

$$R_1=\hat{Q}\,, \tag{3·32}$$

$$R_2=\frac{1}{1-\hat{Q}_1}\hat{Q}\,, \tag{3·33}$$

$$R_3=\frac{1}{1-\hat{Q}_1-\hat{Q}_2\{1/(1-\hat{Q}_1)\}\hat{Q}}\hat{Q}$$

$$= \frac{1}{1-\hat{Q}_1-\hat{Q}_2 R_2}\hat{Q}\,, \tag{3·34}$$

where $\hat{Q}_1$ and $\hat{Q}_2$ have been defined in Eq. (3·6). The general solution is obtained as

$$R_n = \frac{1}{1-\hat{Q}_1-\sum_{m=2}^{n-1}\hat{Q}_m \prod_{k=n-m+1}^{n-1} R_k}\hat{Q}\,. \tag{3·35}$$

The second iterative solution R_2 has a simple interpretation, that is, R_2 agrees with the solution obtained from the application of the Newton-Raphson method to the Bloch-Horowitz equation (2·24). The solution R_n thus obtained corresponds to a certain resummation of the folded diagrams to infinite order. This type of the resummation has already been discussed in Refs. 10) and 24), although the general solution R_n in Eq. (3·35) had not yet been found.

The convergence condition for this iteration procedure is that the eigenvalues of the effective Hamiltonian PH_0P+R converge to those of the full Hamiltonian H nearest to the unperturbed energy E_0. The proof is given as follows: Let $\langle\phi_q|$ and $|\phi_\mu\rangle$ be an eigenbra in Eq. (2·26) and an eigenket in Eq. (2·21) of $Q\mathcal{H}Q$ and $P\mathcal{H}P$, respectively. From Eq. (3·27), we have a relation between the deviation $\delta\omega_n$ and $\delta\omega_{n-1}$

$$\langle\phi_q|\delta\omega_n|\phi_\mu\rangle = \left(\frac{E_0-E_\mu}{E_0-E_q}\right)\langle\phi_q|\delta\omega_{n-1}|\phi_\mu\rangle\,, \tag{3·36}$$

where E_μ and E_q are the eigenvalues of $P\mathcal{H}P$ and $Q\mathcal{H}Q$, respectively. We require for the convergence of the iteration

$$|\langle\phi_q|\delta\omega_n|\phi_\mu\rangle| < |\langle\phi_q|\delta\omega_{n-1}|\phi_\mu\rangle|. \tag{3·37}$$

We then obtain the convergence condition

$$\rho_{E_0} = \left|\frac{E_0-E_\mu}{E_0-E_q}\right| < 1\,. \tag{3·38}$$

Recall that E_q and E_μ are both the ture eigenvalues of H, particularly E_q is not the eigenvalue of the original Q-space Hamiltonian QHQ. The inequality in Eq. (3·38) manifests that the condition is satisfied by d eigenvalues $\{E_\mu\}$ of H nearest to the unperturbed energy E_0.

From the convergence condition in Eq. (3·38), we can say that the admixture in the energy spectrum of the eigenvalues of QHQ and those of the P-space effective Hamiltonian $P\mathcal{H}P$ does not cause instability in this iteration procedure. Therefore, even if there are some intruder states of which eigenvalues are close to the unperturbed energy E_0, they can be produced from the P-space eigenvalue

problem. This is the essential difference between the procedures (A) and (B).

The rate of convergence of this iteration is proportional to the magnitude of ρ_{E_0}. The unperturbed energy E_0 can be chosen to optimize the rate of convergence. This iteration method can reach any eigenvalue of H, if an appropriate value of E_0 is chosen.

The iterative solution R_n in Eq. (3·35) is indeed complicated. However, R_n should be calculated in a correct order. In the following, we shall discuss a counter example that a truncation to Eq. (3·35) may give rise to a serious mistake. We consider a series expansion for R_n, which is actually possible and the first few terms are given by

$$R_n = \hat{V}_Q + \hat{V}_2\hat{V}_Q{}^2 + \hat{V}_3\hat{V}_Q{}^3 + \cdots\cdots + \hat{V}_2\hat{V}_Q\hat{V}_2\hat{V}_Q{}^2 + \hat{V}_3\hat{V}_Q\hat{V}_2\hat{V}_Q{}^3 + \cdots\cdots , \tag{3·39}$$

where

$$\hat{V}_Q = \frac{1}{1-\hat{Q}_1}\hat{Q} , \tag{3·40}$$

$$\hat{V}_m = \frac{1}{1-\hat{Q}_1}\hat{Q}_m . \tag{3·41}$$

The right-hand side of R_n contains only $\hat{V}_m$ with m less than n. In so doing, one can calculate an "approximate" R_n or one can introduce some truncation to R_n. However, any truncation might lead to a serious mistake of inconsistency, especially when the R.S. expansion diverges. Any truncation or approximation to R_n in the iteration procedure does not preserve the equation to be solved. The expansion formula for R_n in Eq. (3·39) may sometimes be advantageous, but it is not advisable to apply to the actual calculation when there are intruder states. Due to the presence of the intruder state, $\hat{Q}$ and $\hat{Q}_m$ become quite large because of the small energy denominator $E_0 - QHQ$ in Eq. (3·5). If $\hat{Q}$ and $\hat{Q}_m$ are large, the series expansion for R_n is meaningless. It is, therefore, important to calculate R_n according to Eq. (3·35). It should be noted that the expression of R_n in Eq. (3·35) contains only operators defined in the P space which has rather small dimension. We believe that the exact calculation of R_n is applicable to the actual problem, if we can calculate the Q-box interaction and its derivative $\hat{Q}_m$.

§ 4. Conclusions and discussion

We have considered, in § 2, the similarity transformation of the Hamiltonian for the derivation of the effective interaction. A general equation has been derived for the energy independent effective interaction. It has been proved that the equation is essentially equivalent to Bloch's equation and the R.S. theory can be reformulated on the basis of the similarity transformation theory.

In order to solve the equation, we have discussed, in § 3, two iteration procedures. It has been shown that a different iteration procedure leads us to a different solution or a different expansion formula for the effective interaction. Our main interest has been how to overcome the difficulty of divergence of the R.S. perturbation expansion due to the presence of the intruder state and how to obtain the convergent result for the effective interaction. We have found that two iteration procedures (A) and (B) bring convergent solutions even if the intruder states are present.

The iteration method (A) corresponds, in essence, to the self-energy insertion procedure which is also equivalent to Krenciglowa and Kuo's iteration scheme.[14] It has been proved that the eigenstates with large overlap with the model space are obtained from the procedure (A). We can expect, therefore, that the procedure (A) would be a very effective way of calculation of the "two-body" effective interaction for the two valence particles in nuclei such as ^{18}O or ^{18}F, because the model space is chosen usually as the set of the shell-model states with the configurations of a few active orbits. If the coupling between the shell-model states and the collective intruder states is weak, the effective interaction would not be changed largely by the intruder states. In this weak coupling case, the procedure (A) would successfully give us the "two-body" effective interaction which includes the renormalization effect induced by the intruder states.

In our study, we have found a very powerful iteration method (B) which is also convergent even when there are some intruder states. The convergence condition for the procedure (B) is satisfied by the eigenstates which have the eigenvalues nearest to the unperturbed energy. The convergence condition is independent of the structure of the wavefunction of the eigenstate to be produced, which is essentially different from the convergence condition for the procedure (A). If the unperturbed energy is chosen as an appropriate value, the iterative solution obtained through the procedure (B) reaches all the low lying states including the intruder states. The procedure (B) derives a new solution for the effective interaction. The effective interaction derived from the procedure (B) would be quite different from that obtained from the procedure (A). If there are some intruder states, the effective interaction in the procedure (B) would accept a very large renormalization and non-Hermiticity, which has already been shown by the authors.[25] Any effort of trying to describe the intruder state in the perturbative approach is bound to fail, but the linearized iteration procedure (B) provides us a stable and convergent method for the calculation of the effective interaction by which the intruder states, as well as the low lying shell-model states, can be produced.

Only remaining problem is how to calculate the Q-box interaction. This problem will be discussed in a subsequent paper. In this respect, the study by Adhikari and Bandō[26] would be encouraging. They have proposed a multiple scattering equation to calculate certain type of diagrams to infinite order which are

included in the Q-box interaction. It is hopeful that we are able to calculate the convergent effective interaction in nuclei in very near future.

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References

1) B. H. Brandow, Rev. Mod. Phys. **39** (1967), 711.
2) B. R. Barrett and M. W. Kirson, *Advances in Nuclear Physics* Eds. M. Baranger and E. Vogt (Plenum Press, New York, 1973), vol. 6, p. 219.
3) T. T. S. Kuo, Ann. Rev. Nucl. Sci. **24** (1974), 101.
4) P. J. Ellis and O. Osnes, Rev. Mod. Phys. **49** (1977), 777 and references therein.
5) T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85** (1966), 40.
G. E. Brown and T. T. S. Kuo, Nucl. Phys. **A92** (1967), 481.
T. T. S. Kuo, Nucl. Phys. **A103** (1967), 71.
6) K. A. Brueckner, C. A. Levinson and H. M. Mahmoud, Phys. Rev. **95** (1954), 217.
K. A. Brueckner, Phys. Rev. **100** (1955), 36.
H. A. Bethe and J. Goldstone, Proc. Roy. Soc. London **A238** (1957), 551.
7) T. T. S. Kuo, S. Y. Lee and K. F. Ratcliff, Nucl. Phys. **A176** (1971), 65.
8) M. B. Johnson and M. Baranger, Ann. of Phys. **62** (1971), 172.
G. Oberlechner, F. Owono-N'-Guema and J. Richert, Nuovo Cim. **B68** (1970), 23.
9) B. R. Barrett and M. W. Kirson, Nucl. Phys. **A148** (1970), 145; **A196** (1972), 638 Errata.
10) T. Schucan and H. A. Weidenmüller, Ann. of Phys. **73** (1972), 108; **76** (1973), 483.
11) H. M. Hofmann, S. Y. Lee, J. Richert, H. A. Weidenmüller and T. H. Schucan, Ann. of Phys. **85** (1974), 410.
12) H. M. Hofmann, Y. Starkand and M. W. Kirson, Nucl. Phys. **A266** (1976), 138.
13) S. Pittel, C. M. Vincent and J. D. Vergados, Phys. Rev. **C13** (1976), 412.
14) E. M. Krenciglowa and T. T. S. Kuo, Nucl. Phys. **A235** (1974), 171; **A240** (1975), 195.
15) M. W. Kirson, Ann. of Phys. **82** (1974), 345.
16) P. J. Ellis and H. A. Mavromatis, Nucl. Phys. **A175** (1971), 309.
17) F. Coester, Nucl. Phys. **7** (1958), 421.
R. Offermann, W. Ey and H. Kümmel, Nucl. Phys. **A273** (1976), 349.
H. Kümmel, K. H. Luhrmann and J. G. Zabolitzky, Phys. Reports **38C** (1978), 1.
18) K. Andō and H. Bandō, Prog. Theor. Phys. **53** (1975), 1711.
K. Andō, H. Bandō and S. Nagata, Prog. Theor. Phys. **57** (1977), 1303.
K. Andō, H. Bandō and E. M. Krenciglowa, Prog. Theor. Phys. Suppl. No. 65 (1979), 38.
19) K. Suzuki, Prog. Theor. Phys. **58** (1977), 1064.
20) C. Bloch, Nucl. Phys. **6** (1958), 329.
21) I. Lindgren, J. of Phys. **B7** (1974), 2441.
22) J. Des Cloizeaux, Nucl. Phys. **20** (1960), 321.
23) M. R. Anastasio and T. T. S. Kuo, Nucl. Phys. **A238** (1975), 79.
24) S. Y. Lee, Thesis, SUNY at Stony Brook, 1972, unpublished.
25) S. Y. Lee and K. Suzuki, Phys. Letters **91B** (1980), 173.
26) S. K. Adhikari and H. Bandō, Phys. Rev. **C22** (1980), 787.