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Formulation of effective interaction in terms of the non-perturbative and analytic $\widehat{Q}$ box

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Abstract. One of the useful and practical methods for solving quantum-mechanical many-body systems is to recast the full problem into a form of the effective interaction acting within a model space of tractable size. Many of the effective-interaction theories in nuclear physics have been formulated by use of the so called $\widehat{Q}$ box introduced by Kuo et al. It has been one of the central problems how to calculate the $\widehat{Q}$ box accurately and efficiently. Introducing new basis states, the Hamiltonian is transformed to a block-tridiagonal form in terms of submatrices with small dimension. With the transformed Hamiltonian we derive a recursion method of calculating the $\widehat{Q}$ box non-perturbatively and analytically. The $\widehat{Q}$ box given in this study corresponds to a non-perturbative solution for the energy-dependent Hamiltonian interaction which is often referred to as the Bloch-Horowitz or the Feshbach form. The present approach has a possibility of resolving many of the theoretical and practical difficulties encountered in the calculation of effective-interaction and/or Hamiltonian.

1. Introduction

In nuclear many-body physics various methods have been proposed, on the basis of the shell model, to solve the Schrödinger equations for nuclear many-body systems starting with realistic nucleon-nucleon(NN) interactions. These methods, which are called the *ab initio* calculations, include the Green's function Monte Carlo method, the no-core shell model, the effective interaction for hyperspherical harmonics method, the coupled cluster method and the unitary-model-operator approach. Much effort has been made also to diagonalize a matrix of a many-body shell-model Hamiltonian in a huge dimensional Hilbert space on the basis of, or alternatively to, the Lanczos method.

The effective interaction theory has been one of the *ab initio* method which has aimed at solving the nuclear properties starting from realistic nucleon-nucleon forces. Most of the effective-interaction theories given to date have been formulated in terms of the $\widehat{Q}$ box introduced by Kuo and his collaborators. Originally the $\widehat{Q}$ box has been defined as the sum of linked and unfolded diagrams. In the algebraic or non-diagrammatical approach the $\widehat{Q}$ box is equivalent to the energy-dependent effective Hamiltonian given by Bloch and Horowitz and Feshbach which has been studied extensively on the Brillouin-Wigner perturbation theory.

It has been established that the effective interaction can be expressed as a series expansion in terms of the $\widehat{Q}$ box and its energy derivatives. The series can be summed up by using either the Krenciglowa-Kuo (KK) or the Lee-Suzuki(LS) methods. It has been known that, in general, two methods have different convergence properties: Many of the numerical calculations have shown that the KK method yields the eigenvalues for the eigenstates which have the largest overlaps with the chosen model space. However, it has been pointed out that the rigorous convergence condition for the KK method has not yet been clarified. On the other hand the LS method reproduces the eigenvalues which lie closest to the chosen unperturbed energy. Both of the two approaches reproduce only certain of the eigenvalues of the original Hamiltonian. This restriction is not, in general, desirable.

Recently a new vertex function, called the $\widehat{Z}$ box, has been introduced to yield the eigenvalues of a given Hamiltonian H regardless of the properties of the eigenstates [1]. The $\widehat{Z}$ box itself has also been defined as a function of the $\widehat{Q}$ box. At present the most important remaining task would be to establish a method of how to calculate the $\widehat{Q}$ box rigorously and efficiently. The perturbative calculation method for the $\widehat{Q}$ box has been established and applied widely. In the derivation of the nuclear effective interaction, the convergence of the order-by-order calculation was confirmed in many of the numerical studies. However, a basic problem of the convergence of its perturbation expansion has not been made clear theoretically for general cases. Main concern of the present study is to propose a non-perturbative method for obtaining the $\widehat{Q}$ box for any of the starting NN interactions. Detailed discussions have been given in Ref.[2].

2. Effective-interaction theory by means of similarity transformation

2.1. Basic equation for effective interaction

Let us begin with a Hamiltonian H defined in a Hilbert space. We divide the space into a model space (P space) and its complementary space (Q space). When all the eigenvalues of an operator H_{eff} given in the P space coincide with those of H, we call H_{eff} an effective Hamiltonian.

There are various ways of constructing H_{eff}. We adopt the following standard one. First we introduce an operator ω that maps states in the P space and those in the Q space to each other, with the properties,

$$\omega = Q\omega P, \tag{2.1}$$

$$\omega^n = 0 \qquad (n \geq 2). \tag{2.2}$$

Suppose that the operator ω satisfies the following equation;

$$QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0. \tag{2.3}$$

This equation for ω was first derived by Okubo. Once a solution ω to Eq.(2.3) is given, H_{eff} is written as

$$H_{\text{eff}} = PHP + PHQ\omega. \tag{2.4}$$

It has been proved that the effective Hamiltonian H_{eff} can be derived as in Eq.(2.4) with the solution ω to Eq.(2.3)

2.2. Krenciglowa-Kuo's solution

Since Eq.(2.3) is a nonlinear matrix equation for ω, it is difficult to find a general solution. The following formal solution, however, has been known and is enough for applications. We rewrite Eq.(2.3) as

$$QHP + QHQ\omega - \omega H_{\text{eff}} = 0, \tag{2.5}$$

using Eq.(2.4). Here the eigenvalue equation for $H_{\rm eff}$ is given by

$$H_{\rm eff}|\phi_k\rangle = E_k|\phi_k\rangle. \tag{2.6}$$

If the operator ω is a solution to Eq.(2.3), we can verify that the eigenstates $\{|\phi_k\rangle\}$ belong to the P space and each eigenvalue E_k coincides with one of those of H.

Using Eq.(2.5), ω is given by

$$\omega = \sum_{k=1}^{d} \frac{1}{E_k - QHQ} QHP|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{2.7}$$

and from Eq.(2.4) $H_{\rm eff}$ becomes

$$H_{\rm eff} = PHP + \sum_{k=1}^{d} PHQ\frac{1}{E_k - QHQ}QHP|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{2.8}$$

where $\langle\tilde{\phi}_k|$ is the biorthogonal states of $|\phi_k\rangle$. Here we introduce an operator in the P space called the $\widehat{Q}$ box

$$\widehat{Q}(E) = PHP + PHQ\frac{1}{E - QHQ}QHP, \tag{2.9}$$

where E is an energy variable. The $\widehat{Q}$ box thus defined is equivalent to the energy-dependent effective Hamiltonian referred to as the Bloch-Horowitz and /or the Feshbach forms. In terms of $\widehat{Q}(E)$, $H_{\rm eff}$ is expressed as

$$H_{\rm eff} = \sum_{k=1}^{d} \widehat{Q}(E_k)|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{2.10}$$

from which the following self-consistent equation can be derived

$$\widehat{Q}(E_k)|\phi_k\rangle = E_k|\phi_k\rangle. \tag{2.11}$$

The $H_{\rm eff}$ in Eq.(2.10) is just a formal solution in the sense that unknown E_k, $|\phi_k\rangle$, and $\langle\widetilde{\phi}_k|$ appear on the right-hand side, but the following method of solving is available: In order that the solutions to Eq.(2.6) coincide with those given by Eq.(2.10), they selfconsistently satisfy the iterative equation

$$\widehat{Q}(E_k^{(n)})|\phi_k^{(n+1)}\rangle = E_k^{(n+1)}|\phi_k^{(n+1)}\rangle, \tag{2.12}$$

where $E_k^{(n+1)}$ and $|\phi_k^{(n+1)}\rangle$ are the $(n+1)$-th order eigenvalue and eigenstate of the $\widehat{Q}$ box, respectively, given by the n-th order eigenvalue $E_k^{(n)}$. This iterative scheme has been called the Kreciglowa-Kuo method.

From Eq.(2.9), we see that $\widehat{Q}(E)$ has poles at energies $\{\varepsilon_q\}$, where ε_q is one of the eigenvalues of QHQ,

$$QHQ|q\rangle = \varepsilon_q|q\rangle. \tag{2.13}$$

These singularities of the $\widehat{Q}$ box lead to some difficulties in numerical calculations. These arguments suggest that some further improvements are desired for the $\widehat{Q}$-box method although it has been applied widely to practical problems.

2.3. The $\widehat{Z}$ box method

In order to resolve the pole problem we have introduced a vertex function $\widehat{Z}$, called the $\widehat{Z}$ box, as[1]

$$\widehat{Z}(E) = \frac{1}{1-\widehat{Q}_1(E)}\left[\widehat{Q}(E) - E\widehat{Q}_1(E)\right], \tag{2.14}$$

where E is an energy variable and

$$\widehat{Q}_1(E) = \frac{d\widehat{Q}(E)}{dE}. \tag{2.15}$$

The $\widehat{Z}$ box has the following properties:

(i) The $\widehat{Z}$ box satisfies the selfconsistent equation

$$\widehat{Z}(E_k)|\phi_k\rangle = E_k|\phi_k\rangle, \tag{2.16}$$

where $\{E_k\}$ are the eigenvalues of H and $\{|\phi_k\rangle\}$ the model-space eigenstates which are the same as in Eqs.(2.10) and (2.11).

(ii) The $\widehat{Z}(\varepsilon_q)$ also satisfies the self-consistent equation for the eigenvalues $\{\varepsilon_q\}$ of QHQ as

$$\widehat{Z}(\varepsilon_q)|\mu_q\rangle = \varepsilon_q|\mu_q\rangle. \tag{2.17}$$

(iii) Both of $\{E_k\}$ and $\{\varepsilon_q\}$ satisfy the selfconsistent equations as in Eqs.(2.16) and (2.17), respectively, but the derivative of the $\widehat{Z}$ box takes different values as

$$\frac{d\widehat{Z}(E)}{dE} = \begin{cases} 0 & \text{for } E = E_k, \\ 2 & \text{for } E = \varepsilon_q. \end{cases} \tag{2.18}$$

Using these properties we can divide the solutions of the selfconsistent equations into two parts, namely, the true eigenvalues $\{E_k\}$ of H and the pole energies $\{\varepsilon_q\}$.

(iv) The $\widehat{Z}(E)$ is finite and differentiable at any energy variable E, even at pole positions $\{\varepsilon_q\}$ of the $\widehat{Q}$ box. This may be clear from Eqs.(2.17) and (2.18).

3. Calculation of the $\widehat{Q}$ box by means of recurrence relations

3.1. Block tridiagonalization of Hamiltonian

Before discussing the calculation procedure of the $\widehat{Q}$ box, we transform the Hamiltonian H into a tractable form by changing basis vectors. First we introduce

$$Y_P = PHQ \cdot QHP. \tag{3.1}$$

The Y_P is an operator in the P space, which is Hermitian and positive semi-definite, that is, $y_k^{(1)} \geq 0$ in the eigenvalue equation

$$Y_P|p_k\rangle = y_k^{(1)}|p_k\rangle. \tag{3.2}$$

Suppose that d_1 eigenvalues are nonzero among $\{y_k^{(1)}\}$. In terms of the eigenvectors $\{|p_k\rangle, k = 1, 2, \cdots, d_1\}$ with nonzero eigenvalues, we define normalized vectors $\{|q_k^{(1)}\rangle\}$ in the Q space as

$$|q_k^{(1)}\rangle = \frac{1}{\sqrt{y_k^{(1)}}}QHP|p_k\rangle, \quad (k = 1, 2, \cdots, d_1). \tag{3.3}$$

They are orthogonal to each other and span the d_1-dimensional subspace Q_1 in the Q space. Then the projection operator onto the Q_1 space becomes

$$Q_1 = \sum_{k=1}^{d_1} |q_k^{(1)}\rangle\langle q_k^{(1)}|. \tag{3.4}$$

The complement of the Q_1 space in the Q space is given by

$$\overline{Q}_1 = Q - Q_1. \tag{3.5}$$

Equation (3.3) indicates that

$$QHP = \sum_{k=1}^{d_1} \sqrt{y_k^{(1)}}|q_k^{(1)}\rangle\langle p_k|, \tag{3.6}$$

then we have

$$QHP = Q_1 HP \tag{3.7}$$

which leads to

$$\overline{Q}_1 HP = 0. \tag{3.8}$$

Next, a similar manipulation with replacing P and Q with Q_1 and $\overline{Q}_1$, respectively, leads to another orthogonal system and the subspace, namely the Q_2 space. Repeating the same procedures leads to the following: Decompose the Q space as

$$Q = Q_1 + Q_2 + \cdots + Q_n + \cdots . \tag{3.9}$$

Basis vectors of the subspace Q_m, namely, $\{|q_k^{(m)}\rangle, k = 1, 2, \cdots, d_m\}$, define the projection operator

$$Q_m = \sum_{k=1}^{d_m} |q_k^{(m)}\rangle\langle q_k^{(m)}|. \tag{3.10}$$

The basis vectors $\{|q_k^{(m)}\rangle\}$ are given as follows: Introduce $Y_{Q_{m-1}}$ as

$$Y_{Q_{m-1}} = Q_{m-1} H \overline{Q}_{m-1} \cdot \overline{Q}_{m-1} H Q_{m-1} \tag{3.11}$$

with

$$\overline{Q}_{m-1} = Q - (Q_1 + Q_2 + \cdots + Q_{m-1}). \tag{3.12}$$

Its eigenvalue equation is

$$Y_{Q_{m-1}}|q_k'^{(m-1)}\rangle = y_k^{(m)}|q_k'^{(m-1)}\rangle. \tag{3.13}$$

In general new orthogonal bases

$$|q_k^{(m)}\rangle = \frac{1}{\sqrt{y_k^{(m)}}} \overline{Q}_{m-1} H Q_{m-1} |q_k'^{(m-1)}\rangle \tag{3.14}$$

are derived from the eigenvectors $\{|q_k'^{(m-1)}\rangle\}$ with nonzero eigenvalues $\{y_k^{(m)}\}$. They span the subspace Q_m. With the projection operators Q_m and Q_{m-1} we obtain, from Eq.(3.14), an expression written as

$$Q_m H Q_{m-1} = \sum_{k=1}^{d_m} \sqrt{y_k^{(m)}} |q_k^{(m)}\rangle\langle q_k'^{(m-1)}|. \tag{3.15}$$

We conclude from the above discussion that

$$PHQ_m = Q_m HP = 0 \quad (m \geq 2), \tag{3.16}$$
$$Q_m H Q_{m+k} = Q_{m+k} H Q_m = 0 \quad (k \geq 2) \tag{3.17}$$

hold for the subspaces $\{P, Q_1, Q_2, \cdots, Q_m, \cdots\}$. This means that the given Hamiltonian H is transformed to a block-tridiagonal matrix

$$H = \begin{pmatrix} PHP & PHQ_1 & 0 & 0 & \cdots \\ Q_1HP & Q_1HQ_1 & Q_1HQ_2 & 0 & \cdots \\ 0 & Q_2HQ_1 & Q_2HQ_2 & Q_2HQ_3 & \cdots \\ 0 & 0 & Q_3HQ_2 & Q_3HQ_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \tag{3.18}$$

where each block matrix is at most d-dimensional.

3.2. Calculation of the $\widehat{Q}$ box
We introduce an operator $\chi(E)$ defined as

$$\chi(E) = \frac{1}{e(E)} QHP \tag{3.19}$$

with

$$e(E) = Q(E - H)Q. \tag{3.20}$$

The Q space is decomposed as in Eq.(3.9), and also $\chi(E)$ is as

$$\chi(E) = \chi_1(E) + \chi_2(E) + \cdots + \chi_n(E) + \cdots, \tag{3.21}$$

where

$$\chi_n(E) = Q_n\, \chi(E) P. \tag{3.22}$$

The operators $\{\chi_n(E)\}$ obey the recursion relation written as[2]

$$Q_1\, e(E)\{\chi_1(E) + \chi_2(E)\} = Q_1 HP, \tag{3.23}$$
$$Q_n\, e(E)\{\chi_{n-1}(E) + \chi_n(E) + \chi_{n+1}(E)\} = 0, \ (n \geq 2). \tag{3.24}$$

Note that, from Eq.(3.7), the $\widehat{Q}$ box in Eq.(2.9) can be written as

$$\widehat{Q}(E) = PHP + PHQ_1\chi_1(E). \tag{3.25}$$

Then the calculation procedure of the $\widehat{Q}$ box is reduced to solving the recursive equations and finding the solution for $\chi_1(E)$.

It has been proved that the solution for $\chi_1(E)$ is given by

$$\chi_1(E) = \frac{1}{\widetilde{e}_1(E)} Q_1 H P, \tag{3.26}$$

where the energy denominator is determined from the following descending recurrence relations;

$$\widetilde{e}_{n-1}(E) = e_{n-1}(E) - H_{n-1,n} \frac{1}{\widetilde{e}_n(E)} H_{n,n-1}. \tag{3.27}$$

with

$$e_{n-1}(E) = Q_{n-1}(E - H)Q_{n-1}, \tag{3.28}$$

$$H_{ij} = Q_i H Q_j. \tag{3.29}$$

Suppose that, for a sufficiently large number N, the condition

$$\| \frac{1}{e_N(E)} H_{N,N-1} \| \ll 1 \tag{3.30}$$

is satisfied, where the symbol $||X||$ means the norm of a matrix X. If we start with $n = N$ in Eq.(3.28), we have a sequence $\{\widetilde{e}_{N-1}(E), \widetilde{e}_{N-2}(E), \cdots\}$ and finally we have $\widetilde{e}_1(E)$. Then we may write the $\widehat{Q}$ box as

$$\widehat{Q}(E) = PHP + PHQ_1 \frac{1}{\widetilde{e}_1(E)} Q_1 H P. \tag{3.31}$$

The above expression indicates that a certain energy denominator $\widetilde{e}_1(E)$ exists such that the $\widehat{Q}(E)$ can be represented by a sum of only second-order perturbation terms[2].

4. Model calculation

We solve the eigenvalue problem for the Hamiltonian H in the framework of the $\widehat{Z}$-box method[1, 2]. The calculation procedure is as follows: We define d functions $\{F_k(E), k = 1, 2, \cdots, d\}$ through the eigenvalue equation for $\widehat{Z}(E)$ as

$$\widehat{Z}(E)|\zeta_k\rangle = F_k(E)|\zeta_k\rangle, \quad k = 1, 2, \cdots, d. \tag{4.32}$$

We further introduce functions $\{F'_k(E), k = 1, 2, \cdots, d\}$ as

$$F'_k(E) = \left\langle \zeta_k \right| \frac{d\widehat{Z}}{dE} \left| \zeta_k \right\rangle. \tag{4.33}$$

Using the properties in Eqs.(2.16)- (2.18), we can prove that the true eigenvalues $\{E_k\}$ of H can be obtained by solving the equation

$$g_k(E) = \left\{ \frac{F_k(E) - E}{F_0} \right\}^2 + \{F'_k(E)\}^2 = 0, \tag{4.34}$$

where F_0 is a parameter chosen suitably. We solve Eq.(4.34) by means of the parabolic-interpolation method given in Ref.[2].

In order to obtain some assessments of the present approach we study a model problem. We start with a model Hamiltonian H of which matrix elements are given by

$$\langle i|H|j\rangle = (\alpha i + \beta i^2)\delta_{ij} + \gamma x_{ij} \tag{4.35}$$

with

$$x_{ij} = 2\left\{\sqrt{\sqrt{2}(i+j)} - \left[\sqrt{\sqrt{2}(i+j)}\right]\right\} - 1, \tag{4.36}$$

where $[X]$ is Gauss's symbol which means the integer part of a real number X. A set of $\{x_{ij}\}$ are recognized as pseudo random numbers satisfying

$$-1 \leq x_{ij} \leq 1. \tag{4.37}$$

The α, β and γ are the parameters chosen suitably. The total dimension of H is taken to be $N_h = 100$. As for the P space we choose a two-dimensional space ($d = 2$) spanned by the two states which have the lowest and second lowest diagonal energies of H. We suppose that the subspaces $\{Q_k,\ k = 1, 2, \cdots, N_q\}$ are all d-dimensional and the number of the subspace $\{Q_k\}$ is given by $N_q = (N_h - 2)/2 = 49$.

In Table 1 we show the results for the lowest two eigenvalues of H calculated by the parabolic-interpolation method[2]. The convergence is markedly fast. With three times of the changes of the interval $[a, b]$, convergence is reached with accuracy better than 10 decimal places.

Table 1. Correct digits of the lowest two eigenvalues of H calculated by the parabolic-interpolation method. Initial intervals are taken to be $[a, b] = [0.0, 1.0]$ and $[2.5, 3.5]$ for E_1 and E_2, respectively. The numbers of repeats means the number of changes of the interval [a, b]. All the values of E_1 and E_2 are dimensionless.

E_i	No. of repeats	Calculated value
E_1	1	0.365
	2	0.365550
	3	0.365550151994574
E_2	1	2.999
	2	2.9994240
	3	2.99942408730107

It would be interesting to examine the dependence of the calculated eigenvalues of H on the number of the subspaces $\{Q_k\}$ taken into consideration. Let $K_{\max}$ be the maximum number of the subspaces $\{Q_k\}$. The dependence on $K_{\max}$ is shown in Figs.1. It is clear that, as $K_{\max}$ approaches to N_q=49, the eigenvalues converge to the exact values. These results suggest a possibility of introducing a new way of truncation in the calculation of effective interaction, instead of making it according to the magnitude of energies of intermediate states.

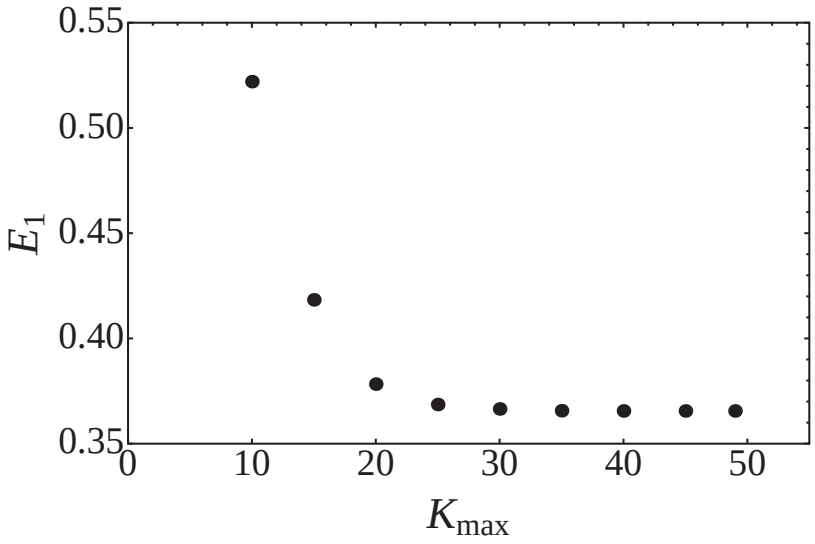

Figure 1. Convergence of E_1 as a function of $K_{\max}$. The $K_{\max}$ denotes the block dimension which means the number of the subspaces $\{Q_k,\ k{=}1,2,\cdots,K_{\max}\}$ taken into calculation. In this model calculation $K_{\max}$ is in the range $1 \leq K_{\max} \leq 49$. The exact value of E_1 is $0.36555\cdots$ as given in Table 1. The value of E_1 is dimensionless.

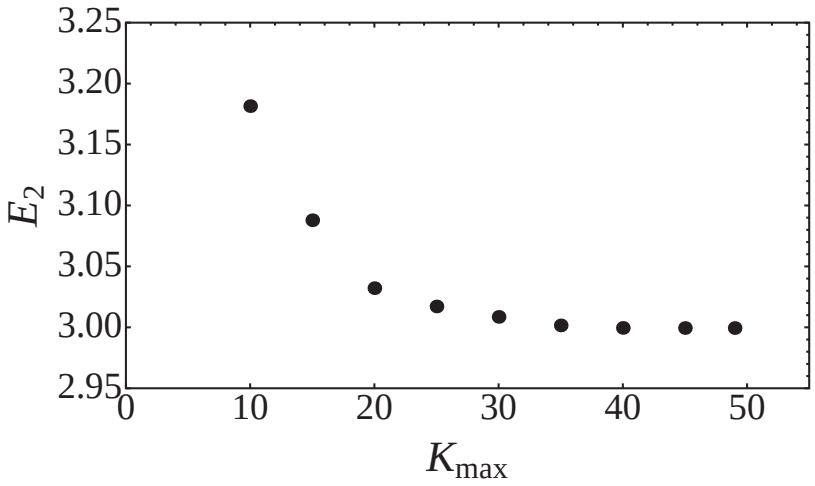

Figure 2. Convergence of E_2 as a function of $K_{\max}$. The exact value of E_2 is $2.9994\cdots$. Other notations are the same as in Fig.1.

5. The relation of the present method to the block Lanczos method

The calculation of the $\widehat{Q}$ box can be carried out without matrix inversion of QHQ which is usually a huge-dimensional matrix. All the procedures for obtaining the $\widehat{Q}$ box are reduced to calculations of small-dimensional submatrices in the block-tridiagonalized Hamiltonian.

Regarding the block tridiagonalization of the Hamiltonian, the present approach has a common aspect to the so called block Lanczos method based on the theory of the Krylov subspaces. For a given model space P and a Hamiltonian H, the subspaces leading to a block-tridiagonal form of H are determined uniquely. Therefore, the subspaces given in the present

study are the same as those of Krylov. However, the choice of basis states of each subspace is ambiguous. For determining the basis states we employ a different calculation procedure from the usual one in the block Lanczos method, as shown in Eq.(3.14). We show that the basis states thus introduced are suitable for the purpose of calculating not only the $\widehat{Q}$ box but also the eigenstates of H[1].

It is well known that roundoff errors makes the Lanczos method somewhat difficult to use in practice[3],[4]. The central problem is a loss of orthogonality among the Lanczos vectors that are produced by iteration. There are several ways, say selective or full reorthonormalization to cope with this problem[3],[4]. However, there is no need of additional orthonormalization of the relevant basis in the present formulation, as long as we concern the effective Hamiltonian and its eigenvalues in the model space.

6. Summary and outlook

The main purpose of the present study has been to derive a new method of calculating the $\widehat{Q}$ box as accurately as possible even if the original Hamiltonian H is given in a huge-dimensional space.

The present formulation[2] consists of two steps: First one is to transform a given Hamiltonian H to a block-tridiagonal form by dividing the complementary space Q of the P space into subspaces $\{Q_k,\ k = 1, 2, \cdots\}$ with tractable dimensions. If the subspaces are chosen suitably the Hamiltonian is transformed to a block-tridiagonal form. With the Hamiltonian thus transformed, the next step is to derive coupled equations for determining the $\widehat{Q}$ box. We have shown that these coupled equations can be solved by means of a recursion method.

Given the $\widehat{Q}$ box, we have applied the $\widehat{Z}$-box method for solving the eigenvalue problem of a Hamiltonian H[2]. In order to assess the present method we have made a test calculation by introducing a 100×100 model Hamiltonian. We have confirmed that the present method reproduces successfully the eigenvalues of the original Hamiltonian.

There would be two applicabilities of the present approach: One is to solve the eigenvalue problem for a Hamiltonian given in a huge dimensional space. Once the $\widehat{Q}$ box is given, the eigenvalues and the corresponding eigenstates can be calculated according to the procedures in the present framework. The other is to apply the present formalism to the derivation of the effective interaction to be used in the shell-model calculations.

The present study is based essentially on the algebraic approach to the effective Hamiltonian. When we want to calculate the effective interaction acting among valence nucleons, it is necessary to represent all the terms contained in the $\widehat{Q}$ box in terms of linked diagrams. A general and rigorous relation is not made clear between the present approach and the linked-and-folded-diagram theory. We note that algebraic approaches can not always exclude unlinked diagrams in general. Therefore, this formal relation is an interesting problem to be clarified.

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