# Formulation of an effective interaction in terms of renormalized vertices and propagators

Kenji Suzuki,[1,*] Hiroo Kumagai,[2,†] Masayuki Matsuzaki,[3,‡] and Ryoji Okamoto[1,§]
[1]*Senior Academy, Kyushu Institute of Technology, Kitakyushu 804-8550, Japan*
[2]*Faculty of Information Engineering, Fukuoka Institute of Technology, Fukuoka 811-0295, Japan*
[3]*Department of Physics, Fukuoka University of Education, Munakata, Fukuoka 811-4192, Japan*
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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. We first show that, introducing new basis states, the Hamiltonian is transformed to a block-tridiagonal form in terms of submatrices with small dimension. With this transformed Hamiltonian, we next prove that the $\widehat{Q}$ box can be expressed in two ways: One is in the form of a continued fraction and the other is a simple series expansion up to second order with respect to renormalized vertices and propagators. This procedure ensures derivation of an exact $\widehat{Q}$ box, if the calculation converges as the dimension of the Hilbert space tends to infinity. The $\widehat{Q}$ box given in this study corresponds to a nonperturbative solution for the energy-dependent effective interaction which is often referred to as the Bloch-Horowitz or the Feshbach form. By applying the $\widehat{Z}$-box approach based on the $\widehat{Q}$ box proposed previously, we introduce a graphical method for solving the eigenvalue problem of the Hamiltonian. The present approach has a possibility of resolving many of the difficulties encountered in the effective-interaction theory.

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## I. 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 interactions. These methods, which are called the *ab initio* calculations, include the Green's function Monte Carlo (GFMC) method [1,2], the no-core shell model (NCSM) [3,4], the effective interaction for hyperspherical harmonics (EIHH) method [5], the coupled cluster method (CCM) [6–8], and the unitary-model-operator approach (UMOA) [9–11]. 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 [12–14].

The shell-model calculations were carried out in the early stage by introducing the phenomenological residual interaction between two nucleons determined from the experimental data [15,16]. These studies have been considered to be useful in accounting for the variety of nuclear properties; such studies were reviewed by Talmi [17]. The next stage of the nuclear shell-model calculation was to employ a realistic nucleon-nucleon (NN) interaction and to derive theoretically a renormalized interaction which takes the repulsive short-range correlations into account. The first attempt of this approach was made by Dowson, Talmi, and Walecka [18] by applying the Brueckner reaction-matrix theory. Soon afterwards corrections to the reaction matrix, such as the core-polarization effect, were estimated by Bertsch [19].

A marked development was attained by Kuo and Brown [20], who performed a second-order perturbative calculation for deriving the effective interaction between two valence nucleons outside the core $^{16}$O. They established that the core-polarization effect has a crucial role in understanding the nuclear properties. Their study attracted increased attention to the evaluation of higher-order perturbative terms. The third-order diagrams were calculated by Barrett and Kirson [21], and many studies were made to sum up the specific series of diagrams to all orders, which include the Padè approximants [22,23], RPA [24], and the induced-interaction method [25–27]. The theoretical formalism for deriving the effective interaction was also developed on the basis of the perturbation theory. The folded-diagram theory by Kuo, Lee, and Ratcliff [28] was proposed and has been recognized to be the basic formalism of deriving microscopically the effective interaction. Much effort has been devoted continuously to progress in the effective-interaction theory and its practical application [29–34]. The present status of these studies was reviewed by recent articles of Coraggio *et al.* [35,36]. This effective-interaction method has been developed to apply to new fields of many-body physics such as quantum dots [37,38] and many-boson systems [39].

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 [32,40,41]. Originally the $\widehat{Q}$ box was defined as the sum of linked and unfolded diagrams [28]. In the algebraic or nondiagrammatical approach the $\widehat{Q}$ box is equivalent to the energy-dependent effective interaction given by Bloch and Horowitz [42] and Feshbach [43], which has

*suz93@mocha.ocn.ne.jp
†kumagai@fit.ac.jp
‡matsuza@fukuoka-edu.ac.jp
§okamoto.ryoji.munakata@gmail.com

 

been studied extensively in the Brillouin-Wigner perturbation theory [44,45].

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) [46] or the Lee-Suzuki(LS) [47–49] method. It has been known that, in general, the 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 [50]. 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 some of the eigenvalues of the original Hamiltonian. This restriction is not, in general, desirable.

Another difficulty encountered in actual calculations is the pole problem. The $\widehat{Q}$ box itself has poles at the energies which are the eigenvalues of $QHQ$, where $Q$ is the projection operator onto the complement ($Q$ space) of the model space ($P$ space). The presence of the poles causes often instability in numerical calculations. Three of the present authors and Fujii [51] have shown that it was indeed possible to resolve these difficulties by introducing a new vertex function $\widehat{Z}(E)$, called the $\widehat{Z}$ box. The $\widehat{Z}$-box approach based on the $\widehat{Q}$ box may have a possibility of resolving many of the difficulties encountered in the effective-interaction theory.

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 [28,32,46]. In the derivation of the nuclear effective interaction, the convergence of the order-by-order calculation was confirmed in many of the numerical studies [35,36]. However, a basic problem of the convergence of its perturbation expansion has not been made clear theoretically for general cases. A main concern of the present study is to propose a nonperturbative method for obtaining a convergent result for any of the starting NN interactions.

The formulation in the present study consists mainly of two parts: The first one is to transform the Hamiltonian to a block-tridiagonal form, where the dimensions of the block submatrices are taken to be equal to or less than the dimension of the $P$ space. With the block-tridiagonalized Hamiltonian, the next step is to derive a set of coupled equations for determining the $\widehat{Q}$ box. We show that the coupled equations can be solved by employing two different recursion methods: The first solution is represented in the form of a continued fraction, and the second one is expressed as a sum of terms up to second order with respect to renormalized vertices and propagators. In both of the methods 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 [13]. 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. Different basis states are introduced, and we show that they are suitable for the purpose of calculating not only the $\widehat{Q}$ box but also the eigenstates of $H$.

The construction of the present article is as follows: In Sec. II some basic elements of the effective-interaction theory are reviewed. Section III is devoted to the formulation of rigorous calculation of the $\widehat{Q}$ box. A set of coupled equations for determining the $\widehat{Q}$ box are given. The equations are solved by employing recursion methods and two kinds of solutions for the $\widehat{Q}$ box are derived. In Sec. IV, a method is given for the problem of how to calculate eigenstates of $H$ within the framework of the effective-interaction theory. In Sec. V a short review of the $\widehat{Z}$-box theory is given. In Sec. VI, by applying the $\widehat{Z}$-box theory, we make a numerical calculation with a model Hamiltonian to assess the present approach. We propose a graphical method and show that it works well for finding the eigenvalues of $H$. A summary of the present study and some remarks are given in the last section. In Appendices A and B the derivatives of the $\widehat{Q}$ box are given for the two recursive solutions, which are necessary for calculating the $\widehat{Z}$ box.

## II. EFFECTIVE-INTERACTION THEORY BY MEANS OF SIMILARITY TRANSFORMATION

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 $H_{\rm eff}$ given in the $P$ space coincide with those of $H$, we call $H_{\rm eff}$ an effective Hamiltonian. In the following, we do not impose any particular conditions on $H$ and states belonging to the $P$ space nor assume degeneracy of their unperturbed energies.

There are various ways of constructing $H_{\rm eff}$. We adopt the following standard one. First we introduce an operator $\omega$ that maps states in the $P$ space and those in the $Q$ space to each other, with the properties [48]

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

$$\omega^n = 0 \quad (n \geqslant 2). \tag{2.2}$$

The operator $\omega$ defines a similarity transformation of $H$,

$$\widetilde{H} = e^{-\omega} H e^{\omega}. \tag{2.3}$$

This reduces to

$$\widetilde{H} = (1-\omega)H(1+\omega) \tag{2.4}$$

by virtue of Eq. (2.2).

The condition that $P\widetilde{H}P$ be a model-space effective Hamiltonian $H_{\rm eff}$ is that $\widetilde{H}$ should be decoupled between the $P$ and $Q$ spaces as

$$Q\widetilde{H}P = 0. \tag{2.5}$$

This condition is rewritten as

$$QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0, \tag{2.6}$$

with the aid of Eqs. (2.1) and (2.4). This equation for $\omega$ was first derived by Okubo [52] in a different way. Once a solution $\omega$ to Eq. (2.6) is given, $H_{\rm eff}$ is written as

$$H_{\rm eff} = PHP + PHQ\omega. \tag{2.7}$$

Dividing $PHP$ into the unperturbed part $PH_0P$ and the interaction $PVP$, we write

$$PHP = PH_0P + PVP. \tag{2.8}$$

The model-space effective interaction $V_{\rm eff}$ is defined as

$$V_{\rm eff} = H_{\rm eff} - PH_0P = PVP + PHQ\omega. \tag{2.9}$$

From the definition of $H_{\rm eff}$ and $V_{\rm eff}$ we see that a central part of determining them is to find a solution for $\omega$ in Eq. (2.6).

Since Eq. (2.6) is a nonlinear matrix equation for $\omega$, it is difficult to find a general solution. The following formal solution, however, has been known and is enough for applications. We rewrite Eq. (2.6) as

$$QHP + QHQ\omega - \omega H_{\rm eff} = 0, \tag{2.10}$$

using Eq. (2.7). Here the eigenvalue equation for $H_{\rm eff}$ is given by

$$H_{\rm eff}|\phi_k\rangle = E_k|\phi_k\rangle. \tag{2.11}$$

If the operator $\omega$ is a solution to Eq. (2.6), 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 $H$. The effective Hamiltonian $H_{\rm eff}$ is not Hermitian in general; the eigenstates $\{|\phi_k\rangle,\ k = 1, 2, \ldots, d\}$ are not orthogonal to each other. Then we introduce the adjoint states $\{\langle\widetilde{\phi}_k|,\ k = 1, 2, \ldots, d\}$ according to the biorthogonality condition

$$\langle\widetilde{\phi}_k|\phi_{k'}\rangle = \delta_{kk'}, \tag{2.12}$$

where $d$ is the dimension of the $P$ space. The projection operator onto the $P$ space is written as

$$P = \sum_{k=1}^{d} |\phi_k\rangle\langle\widetilde{\phi}_k|. \tag{2.13}$$

Then, using Eqs. (2.10)–(2.13), $\omega$ is given by

$$\omega = \sum_{k=1}^{d} \frac{1}{E_k - QHQ} QHP|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{2.14}$$

and from Eq. (2.7) $H_{\rm eff}$ becomes

$$H_{\rm eff} = PHP + \sum_{k=1}^{d} PHQ \frac{1}{E_k - QHQ} QHP|\phi_k\rangle\langle\widetilde{\phi}_k|. \tag{2.15}$$

Here we introduce an operator in the $P$ space called the $\widehat{Q}$ box,

$$\widehat{Q}(E) = PHP + PHQ\frac{1}{E - QHQ}QHP, \tag{2.16}$$

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 [42] and/or the Feshbach [43] forms. In terms of $\widehat{Q}(E)$, $H_{\rm eff}$ is expressed as

$$H_{\rm eff} = \sum_{k=1}^{d} \widehat{Q}(E_k)|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{2.17}$$

from which the following self-consistent equation can be derived:

$$\widehat{Q}(E_k)|\phi_k\rangle = E_k|\phi_k\rangle. \tag{2.18}$$

The $H_{\rm eff}$ in Eq. (2.17) 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. (2.11) coincide with those given by Eq. (2.17), they self-consistently satisfy the iterative equation

$$\widehat{Q}\big(E_k^{(n)}\big)\big|\phi_k^{(n+1)}\big\rangle = E_k^{(n+1)}\big|\phi_k^{(n+1)}\big\rangle, \tag{2.19}$$

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 $E_k^{(n)}$. There have been a lot of studies about the convergence of this iterative method [46–50]. But the condition of convergence is rather complicated and it has been known that only some specific solutions are obtained.

In addition, $\widehat{Q}(E)$ has poles at energies $\{\varepsilon_q\}$, where $\varepsilon_q$ is one of the eigenvalues of $QHQ$,

$$QHQ|q\rangle = \varepsilon_q|q\rangle. \tag{2.20}$$

These singularities of the $\widehat{Q}$ box lead to some difficulties in numerical calculations [51]. These arguments suggest that some further improvements are desired for the $\widehat{Q}$-box method although it has been applied widely to practical problems.

## III. CALCULATION OF THE $\widehat{Q}$ BOX BY MEANS OF RECURRENCE RELATIONS

Most of the effective-interaction theories formulated so far are based on the $\widehat{Q}$ box. The $\widehat{Q}$ box has been calculated via the perturbative expansion methods, but their convergence properties and accuracies have not been well understood yet. This is because, as a matter of fact, it is impossible to solve the eigenvalue problem of $QHQ$ or to calculate the inverse of $(E - QHQ)$ when the dimension of the $Q$ space is huge. The accuracy of the $\widehat{Q}$ box determines that of $H_{\rm eff}$ and $V_{\rm eff}$, because errors that arise in the calculations of operators and/or matrices in the $P$ space with small dimension are considered to be negligible.

In the following subsections we describe a method of how to calculate accurately and efficiently the $\widehat{Q}$ box. We first transform $H$ to a block-tridiagonal form. With this transformed Hamiltonian we derive a set of coupled equations for determining the operator $\omega$. We shall show that these

coupled equations can be solved in two ways by introducing two types of recurrence relations. The properties of two solutions for the $\widehat{Q}$ box are discussed.

### A. Block tridiagonalization of Hamiltonian

We transform the Hamiltonian $H$ into a tractable form by changing basis vectors. First we introduce

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

The $Y_P$ is an operator in the $P$ space, which is Hermitian and positive semidefinite, that is, $y_k^{(1)} \geqslant 0$ 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 $\{|p_k\rangle,\ k = 1, 2, \ldots, d_1\}$ with nonzero eigenvalues, we define normalized vectors $\{|q_k^{(1)}\rangle\}$ in the $Q$ space as

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

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

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

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

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

then we have

$$QHP = Q_1HP \tag{3.7}$$

which leads to

$$\overline{Q}_1HP = 0. \tag{3.8}$$

Thus the image $H(P)$ by the mapping $H$ is given as a sum of the $P$ and $Q_1$ spaces as depicted in Fig. 1.

Next, a similar manipulation replacing $P$ and $Q$ with $Q_1$ and $\overline{Q}_1$, respectively, leads to another orthogonal system. We introduce

$$Y_{Q_1} = Q_1H\overline{Q}_1 \times \overline{Q}_1HQ_1, \tag{3.9}$$

and write its eigenvalue equation as

$$Y_{Q_1}\left|q_k^{\prime(1)}\right\rangle = y_k^{(2)}\left|q_k^{\prime(1)}\right\rangle. \tag{3.10}$$

The eigenvectors $\{|q_k^{\prime(1)}\rangle\}$ belong to the $Q_1$ space and accordingly are given as linear combinations of $\{|q_k^{(1)}\rangle,\ k = 1, 2, \ldots, d_1\}$ in Eq. (3.3). Suppose also that $d_2$ eigenvalues are nonzero among $\{y_k^{(2)}\}$. New orthogonal bases

$$\left|q_k^{(2)}\right\rangle = \frac{1}{\sqrt{y_k^{(2)}}} \overline{Q}_1HQ_1\left|q_k^{\prime(1)}\right\rangle \quad (k = 1, 2, \ldots, d_2) \tag{3.11}$$

are derived. The $d_2$-dimensional subspace $Q_2$ is defined by them and the projection operator onto the $Q_2$ space is expressed as

$$Q_2 = \sum_{k=1}^{d_2} \left|q_k^{(2)}\right\rangle\left\langle q_k^{(2)}\right|. \tag{3.12}$$

The projection operator $Q_2$ has the properties

$$Q_2HP = 0, \tag{3.13}$$
$$\overline{Q}_1HQ_1 = Q_2HQ_1, \tag{3.14}$$
$$\overline{Q}_2HQ_1 = 0, \tag{3.15}$$

where $\overline{Q}_2$, the complementary space to $Q_1 + Q_2$ in the $Q$ space, is written as

$$\overline{Q}_2 = Q - Q_1 - Q_2. \tag{3.16}$$

Repeating these manipulations leads to the following: Decompose the $Q$ space as

$$Q = Q_1 + Q_2 + \cdots + Q_n + \cdots. \tag{3.17}$$

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

$$Q_m = \sum_{k=1}^{d_m} \left|q_k^{(m)}\right\rangle\left\langle q_k^{(m)}\right|. \tag{3.18}$$

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

$$Y_{Q_{m-1}} = Q_{m-1}H\overline{Q}_{m-1} \times \overline{Q}_{m-1}HQ_{m-1} \tag{3.19}$$

with

$$\overline{Q}_{m-1} = Q - (Q_1 + Q_2 + \cdots + Q_{m-1}). \tag{3.20}$$

Its eigenvalue equation is

$$Y_{Q_{m-1}}\left|q_k^{\prime(m-1)}\right\rangle = y_k^{(m)}\left|q_k^{\prime(m-1)}\right\rangle. \tag{3.21}$$

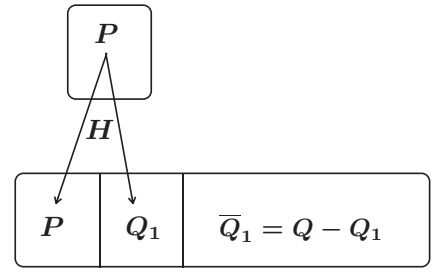


FIG. 1. The image $H(P)$ by the mapping $H$. Here, $H$ denotes the Hamiltonian, $P$ the model space, and $Q_1$ the $Q$-space part of the image $H(P)$.

In general new orthogonal bases

$$\left|q_k^{(m)}\right\rangle = \frac{1}{\sqrt{y_k^{(m)}}}\overline{Q}_{m-1} H Q_{m-1}\left|q_k^{\prime(m-1)}\right\rangle \tag{3.22}$$

are derived from the eigenvectors $\{|q_k^{\prime(m-1)}\rangle\}$ with nonzero eigenvalues $\{y_k^{(m)}\}$. They span the subspace $Q_m$. When all the eigenvalues $\{y_k^{(m)}\}$ are zero, the procedure ends because the eigenstates of $H$ reside in the subspace $P + Q_1 + Q_2 + \cdots + Q_{m-1}$. Here we note that we are not interested in any eigenstates that are decoupled from the states in the $P$ space. With the projection operators $Q_m$ and $Q_{m-1}$ we obtain, from Eq. (3.22), an expression written as

$$Q_m H Q_{m-1} = \sum_{k=1}^{d_m} \sqrt{y_k^{(m)}}\left|q_k^{(m)}\right\rangle\left\langle q_k^{\prime(m-1)}\right|. \tag{3.23}$$

We conclude from the above discussion that

$$PHQ_m = Q_m HP = 0 \quad (m \geqslant 2), \tag{3.24}$$

$$Q_m H Q_{m+k} = Q_{m+k} H Q_m = 0 \quad (k \geqslant 2) \tag{3.25}$$

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

$$H = \begin{pmatrix} PHP & PHQ_1 & 0 & 0 & \cdots \\ Q_1HP & Q_1HQ_1 & Q_1HQ_2 & 0 & \cdots \\ 0 & Q_2HQ_1 & Q_2HQ_2 & Q_2HQ_3 & \cdots \\ 0 & 0 & Q_3HQ_2 & Q_3HQ_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \tag{3.26}$$

where each block matrix is at most $d$ dimensional. Thus the image $H(Q_m)$ by the mapping $H$ is a sum of adjacent subspaces $Q_{m-1}$, $Q_m$, and $Q_{m+1}$ as depicted in Fig. 2.

From Figs. 1 and 2 it is easy to see that the image of the mapping $H$ of the $P$ space becomes

$$H(P) = P + Q_1. \tag{3.27}$$

The image of the successive mapping is given by

$$H^2(P) = H(P + Q_1) = P + Q_1 + Q_2 \tag{3.28}$$

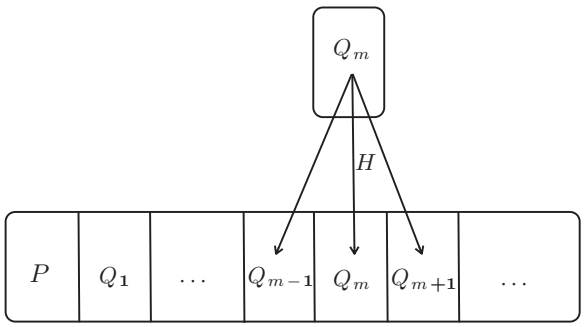


FIG. 2. The image $H(Q_m)$ by the mapping $H$ for $m \geqslant 2$. The $Q_{m-1}$, $Q_m$, and $Q_{m+1}$ are the subspaces of the $Q$ space which constitute the image $H(Q_m)$.

and generally

$$H^m(P) = P + Q_1 + Q_2 + \cdots + Q_m. \tag{3.29}$$

The above relations mean that the mapping $H^m(P)$ generates an additional subspace $Q_m$. The sequence $\{P, H(P), \ldots, H^m(P)\}$ is called the Krylov subspaces [13]. It may be clear that the subspaces $\{P, Q_1, \ldots, Q_m\}$ determine a unique block-tridiagonal form of $H$. In this sense the subspaces introduced in the present approach are essentially the same as those of Krylov. However, the basis states of each subspace $Q_k$ are ambiguous. Determination of the basis states depends on the purpose; that is, what problem we want to solve after the block tridiagonalization of the Hamiltonian. We show, in the later sections, that the basis states introduced in the present study are useful for the formulation of the effective-interaction theory.

### B. Expression of the $\widehat{Q}$ box in terms of the $\omega$ operator

Here we define two operators

$$e(E) = Q(E - H)Q, \tag{3.30}$$

$$\chi(E) = \frac{1}{e(E)}QHP = \frac{1}{E - QHQ}QHP. \tag{3.31}$$

In terms of $\chi(E)$, the $\widehat{Q}$ box in Eq. (2.16) is expressed as

$$\widehat{Q}(E) = PHP + PHQ\chi(E), \tag{3.32}$$

and the solution $\omega$ in Eq. (2.14) to the decoupling equation (2.6) is given by

$$\omega = \sum_{k=1}^{d} \chi(E_k)|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{3.33}$$

where $|\phi_k\rangle$ and $\langle\widetilde{\phi}_k|$ have been defined in Eqs. (2.11) and (2.12). Consequently calculating $\widehat{Q}(E)$ reduces to calculating $\chi(E)$. When the $Q$ space is decomposed as in Eq. (3.17), also $\chi(E)$ is as

$$\chi(E) = \chi_1(E) + \chi_2(E) + \cdots + \chi_n(E) + \cdots, \tag{3.34}$$

where

$$\chi_n(E) = Q_n\,\chi(E)P. \tag{3.35}$$

Coupled equations for $\{\chi_n(E)\}$

$$Q_1\,e(E)\{\chi_1(E) + \chi_2(E)\} = Q_1 HP, \tag{3.36}$$

$$Q_2\,e(E)\{\chi_1(E) + \chi_2(E) + \chi_3(E)\} = 0, \tag{3.37}$$

$$\vdots$$

$$Q_n\,e(E)\{\chi_{n-1}(E) + \chi_n(E) + \chi_{n+1}(E)\} = 0, \tag{3.38}$$

$$\vdots$$

are derived from Eq. (3.31) using Eqs. (3.7), (3.24), and (3.25). Since the $\widehat{Q}$ box is expressed as

$$\widehat{Q}(E) = PHP + PHQ_1\chi_1(E) \tag{3.39}$$

by using Eq. (3.7), calculating the $\widehat{Q}$ box reduces to calculating $\chi_1(E)$.

### C. Expansion in terms of continued fraction

We show that the $\widehat{Q}$ box is expanded by a continued fraction [53] of small-dimensional matrices by solving Eqs. (3.36)–(3.38). We assume $\chi_m(E) = 0$ for $m \geqslant 2$; then we have

$$\chi_1(E) = \frac{1}{e_1(E)} Q_1 H P \tag{3.40}$$

from Eq. (3.36), where

$$e_1(E) = Q_1(E - H)Q_1. \tag{3.41}$$

Hereafter we use the notation

$$e_m(E) = Q_m(E - H)Q_m. \tag{3.42}$$

The solution (3.40) gives the $\widehat{Q}$ box in the first approximation as

$$\widehat{Q}^{(1)}(E) = PHP + PHQ_1 \frac{1}{e_1(E)} Q_1 H P. \tag{3.43}$$

Next we have

$$\chi_2(E) = \frac{1}{e_2(E)} Q_2 H Q_1 \chi_1(E) \tag{3.44}$$

from Eq. (3.37) by assuming $\chi_m(E) = 0$ for $m \geqslant 3$. Substituting this into Eq. (3.36) leads to

$$\chi_1(E) = \frac{1}{e_1(E) - Q_1 H Q_2 \frac{1}{e_2(E)} Q_2 H Q_1} Q_1 H P, \tag{3.45}$$

and then the $\widehat{Q}$ box is given as

$$\widehat{Q}^{(2)}(E) = PHP + PHQ_1 \frac{1}{e_1(E) - Q_1 H Q_2 \frac{1}{e_2(E)} Q_2 H Q_1} Q_1 H P \tag{3.46}$$

in the second approximation. Repeating similar manipulations, we finally have a general form

$$\widehat{Q}(E) = PHP + PHQ_1 \frac{1}{e_1 - H_{12} \frac{1}{e_2 - H_{23} \frac{1}{e_3 - H_{34} \frac{1}{e_4 - \cdots} H_{43}} H_{32}} H_{21}} Q_1 H P \tag{3.47}$$

with $e_m = e_m(E)$ and

$$H_{ij} = Q_i H Q_j. \tag{3.48}$$

Here we consider a case in which the $Q$ space for a system of interest is well described by finite number of subspaces. We denote the maximum of $n$ by $N$ in Eq. (3.17). We introduce $\{\widetilde{e}_n(E)\}$ given through a descending recurrence relation starting from $n = N$ as

$$\widetilde{e}_{n-1}(E) = e_{n-1}(E) - H_{n-1,n} \frac{1}{\widetilde{e}_n(E)} H_{n,n-1}, \tag{3.49}$$

where we define

$$\widetilde{e}_N(E) = Q_N(E - H)Q_N. \tag{3.50}$$

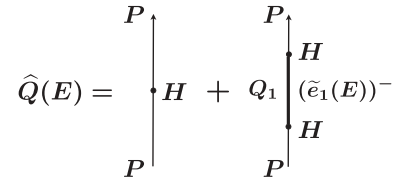


FIG. 3. Diagrammatical expression of the $\widehat{Q}$ box in terms of the renormalized propagator $[\widetilde{e}_1(E)]^{-1}$ which is composed of the continued fraction. The $H$ denotes the Hamiltonian. The $P$ and $Q_1$ are the projection operators onto the model space and the $Q_1$ space, respectively, where the $Q_1$ space is the $Q$-space part of the image $H(P)$. The thick line expresses the propagation of $Q_1$-space states with the propagator $[\widetilde{e}_1(E)]^{-1}$.

From Eq. (3.49) we have a sequence $\widetilde{e}_{N-1}(E)$, $\widetilde{e}_{N-2}(E)$, ..., and $\widetilde{e}_1(E)$. Then the $\widehat{Q}$ box is expressed as

$$\widehat{Q}(E) = PHP + PHQ_1 \frac{1}{\widetilde{e}_1(E)} Q_1 H P. \tag{3.51}$$

Diagrammatical expression of $\widehat{Q}(E)$ is shown in Fig. 3. It is a remarkable fact that the above result for the $\widehat{Q}$ box indicates the existence of the renormalized inverse propagator $\widetilde{e}_1(E)$ such that the $\widehat{Q}$ box can be represented by a sum of only two terms, namely, the unperturbed part and the second-order term.

If the dimension of the $Q$ space is finite, the number of the subspaces $\{Q_m\}$ is also finite and the $\widehat{Q}$ box given in Eq. (3.51) is exact. On the other hand, if the dimension of the $Q$ space is infinite, the number of the subspaces $\{Q_m\}$ is, in general, infinite. For this case we introduce a truncation of the $Q$ space. We consider a finite-dimensional subspace $Q_1 + Q_2 + \cdots + Q_N$, where the subspaces $\{Q_m,\ 1 \leqslant m \leqslant N\}$ lead to a block-tridiagonal form of $H$ as in Eq. (3.26). The operator $\widetilde{e}_1(E)$ that is determined through the recurrence relation in Eq. (3.49) starting with $n = N$ is a function of $N$ and we write it as $\widetilde{e}_1^{(N)}(E)$. If $\widetilde{e}_1^{(N)}(E)$ converges as $N$ tends to infinity, we can write the $\widehat{Q}$ box as

$$\widehat{Q}(E) = PHP + PHQ_1 \frac{1}{\widetilde{e}_1^{(\infty)}(E)} Q_1 H P, \tag{3.52}$$

where

$$\widetilde{e}_1^{(\infty)}(E) = \lim_{N \to \infty} \widetilde{e}_1^{(N)}(E). \tag{3.53}$$

We discuss the meaning of Eq. (3.52) in more detail. We consider an application of the present formalism to the calculation of the effective interaction between two valence nucleons outside a core, such as $^{16}$O. Many of the numerical calculations have shown that the second-order diagrams make dominant contributions [54,55] and the third- and higher-order terms are less important. It should be pointed out that, in many of such calculations, the experimental single-particle (s.p.) energies have been employed. As shown in Eqs. (3.51) and (3.52) the $\widehat{Q}$ box can be expressed finally as the second-order diagrams with the unchanged (not renormalized) vertex $PHQ_1$ ($=PHQ$) and the renormalized inverse propagator $\widetilde{e}_1(E)$. This fact means that, if we use a proper $\widetilde{e}_1(E)$, the exact $\widehat{Q}$ box can be given by the second-order term. There is a

possibility that $\widetilde{e}_1(E)$ can be replaced approximately with the energy denominator determined from the experimental s.p. energies. We mention that the expression of the $\widehat{Q}$ box in Eqs. (3.51) or (3.52) would give an explanation for the reason why the second-order diagrams make dominant contributions and lead to fairly good agreement with the experimental spectra.

### D. Expansion in terms of renormalized vertices and propagators

We here consider a method of calculation by an ascending recurrence relation for $\{\chi_n(E)\}$ and derive another solution for the $\widehat{Q}$ box. By using Eqs. (3.30) and (3.48), the coupled equations Eqs. (3.36)–(3.38) for the operators $\{\chi_n(E)\}$ are written as

$$e_1(E)\chi_1(E) = H_{10} + H_{12}\chi_2(E), \tag{3.54}$$
$$e_2(E)\chi_2(E) = H_{21}\chi_1(E) + H_{23}\chi_3(E), \tag{3.55}$$
$$\vdots$$
$$e_n(E)\chi_n(E) = H_{n,n-1}\chi_{n-1}(E) + H_{n,n+1}\chi_{n+1}(E), \tag{3.56}$$
$$\vdots$$

with

$$H_{10} = Q_1 H P. \tag{3.57}$$

Equations (3.56) is a linear relation of three operators $\chi_{n-1}$, $\chi_n$, and $\chi_{n+1}$, which can be cast into those of two operators as follows: First we rewrite (3.54) as

$$\chi_1(E) = \alpha_1(E) + \beta_1(E)\chi_2(E) \tag{3.58}$$

with

$$\alpha_1(E) = \frac{1}{e_1(E)} H_{10}, \tag{3.59}$$
$$\beta_1(E) = \frac{1}{e_1(E)} H_{12}. \tag{3.60}$$

By substituting this into Eq. (3.55), $\chi_2(E)$ is expressed as linear with $\chi_3(E)$,

$$\chi_2(E) = \alpha_2(E) + \beta_2(E)\chi_3(E), \tag{3.61}$$

where

$$\alpha_2(E) = \frac{1}{e_2(E) - H_{21}\frac{1}{e_1(E)}H_{12}} H_{21}\frac{1}{e_1(E)}H_{10} = \frac{1}{e_2(E) - H_{21}\beta_1(E)} H_{21}\alpha_1(E), \tag{3.62}$$
$$\beta_2(E) = \frac{1}{e_2(E) - H_{21}\frac{1}{e_1(E)}H_{12}} H_{23} = \frac{1}{e_2(E) - H_{21}\beta_1(E)} H_{23}. \tag{3.63}$$

In general, we define the operators $\alpha_n(E)$ and $\beta_n(E)$ that obey the following ascending recurrence relations:

$$\alpha_n(E) = \frac{1}{e_n(E) - H_{n,n-1}\beta_{n-1}(E)} H_{n,n-1}\alpha_{n-1}(E), \tag{3.64}$$
$$\beta_n(E) = \frac{1}{e_n(E) - H_{n,n-1}\beta_{n-1}(E)} H_{n,n+1}. \tag{3.65}$$

We then have a linear relation

$$\chi_n(E) = \alpha_n(E) + \beta_n(E)\chi_{n+1}(E). \tag{3.66}$$

Equations (3.64) and (3.65) determine $\{\alpha_n(E), \beta_n(E),\ n = 1, 2, \dots\}$ with the initial values $\alpha_1(E)$ and $\beta_1(E)$ in Eqs. (3.59) and (3.60), respectively. We finally have a solution for $\chi_1(E)$ as

$$\begin{aligned}\chi_1(E) &= \alpha_1(E) + \beta_1(E)\alpha_2(E) + \cdots \\ &\quad + \beta_1(E)\beta_2(E)\cdots\beta_{n-1}(E)\alpha_n(E) + \cdots \\ &= \sum_{k=1}^{\infty}\left\{\prod_{m=1}^{k-1}\beta_m(E)\right\}\alpha_k(E).\end{aligned} \tag{3.67}$$

Consequently the $\widehat{Q}$ box is given by

$$\widehat{Q}(E) = PHP + PHQ_1\left[\sum_{k=1}^{\infty}\left\{\prod_{m=1}^{k-1}\beta_m(E)\right\}\alpha_k(E)\right]. \tag{3.68}$$

In order to rewrite $\{\alpha_n(E)\}$, $\{\beta_n(E)\}$, and the $\widehat{Q}$ box in terms of $\{e_i(E)\}$ and $\{H_{ij}\}$, we introduce another inverse propagator $\overline{e}_m(E)$ defined through the recurrence relation

$$\overline{e}_m(E) = e_m(E) - H_{m,m-1}\frac{1}{\overline{e}_{m-1}(E)}H_{m-1,m} \tag{3.69}$$

with the initial value

$$\overline{e}_1(E) = e_1(E) = Q_1(E - H)Q_1. \tag{3.70}$$

We note that $\overline{e}_m(E)$ in Eq. (3.69) obeys an ascending recurrence relation, which differs from $\widetilde{e}_m(E)$ in Eq. (3.49). In terms of $\{\overline{e}_m(E)\}$, the operators $\{\alpha_n(E)\}$ and $\{\beta_n(E)\}$ are written as

$$\alpha_1(E) = \frac{1}{\overline{e}_1(E)} H_{10}, \tag{3.71}$$
$$\alpha_2(E) = \frac{1}{\overline{e}_2(E)} H_{21}\frac{1}{\overline{e}_1(E)}H_{10}, \tag{3.72}$$
$$\vdots$$
$$\alpha_n(E) = \frac{1}{\overline{e}_n(E)} H_{n,n-1}\frac{1}{\overline{e}_{n-1}(E)}H_{n-1,n-2}\cdots H_{21}\frac{1}{\overline{e}_1(E)}H_{10}, \tag{3.73}$$
$$\vdots$$
$$\beta_1(E) = \frac{1}{\overline{e}_1(E)} H_{12}, \tag{3.74}$$
$$\beta_2(E) = \frac{1}{\overline{e}_2(E)} H_{23}, \tag{3.75}$$
$$\vdots$$

$$\beta_n(E) = \frac{1}{\bar{e}_n(E)} H_{n,n+1}, \tag{3.76}$$
$$\vdots$$

Then the $\widehat{Q}$ box in Eq. (3.68) is expressed explicitly as

$$\begin{aligned}\widehat{Q}(E) = {} & PHP + H_{01}\frac{1}{\bar{e}_1(E)}H_{10} + H_{01}\frac{1}{\bar{e}_1(E)}H_{12}\frac{1}{\bar{e}_2(E)} \\ & \times H_{21}\frac{1}{\bar{e}_1(E)}H_{10} + \cdots + H_{01}\frac{1}{\bar{e}_1(E)}H_{12}\cdots H_{n-1,n} \\ & \times \frac{1}{\bar{e}_n(E)}H_{n,n-1}\cdots H_{21}\frac{1}{\bar{e}_1(E)}H_{10} + \cdots . \end{aligned} \tag{3.77}$$

A simpler expression of the $\widehat{Q}$ box can be obtained by utilizing $\{\overline{H}_k(E)\}$ defined through

$$\begin{aligned}\overline{H}_k(E) &= H_{01}\frac{1}{\bar{e}_1(E)}H_{12}\frac{1}{\bar{e}_2(E)}H_{23}\cdots\frac{1}{\bar{e}_{k-1}(E)}H_{k-1,k} \\ &= \overline{H}_{k-1}(E)\frac{1}{\bar{e}_{k-1}(E)}H_{k-1,k} \end{aligned} \tag{3.78}$$

with the initial value

$$\overline{H}_1(E) = PHQ_1. \tag{3.79}$$

The $\overline{H}_k(E)$ interconnecting the $P$ and $Q_k$ spaces is a $d \times d_k$ matrix. The $\widehat{Q}(E)$ in Eq. (3.77) is further reduced to

$$\begin{aligned}\widehat{Q}(E) &= PHP + \overline{H}_1(E)\frac{1}{\bar{e}_1(E)}\overline{H}_1^{\dagger}(E) + \cdots \\ &\quad + \overline{H}_n(E)\frac{1}{\bar{e}_n(E)}\overline{H}_n^{\dagger}(E) + \cdots \\ &= PHP + \sum_{k=1}^{\infty}\overline{H}_k(E)\frac{1}{\bar{e}_k(E)}\overline{H}_k^{\dagger}(E). \end{aligned} \tag{3.80}$$

This expression can be interpreted as that the $\widehat{Q}$ box is given by a sum up to second order in the usual perturbation theory as schematically depicted in Fig. 4 in terms of the renormalized inverse propagators $\{\bar{e}_k(E)\}$ and the renormalized vertices $\{\overline{H}_k(E)\}$.

Equation (3.80) shows clearly that there exist the renormalized inverse propagators $\{\bar{e}_k(E)\}$ and the renormalized vertices $\{\bar{H}_k(E)\}$ such that the $\widehat{Q}$ box can be represented by a second-order perturbation form which is the lowest-order interaction terms.

If a system with a Hamiltonian $H$ can be well described in a finite-dimensional space, the $\widehat{Q}$ box in Eq. (3.77) is given by a sum of a finite number of terms and should coincide with the result in Eq. (3.51). Compairing two solutions for the $\widehat{Q}$ box, we have an expression of the renormalized propagator $\{\widetilde{e}_1(E)\}^{-1}$ as

$$\begin{aligned}&\frac{1}{\widetilde{e}_1(E)} \\ &\quad = \frac{1}{\bar{e}_1(E)} + \frac{1}{\bar{e}_1(E)}H_{12}\frac{1}{\bar{e}_2(E)}H_{21}\frac{1}{\bar{e}_1(E)} + \cdots \\ &\qquad + \frac{1}{\bar{e}_1(E)}H_{12}\cdots H_{N-1,N}\frac{1}{\bar{e}_N(E)}H_{N,N-1}\cdots H_{21}\frac{1}{\bar{e}_1(E)}, \end{aligned} \tag{3.81}$$

where $N$ is the number of the subspaces $\{Q_k\}$. The above $\widetilde{e}_1(E)$ can be a solution to the recursive equation (3.49) and gives an expansion formula in terms of $\{H_{k-1,k}\}$, $\{H_{k,k-1}\}$, and $\{\bar{e}_k(E)\}$ which are defined with the subspaces $\{Q_k\}$. Recall that the calculation of the $\widehat{Q}$ box is reduced to that of $\widetilde{e}_1(E)$ as in Eq. (3.51). The expression of $\{\widetilde{e}_1(E)\}^{-1}$ in Eq. (3.81) makes it clear how the subspaces $\{Q_k\}$ contribute to $\widetilde{e}_1(E)$ and, equivalently, to the $\widehat{Q}$ box. Therefore, when we consider introducing an approximation in a practical problem, Eq. (3.81) would provide us with a basic formula for $\{\widetilde{e}_1(E)\}^{-1}$.

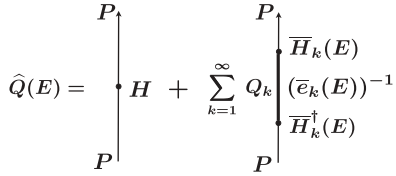


FIG. 4. Diagrammatical expression of the $\widehat{Q}$ box in terms of the renormalized vertices $\overline{H}_k(E)$ and the propagators $[\bar{e}_k(E)]^{-1}$. Other notations are the same as in Fig. 3.

## IV. RECURSIVE SOLUTION FOR THE $\chi(E)$ OPERATOR

We here discuss how to calculate the operator $\chi_n(E)$ in Eq. (3.35) which are necessary for obtaining a true eigenstate, namely, $|\Phi_k\rangle$ with the eigenvalue $E = E_k$. The basic equations for determining $\{\chi_n(E)\}$ have been given in Secs. III B and III D. In the similarity-transformation theory for the effective interaction, the relationship between $|\Phi_k\rangle$ and the model-space eigenstate $|\phi_k\rangle$ is

$$|\Phi_k\rangle = e^{\omega}|\phi_k\rangle = |\phi_k\rangle + \omega|\phi_k\rangle. \tag{4.1}$$

Using Eq. (3.33) for $\omega$ in terms of $\chi(E_k)$, $|\Phi_k\rangle$ is also expressed as

$$|\Phi_k\rangle = |\phi_k\rangle + \chi(E_k)|\phi_k\rangle. \tag{4.2}$$

Therefore, if we want to obtain $|\Phi_k\rangle$, we have to solve $\chi(E_k)$. We decompose $\chi(E_k)$ into $\{\chi_n(E_k)\}$ as in Eq. (3.34). The sequence $\{\chi_1(E_k), \chi_2(E_k), \ldots\}$ obeys Eqs. (3.54)–(3.56). From Eq. (3.56) the following recurrence relation is obtained for $\{\chi_n(E_k)\}$;

$$\begin{aligned}&\chi_{n+1}(E_k) \\ &\quad = K_{n+1,n}\{e_n(E_k)\chi_n(E_k) - H_{n,n-1}\chi_{n-1}(E_k)\} \quad (n \geqslant 2), \end{aligned} \tag{4.3}$$

where $K_{n+1,n}$ is defined as

$$K_{n+1,n} = \sum_{k=1}^{d_{n+1}} \frac{1}{\sqrt{y_k^{(n+1)}}} \left|q_k^{(n+1)}\right\rangle\left\langle q'^{(n)}_k\right|. \tag{4.4}$$

It is easy to see, using Eqs. (3.23) and (3.48) for $H_{n,n+1}$,

$$K_{n+1,n} \times H_{n,n+1} = Q_{n+1}, \tag{4.5}$$

from which Eq. (4.3) is derived. For the calculation of $\{\chi_n(E_k)\}$ with $n \geqslant 3$, $\chi_1(E_k)$ and $\chi_2(E_k)$ are necessary as initial values.

In this stage we suppose that $\widehat{Q}(E_k)$ is given beforehand and use Eq. (3.39) to obtain

$$\chi_1(E_k) = K_{10}(\widehat{Q}(E_k) - PHP) \tag{4.6}$$

with

$$K_{10} = \sum_{k=1}^{d_1} \frac{1}{\sqrt{y_k^{(1)}}} |q_k^{(1)}\rangle\langle p_k|, \tag{4.7}$$

where $\langle p_k|$ and $|q_k^{(1)}\rangle$ are given in Eqs. (3.2) and (3.3), respectively. In a similar manner, the operator $\chi_2(E_k)$ is solved, using Eq. (3.54), as

$$\chi_2(E_k) = K_{21}\{e_1(E_k)\chi_1(E_k) - H_{1,0}\} \tag{4.8}$$

with

$$K_{21} = \sum_{k=1}^{d_2} \frac{1}{\sqrt{y_k^{(2)}}} |q_k^{(2)}\rangle\langle q'^{(1)}_k|, \tag{4.9}$$

where $\langle q'^{(1)}_k|$ and $|q_k^{(2)}\rangle$ are given in Eqs. (3.10) and (3.11), respectively. Substituting $\chi_1(E_k)$ and $\chi_2(E_k)$, the sequence $\chi_3(E_k)$, $\chi_4(E_k)$, $\cdots$ are obtained from the recurrence relation in Eq. (4.3).

The eigenstate $|\Phi_k\rangle$ of $H$ with the eigenvalue $E_k$ is finally given by

$$|\Phi_k\rangle = |\phi_k\rangle + \sum_n \chi_n(E_k)|\phi_k\rangle. \tag{4.10}$$

The usual normalization in the effective-interaction theory is $\langle\phi_k|\phi_{k'}\rangle = \delta_{k,k'}$. Therefore, the normalized true eigenstate denoted by $|\Psi_k\rangle$ is given by

$$|\Psi_k\rangle = \frac{1}{N_k}|\Phi_k\rangle, \tag{4.11}$$

where the normalization factor $N_k$ is

$$N_k = \sqrt{1 + \sum_n \langle\phi_k|\chi_n^\dagger(E_k)\chi_n(E_k)|\phi_k\rangle}. \tag{4.12}$$

## V. THE $\widehat{Z}$-BOX METHOD AND EFFECTIVE HAMILTONIAN

The $\widehat{Z}$ box has been defined in the previous paper [51] as

$$\widehat{Z}(E) = \frac{1}{1 - \widehat{Q}_1(E)}[\widehat{Q}(E) - E\,\widehat{Q}_1(E)] \tag{5.1}$$

with

$$\widehat{Q}_1(E) = \frac{d\widehat{Q}(E)}{dE} = -PHQ\frac{1}{(E - QHQ)^2}QHP, \tag{5.2}$$

in order to overcome some defects that inevitably accompany the $\widehat{Q}$-box approach. The $\widehat{Z}$ box has the following properties:

(i) The operator

$$H_{\rm eff} = \sum_{k=1}^{d} \widehat{Z}(E_k)|\phi_k\rangle\langle\widetilde{\phi}_k|, \tag{5.3}$$

which is obtained by replacing $\widehat{Q}(E)$ in Eq. (2.17) with $\widehat{Z}(E)$, can be an effective Hamiltonian if $\{E_k,\ k = 1, 2, \ldots, d\}$ are the eigenvalues of $H$. Therefore, $\widehat{Z}(E_k)$ satisfies the self-consistent equation

$$\widehat{Z}(E_k)|\phi_k\rangle = E_k|\phi_k\rangle. \tag{5.4}$$

(ii) The derivative of $\widehat{Z}(E)$ is given by

$$\frac{d\widehat{Z}(E)}{dE} = \frac{2}{1 - \widehat{Q}_1(E)}\widehat{Q}_2(E)[\widehat{Z}(E) - EP] \tag{5.5}$$

with

$$\widehat{Q}_2(E) = \frac{1}{2!}\frac{d^2\widehat{Q}(E)}{dE^2} = PHQ\frac{1}{(E - QHQ)^3}QHP. \tag{5.6}$$

Then

$$\left.\frac{d\widehat{Z}(E)}{dE}\right|_{E=E_k}|\phi_k\rangle = 0 \tag{5.7}$$

holds for the eigenvalue $E_k$ and the corresponding eigenstate $|\phi_k\rangle$ of $H_{\rm eff}$.

(iii) For the eigenvalue $\varepsilon_q$ of $QHQ$ determined by Eq. (2.20), $\widehat{Z}(\varepsilon_q)$ satisfies the self-consistent equation

$$\widehat{Z}(\varepsilon_q)|\mu_q\rangle = \varepsilon_q|\mu_q\rangle. \tag{5.8}$$

Here we note that $|\mu_q\rangle$ belongs to the $P$ space.

(iv) Contrary to Eq. (5.7),

$$\left.\frac{d\widehat{Z}(E)}{dE}\right|_{E=\varepsilon_q}|\mu_q\rangle = 2|\mu_q\rangle \tag{5.9}$$

holds for the derivative of $\widehat{Z}(E)$ at $E = \varepsilon_q$.

These properties lead to the conclusions that $\widehat{Z}(E)$ is finite and differentiable even at $E = \varepsilon_q$, a pole of $\widehat{Q}(E)$. Although $E = \varepsilon_q$ is also a solution of the self-consistent equation for $\widehat{Z}(E)$, it can be easily discriminated from true eigenvalues $\{E_k\}$ of $H$ with the aid of their derivatives in Eqs. (5.7) and (5.9). The $\widehat{Z}$-box method has been applied recently to a realistic calculation of the effective interaction by Coraggio *et al.* [36].

In order to calculate the $\widehat{Z}$ box we need the first and second derivatives of the $\widehat{Q}$ box. These derivatives can be calculated analytically and are derived in Appendices A and B corresponding to two expressions of the $\widehat{Q}$ box given in Secs. III C and III D, respectively.

## VI. MODEL CALCULATION

### A. Graphical method for eigenvalues of $H$

We shall solve the eigenvalue problem for the Hamiltonian $H$ in the framework of the $\widehat{Z}$-box theory. We note that the $\widehat{Z}$ box is a $d$-dimensional operator acting in the $P$ space and has $d$ eigenvalues. We have assumed that the operator $\widehat{Z}(E)$ for an arbitrary energy variable $E$ has $d$ different eigenvalues. In the present calculation we do not discuss the case that $\widehat{Z}(E)$ has some degenerate eigenvalues. The eigenvalues of $\widehat{Z}(E)$ are

functions of $E$. We write the eigenvalue equation for $\widehat{Z}(E)$ as

$$\widehat{Z}(E)|\zeta_k\rangle = F_k(E)|\zeta_k\rangle \quad (k = 1, 2, \ldots, d). \tag{6.1}$$

The above eigenvalue equation defines $d$ functions $\{F_k(E),\ k = 1, 2, \ldots, d\}$. We label $\{F_k(E)\}$ in order of energy as $F_1(E) < F_2(E) < \cdots < F_d(E)$. From Eq. (5.4) we see that the solutions for the eigenvalues of $H$ can be obtained by solving

$$F_k(E) = E. \tag{6.2}$$

As shown in the previous section, Eq. (5.4) has two kinds of solutions, namely, $E = E_i$ and $E = \varepsilon_j$, where $E_i$ and $\varepsilon_j$ are the eigenvalues of $H$ and $QHQ$, respectively. We distinguish the eigenvalues $\{\varepsilon_j\}$ from $\{E_i\}$ according to the condition that the energy derivative $d\widehat{Z}/dE$ takes different values for $E = E_i$ and $E = \varepsilon_j$. We define functions $\{F'_k(E),\ k = 1, 2, \ldots, d\}$ as

$$F'_k(E) = \left\langle \zeta_k \left| \frac{d\widehat{Z}}{dE} \right| \zeta_k \right\rangle, \tag{6.3}$$

where $|\zeta_k\rangle$ is the eigenstate given in Eq. (6.1). The functions $\{F'_k(E)\}$ take the values

$$F'_k(E) = 0 \quad \text{for} \quad E = E_i, \tag{6.4}$$

$$F'_k(E) = 2 \quad \text{for} \quad E = \varepsilon_j. \tag{6.5}$$

From the above properties of $\{F'_k(E)\}$ we see that the eigenvalues $\{E_i\}$ of $H$ can be obtained by calculating the solutions satisfying Eqs. (6.2) and (6.4) simultaneously. A simple expression of the equation to be solved may be written as

$$g_k(E) = \left\{ \frac{F_k(E) - E}{F_0} \right\}^2 + \{F'_k(E)\}^2 = 0, \tag{6.6}$$

where $F_0$ is a parameter chosen suitably such that the two terms on the right-hand side take values of the same order of magnitude.

The solutions to Eq. (6.6) can be obtained by a graphical method. We define a function $f_k(E)$ as

$$f_k(E) = \frac{1}{g_k(E) + \Delta^2}, \tag{6.7}$$

where $\Delta$ is a small number. The function $f_k(E)$ has the properties

$$\lim_{E \to E_i} f_k(E) = \frac{1}{\Delta^2} \tag{6.8}$$

and

$$\lim_{E \to \varepsilon_j} f_k(E) = \frac{1}{4 + \Delta^2}, \tag{6.9}$$

for the eigenvalues $E_i$ of $H$ and $\varepsilon_j$ of $QHQ$, which may be obvious from Eqs. (6.2)–(6.6). If the parameter $\Delta$ is taken to be small enough, the function $f_k(E)$ behaves like a resonance at $E = E_i$. By drawing the graph of $\{f_k(E),\ k = 1, 2, \ldots, d\}$ and finding resonance positions, we obtain eigenvalues of $H$.

### B. Numerical calculation

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

$$\langle i|H|j\rangle = (\alpha i + \beta i^2)\delta_{ij} + \gamma x_{ij} \tag{6.10}$$

with

$$x_{ij} = 2\left\{\sqrt{\sqrt{2}(i+j)} - \left[\sqrt{\sqrt{2}(i+j)}\right]\right\} - 1, \tag{6.11}$$

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

$$-1 \leqslant x_{ij} \leqslant 1. \tag{6.12}$$

The $\alpha$, $\beta$, and $\gamma$ are the dimensionless 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 here do not consider a case that some of the eigenvalues $\{y_k^{(m)}\}$ in Eqs. (3.10) and (3.21) become zero, because $\{x_{ij}\}$ are pseudorandom numbers and $H$ does not have any definite symmetry. Therefore, the subspaces $\{Q_k,\ k = 1, 2, \ldots, N_q\}$ are all $d$ dimensional and the number of the subspace $\{Q_k\}$ is given by $N_q = (N_h - 2)/2 = 49$.

We first calculate the $\widehat{Q}$ box and its energy derivatives $\widehat{Q}_1(E)$ and $\widehat{Q}_2(E)$ according to the continued-fraction method and the renormalized vertex method formulated in Secs. III C and III D, respectively. We have confirmed numerically that the calculations using these two methods agree with each other. With $\widehat{Q}(E)$, $\widehat{Q}_1(E)$, and $\widehat{Q}_2(E)$ we calculate the $\widehat{Z}$ box and its energy derivative $d\widehat{Z}(E)/dE$ according to Eqs. (5.1) and (5.5).

We next calculate the functions $F_k(E)$ and $F'_k(E)$ given in Eqs. (6.1) and (6.3), respectively. We finally obtain the functions $\{f_k(E),\ k = 1, 2, \ldots, d\}$ and draw graphs of these functions. Since the dimension of the $P$ space is taken to be $d = 2$, we have two graphs of $f_1(E)$ and $f_2(E)$. These graphs are shown in Fig. 5. From these figures we can specify the

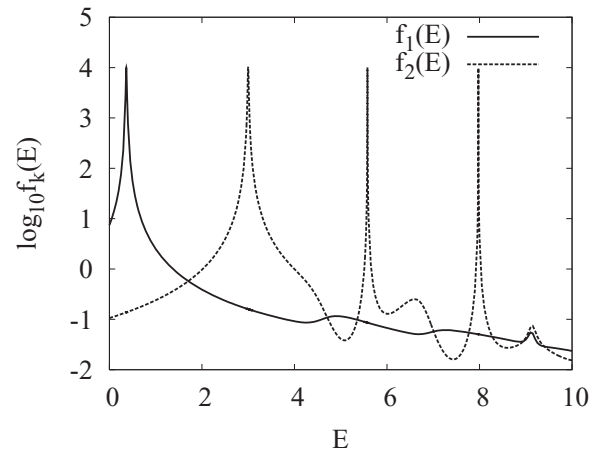


FIG. 5. Resonance-like behavior of the functions $f_1(E)$ and $f_2(E)$ in the case of $\alpha = 1.2$, $\beta = 0.2$, $\gamma = 1.4$, $\Delta = 10^{-2}$, and $F_0 = 1.0$. The values of $E$ at the resonance positions correspond to the eigenvalues of the Hamiltonian.

eigenvalues of $H$ as the resonance positions. From Fig. 5, we can estimate four eigenvalues of $H$ on the interval [0, 10].

The accurate solution, namely $E_i$, can be obtained in the following way: We suppose that the solution $E_i$ lies on the interval $[a, b]$ and there are no other solutions on this interval. The parabolic-interpolation method [56] is applied here. If the difference $|E - E_i|$ is sufficiently small, the approximate form of $g_k(E)$ in Eq. (6.6) becomes a parabolic function written as

$$g_k(E) = \frac{1 + \{F_0 F_k''(E_i)\}^2}{F_0^2}(E - E_i)^2. \tag{6.13}$$

Therefore we approximate $g_k(E)$ to be a parabolic function and solve the energy $E_i$ to give the minimum of $g_k(E)$. We note here that the parabolic function $A(x - \alpha)^2$ passing through two points $(a, g_k(a))$ and $(b, g_k(b))$ takes the minimum at the point $\alpha$ given by

$$\alpha = \frac{a\sqrt{g_k(b)} + b\sqrt{g_k(a)}}{\sqrt{g_k(a)} + \sqrt{g_k(b)}}, \tag{6.14}$$

where we have assumed $a < \alpha < b$. We utilize this fact to solve Eq. (6.6).

The calculation procedure employed in this numerical calculation is as follows:

(i) Determine an interval $[a, b]$ on which only one solution $E_i$ exists.

(ii) Divide $[a, b]$ into equal intervals and define five points $(E_1, E_2, E_3, E_4, E_5)$ as

$$E_k = a + (k - 1)\Delta E, \quad 1 \leqslant k \leqslant 5 \tag{6.15}$$

with $\Delta E = (b - a)/4$.

(iii) Consider all the intervals $[E_i, E_j]$ by selecting $E_i$ and $E_j$ among $\{E_1, E_2, \ldots, E_5\}$ and calculate

$$E_{ij} = \frac{E_i\sqrt{g_k(E_j)} + E_j\sqrt{g_k(E_i)}}{\sqrt{g_k(E_j)} + \sqrt{g_k(E_i)}}. \tag{6.16}$$

(iv) There are ten combinations of the energies $\{E_{ij}\}$. Arrange $\{E_{ij}\}$ in order of energy and write them as $u_1 < u_2 < \cdots < u_{10}$.

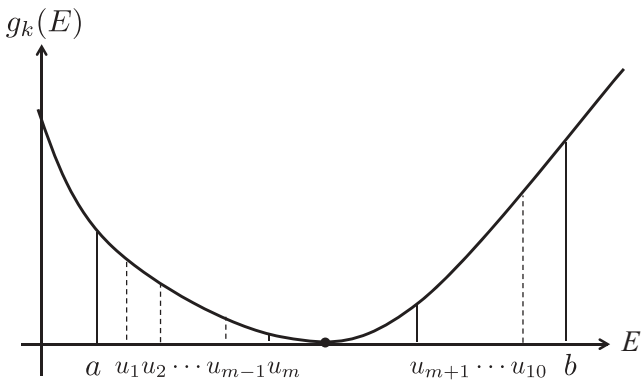


FIG. 6. Illustration of determining a new interval for finding the minimum point of the function $g_k(E)$. If $g_k(u_m)$ is the minimum value among $\{g_k(u_n),\ n = 1, 2, \ldots, 10\}$, then the new interval is given by $[a, b] = [u_{m-1}, u_{m+1}]$.

TABLE I. Correct digits of the lowest two eigenvalues of $H$ calculated by the parabolic-interpolation method. The parameters $\alpha$, $\beta$, and $\gamma$ are taken to be the same as in Fig. 5. Initial intervals are taken to be $[a, b] = [0.0, 1.0]$ and $[2.5, 3.5]$ for $E_1$ and $E_2$, respectively.

| $E_i$ | 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 |

(v) Calculate the values $\{g_k(u_n),\ n = 1, 2, \ldots, 10\}$ and find the minimum $g_k(u_m)$ as shown in Fig. 6. We determine a new interval $[a, b]$ according to

$$\begin{aligned} &a = u_{m-1}, \quad b = u_{m+1} \quad \text{if} \quad 2 \leqslant m \leqslant 9, \\ &a = a, \quad b = u_2 \quad \text{if} \quad m = 1, \\ &a = u_9, \quad b = b \quad \text{if} \quad m = 10. \end{aligned} \tag{6.17}$$

(vi) Repeat the procedure until the convergence, $|g_k(u_m)| < \delta$, is attained for an appropriate small number $\delta$.

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

As has been shown in Eq. (3.80), the $\widehat{Q}$ box is given by a sum over the number $k$. In this model calculation the maximum number of $k$ is equal to $N_q = 49$. Introducing a number $K_{\max}$, we consider a truncation as $k \leqslant K_{\max}$ in the calculation of the $\widehat{Q}$ box in Eq. (3.80). It would be interesting to examine the dependence of the calculated eigenvalues of $H$ on $K_{\max}$. The results are shown in Figs. 7 and 8. 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 series expansion for the $\widehat{Q}$ box, instead of making it according to the magnitude of energies of intermediate states as in the usual perturbative calculations.

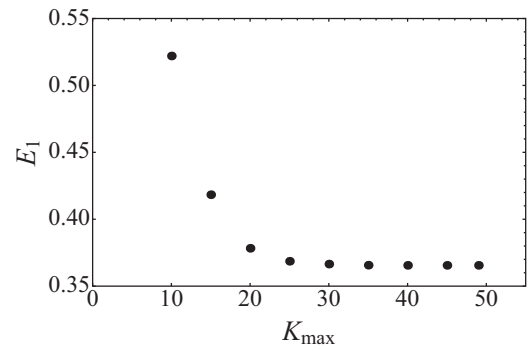


FIG. 7. Convergence of $E_1$ as a function of $K_{\max}$. The $K_{\max}$ denotes the block dimension which means the number of the subspaces $\{Q_k,\ k = 1, 2, \ldots, K_{\max}\}$ taken into the calculation. In this model calculation $K_{\max}$ is in the range $1 \leqslant K_{\max} \leqslant 49$. The exact value of $E_1$ is 0.36555. . . as given in Table I.

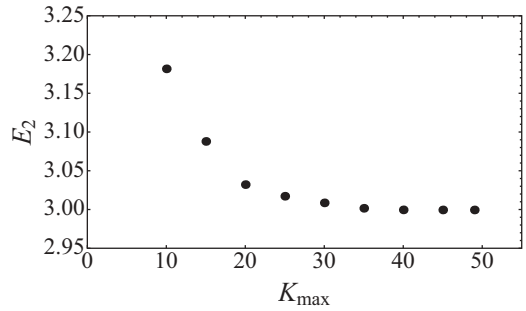


FIG. 8. Convergence of $E_2$ as a function of $K_{\max}$. The exact value of $E_2$ is 2.9994.... Other notations are the same as in Fig. 7.

## VII. CONCLUDING REMARKS

We have proposed a new approach to the effective interaction and/or Hamiltonian acting within a model space $P$. In the present stage of the effective-interaction theory one of the central problems has been how to calculate accurately the $\widehat{Q}$ box which has been used as a building block of the formulation. The main concern 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 formulation consists of two steps: The 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 $\{Q_k,\ k = 1, 2, \dots\}$ 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. By solving these coupled equations we have proved that the $\widehat{Q}$ box can be represented in two ways: The first one is that the $\widehat{Q}$ box is expanded into the form of a continued fraction in terms of the submatrices which are the elements of the block-tridiagonalized Hamiltonian. It has been proved that if a quantum system can be well described by a Hamiltonian given in a finite dimensional space, the continued fraction can be reduced to only one term with a renormalized propagator which can be calculated by using a descending recurrence relation. The other solution is obtained by using ascending recurrence relations for solving the coupled equations. The resultant $\widehat{Q}$ box can be shown to be given by only two terms such as $PHP$ and a sum of second-order terms with respect to renormalized vertices and propagators. This reduction of the $\widehat{Q}$ box has clarified that there exists a method of determining renormalized vertices and propagators such that the $\widehat{Q}$ box can be given by a sum of terms up to second order.

Given the $\widehat{Q}$ box, we have applied the $\widehat{Z}$-box method for solving the eigenvalue problem of a Hamiltonian $H$. We have introduced functions of energy variable $E$ as $\{f_k(E),\ k = 1, 2, \dots, d\}$ such that $f_k(E)$ behaves like a resonance at $E = E_i$ which is one of the eigenvalues of $H$. Here the number $d$ is the dimension of the model space. In this approach the eigenvalues of $H$ can be given by the resonance positions of the functions $\{f_k(E),\ k = 1, 2, \dots, d\}$. This approach enables us to solve the eigenvalue equation of $H$ in a graphical way.

We here emphasize that there would be an applicability of the present approach to solving the eigenvalue problem for a Hamiltonian given in a huge-dimensional shell-model space, because the calculation procedures include only manipulations of matrices with dimensions less than or equal to $d$.

In order to assess the present method we have made a test calculation by introducing a $100\times100$ model Hamiltonian. We have performed the calculation of the $\widehat{Q}$ box by employing two methods, namely, the continued-fraction expansion and the expansion with the renormalized vertices and propagators. We have confirmed that both the two methods have reproduced the exact eigenvalues of the original Hamiltonian $H$.

The present nonperturbative method would have another possibility of application to the derivation of the effective interaction to be used in the shell-model calculations. The reduction of the $\widehat{Q}$ box to simple second-order diagrams may attain a simplification of the calculation of the effective interaction. We here note, however, that the present study is based essentially on the algebraic approach to the effective Hamiltonian. For the calculation of the effective interaction among valence particles outside the core, it is necessary to represent the $\widehat{Q}$ box in terms of linked diagrams. A general relation is not clear between the present approach and the linked-and-folded-diagram theory. Therefore, this formal relation is an important problem to be clarified.

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## APPENDIX A: DERIVATIVES OF THE $\widehat{Q}$ BOX IN EQ. (3.51)

The first and second derivatives of the $\widehat{Q}$ box are given, respectively, by

$$\frac{d\widehat{Q}(E)}{dE} = -PHQ_1\frac{1}{\widetilde{e}_1(E)}\widetilde{k}_1(E)\frac{1}{\widetilde{e}_1(E)}Q_1HP, \tag{A1}$$

$$\frac{d^2\widehat{Q}(E)}{dE^2} = 2PHQ_1\frac{1}{\widetilde{e}_1(E)}\widetilde{k}_1(E)\frac{1}{\widetilde{e}_1(E)}\widetilde{k}_1(E)\frac{1}{\widetilde{e}_1(E)}Q_1HP - PHQ_1\frac{1}{\widetilde{e}_1(E)}\widetilde{l}_1(E)\frac{1}{\widetilde{e}_1(E)}Q_1HP. \tag{A2}$$

Here $\widetilde{e}_1(E)$, $\widetilde{k}_1(E)$, and $\widetilde{l}_1(E)$ are given through the following recurrence relations: We consider the energy derivative of $\widetilde{e}_n(E)$ in Eq. (3.49) and write

$$\widetilde{k}_n(E) = \frac{d\widetilde{e}_n(E)}{dE}. \tag{A3}$$

Noting a relation

$$\frac{d}{dE}\left\{\frac{1}{\widetilde{e}_n(E)}\right\} = -\frac{1}{\widetilde{e}_n(E)}\frac{d\widetilde{e}_n(E)}{dE}\frac{1}{\widetilde{e}_n(E)} = -\frac{1}{\widetilde{e}_n(E)}\widetilde{k}_n(E)\frac{1}{\widetilde{e}_n(E)}, \tag{A4}$$

we can derive

$$\widetilde{k}_n(E) = Q_n + H_{n,n+1}\frac{1}{\widetilde{e}_{n+1}(E)}\widetilde{k}_{n+1}(E)\frac{1}{\widetilde{e}_{n+1}(E)}H_{n+1,n}, \tag{A5}$$

where we have used the energy derivative of $e_m(E)$ in Eq. (3.42),

$$\frac{de_m(E)}{dE} = Q_m. \tag{A6}$$

The $H_{n,n+1}$ and $H_{n+1,n}$ are defined in Eq. (3.48). For the maximum number of $n$, denoted by $N$, $\widetilde{k}_N(E)$ is given by

$$\widetilde{k}_N(E) = \frac{d\widetilde{e}_N(E)}{dE} = Q_N, \tag{A7}$$

which is derived from Eq. (3.50) for $\widetilde{e}_N(E)$. Starting with $\widetilde{k}_N(E)$, the recurrence relation determines a sequence $\widetilde{k}_N(E)$, $\widetilde{k}_{N-1}(E), \ldots, \widetilde{k}_1(E)$.

We write the second derivative of $\widetilde{e}_n(E)$ as

$$\widetilde{l}_n(E) = \frac{d^2\widetilde{e}_n(E)}{dE^2} = \frac{d\widetilde{k}_n(E)}{dE}. \tag{A8}$$

From Eq. (A5) for $\{\widetilde{k}_n(E)\}$ a recurrence formula for $\{\widetilde{l}_n(E)\}$ can be derived as

$$\begin{aligned}\widetilde{l}_n(E) = {} & -2H_{n,n+1}\frac{1}{\widetilde{e}_{n+1}(E)}\widetilde{k}_{n+1}(E)\frac{1}{\widetilde{e}_{n+1}(E)}\widetilde{k}_{n+1}(E) \\ & \times\frac{1}{\widetilde{e}_{n+1}(E)}H_{n+1,n} + H_{n,n+1}\frac{1}{\widetilde{e}_{n+1}(E)}\widetilde{l}_{n+1}(E) \\ & \times\frac{1}{\widetilde{e}_{n+1}(E)}H_{n+1,n}.\end{aligned} \tag{A9}$$

For the maximum number $n = N$ the $\widetilde{l}_N(E)$ is given, from Eqs. (A7) and (A8), by

$$\widetilde{l}_N(E) = 0. \tag{A10}$$

The recurrence formula Eq. (A9) determines a sequence $\widetilde{l}_N(E), \widetilde{l}_{N-1}(E), \ldots, \widetilde{l}_1(E)$. Substituting the operators $\widetilde{e}_1(E)$, $\widetilde{k}_1(E)$, and $\widetilde{l}_1(E)$ into Eqs. (A1) and (A2) the first and second derivatives of the $\widehat{Q}$ box can be calculated.

Here it should be noted that the first and second derivatives of the $\widehat{Q}$ box can be expressed by using only small-dimensional matrices. The $\widetilde{e}_1(E)$, $\widetilde{k}_1(E)$, and $\widetilde{l}_1(E)$ are the operators on the subspace $Q_1$ which are represented by $d_1 \times d_1$ matrices. The operator $PHQ_1$ is a mapping between the $P$ and $Q_1$ spaces and has a $d \times d_1$ matrix representation.

## APPENDIX B: DERIVATIVES OF THE $\widehat{Q}$ BOX IN EQ. (3.80)

We derive the first and second derivatives of the $\widehat{Q}$ box with respect to energy variable $E$ as

$$\begin{aligned}\frac{d\widehat{Q}(E)}{dE} = {} & \sum_{k=1}^{\infty}\{[\overline{H}'_k(E)\lambda_k(E)\overline{H}^{\dagger}_k(E) + \text{H.c.}] \\ & + \overline{H}_k(E)\lambda'_k(E)\overline{H}^{\dagger}_k(E)\},\end{aligned} \tag{B1}$$

$$\begin{aligned}\frac{d^2\widehat{Q}(E)}{dE^2} = {} & \sum_{k=1}^{\infty}\{2\overline{H}'_k(E)\lambda_k(E)\overline{H}'^{\dagger}_k(E) + [\overline{H}''_k(E)\lambda_k(E)\overline{H}^{\dagger}_k(E) \\ & + \text{H.c.}] + 2[\overline{H}'_k(E)\lambda'_k(E)\overline{H}^{\dagger}_k(E) + \text{H.c.}] \\ & + \overline{H}_k(E)\lambda''_k(E)\overline{H}^{\dagger}_k(E)\}\end{aligned} \tag{B2}$$

with

$$\overline{H}'_k(E) = \frac{d\widehat{H}_k(E)}{dE}, \tag{B3}$$

$$\overline{H}''_k(E) = \frac{d^2\widehat{H}_k(E)}{dE^2}, \tag{B4}$$

$$\lambda_k(E) = \frac{1}{\overline{e}_k(E)}, \tag{B5}$$

$$\lambda'_k(E) = \frac{d\lambda_k(E)}{dE} = -\frac{1}{\overline{e}_k(E)}\frac{d\overline{e}_k(E)}{dE}\frac{1}{\overline{e}_k(E)}, \tag{B6}$$

$$\begin{aligned}\lambda''_k(E) = {} & \frac{d^2\lambda_k(E)}{dE^2} = 2\frac{1}{\overline{e}_k(E)}\frac{d\overline{e}_k(E)}{dE}\frac{1}{\overline{e}_k(E)}\frac{d\overline{e}_k(E)}{dE}\frac{1}{\overline{e}_k(E)} \\ & - \frac{1}{\overline{e}_k(E)}\frac{d^2\overline{e}_k(E)}{dE^2}\frac{1}{\overline{e}_k(E)}.\end{aligned} \tag{B7}$$

These expressions indicate that the calculation of the derivatives of $\widehat{Q}(E)$ is reduced to that of $\{\overline{H}_k(E)\}$, $\{\lambda_k(E)\}$, and their derivatives; $\{\overline{H}_k(E)\}$ is given through the recurrence relation Eq. (3.78) and accordingly its derivatives are

$$\overline{H}'_k(E) = \{\overline{H}'_{k-1}(E)\lambda_{k-1}(E) + \overline{H}_{k-1}(E)\lambda'_{k-1}(E)\}H_{k-1,k}, \tag{B8}$$

$$\begin{aligned}\overline{H}''_k(E) = {} & \{\overline{H}''_{k-1}(E)\lambda_{k-1}(E) + 2\overline{H}'_{k-1}(E)\lambda'_{k-1}(E) \\ & + \overline{H}_{k-1}(E)\lambda''_{k-1}(E)\}H_{k-1,k},\end{aligned} \tag{B9}$$

and $\{\lambda_k(E)\}$ is given by

$$\lambda_k(E) = \{e_k(E) - H_{k,k-1}\lambda_{k-1}(E)H_{k-1,k}\}^{-1} \tag{B10}$$

from Eqs. (3.69) and (B5), and accordingly its derivatives are

$$\lambda'_k(E) = -\lambda_k^2(E) + \lambda_k(E)H_{k,k-1}\lambda'_{k-1}(E)H_{k-1,k}\lambda_k(E), \tag{B11}$$

$$\begin{aligned}\lambda''_k(E) = {} & -[\lambda'_k(E)\lambda_k(E) + \text{H.c.}] \\ & + \{\lambda'_k(E)H_{k,k-1}\lambda'_{k-1}(E)H_{k-1,k}\lambda_k(E) + \text{H.c.}\} \\ & + \lambda_k(E)H_{k,k-1}\lambda''_{k-1}(E)H_{k-1,k}\lambda_k(E).\end{aligned} \tag{B12}$$

Their initial values are given in Eq. (3.79) for $\{\overline{H}_k(E)\}$, $\overline{H}'_1(E) = \overline{H}''_1(E) = 0$, and

$$\lambda_1(E) = \frac{1}{e_1(E)} = (E - Q_1HQ_1)^{-1}, \tag{B13}$$

$$\lambda'_1(E) = -(E - Q_1HQ_1)^{-2}, \tag{B14}$$

$$\lambda''_1(E) = 2(E - Q_1HQ_1)^{-3}. \tag{B15}$$

The way of calculating the derivatives of the $\widehat{Q}$ box is summarized as follows: First, $\{\lambda_k(E)\}$ is calculated by Eq. (B10), then its derivatives are determined by Eqs. (B11) and (B12). Next $\{\overline{H}'_k(E)\}$ and $\{\overline{H}''_k(E)\}$ are determined by Eqs. (B8) and (B9); finally we obtain the derivatives of the $\widehat{Q}$ box. Here $\lambda_k(E)$, $\lambda'_k(E)$, and $\lambda''_k(E)$ are $d_k \times d_k$ matrices, while $\overline{H}_k(E)$, $\overline{H}'_k(E)$, and $\overline{H}''_k(E)$ are $d \times d_k$ matrices.

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