Graphical method for deriving an effective interaction with a new vertex function

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(Received 11 January 2011; published 10 February 2011)

Introducing a new vertex function, $\hat{Z}(E)$, of an energy variable E, we derive a new equation for the effective interaction. The equation is obtained by replacing the $\hat{Q}$ box in the Krenciglowa-Kuo (KK) method with $\hat{Z}(E)$. This new approach can be viewed as an extension of the KK method. We show that this equation can be solved both in iterative and noniterative ways. We observe that the iteration procedure with $\hat{Z}(E)$ brings about fast convergence compared to the usual KK method. It is shown that, as in the KK approach, the procedure of calculating the effective interaction can be reduced to determining the true eigenvalues of the original Hamiltonian H and they can be obtained as the positions of intersections of graphs generated from $\hat{Z}(E)$. We find that this graphical method yields always precise results and reproduces any of the true eigenvalues of H. The calculation in the present approach can be made regardless of overlaps with the model space and energy differences between unperturbed energies and the eigenvalues of H. We find also that $\hat{Z}(E)$ is a well-behaved function of E and has no singularity. These characteristics of the present approach ensure stability in actual calculations and would be helpful to resolve some difficulties due to the presence of poles in the $\hat{Q}$ box. Performing test calculations, we verify numerically theoretical predictions made in the present approach.

DOI: 10.1103/PhysRevC.83.024304 PACS number(s): 21.60.De, 24.10.Cn, 02.30.Vv, 02.60.Cb

I. INTRODUCTION

In nuclear, atomic, and chemical physics, it is often useful to introduce an effective interaction acting in a chosen model space (P space) of tractable dimension. In nuclear physics, much effort has been made with regard to both formal theories and their applications [1–8]. Recently, the effective interaction method has been applied to new fields of many-body physics, such as quantum dots [9,10] and many-boson systems [11].

Among many approaches, we here direct our attention to the Krenciglowa-Kuo (KK) [12,13] and the Lee-Suzuki (LS) [14,15] methods. These two methods are constructed in terms of the so-called $\hat{Q}$ box as a building block of formulation. The KK approach has a very simple structure and the effective interaction is obtained in an iterative way. If the iteration converges, in almost all numerical calculations, eigenvalues are given for the states which have the largest overlaps with the chosen model space. On the other hand, the LS method reproduces eigenvalues for the states which lie closest to the chosen unperturbed energy. Originally the LS method had been presented to resolve the difficulty of divergence in the perturbation expansion. The LS method is rather complicated in structure and higher derivatives of the $\hat{Q}$ box with respect to starting energy are necessary if one wishes to obtain more accurate solutions.

Both of the two theories yield only certain of the true eigenvalues of the original Hamiltonian. This restriction is not desirable. In a formal point of view, the $\hat{Q}$ box itself contains information regarding all of the true eigenvalues. For a given model space of dimension d, there would be a method of reproducing any d eigenvalues among all the true eigenvalues.

In many cases where the effective interaction theories have been applied an iteration or a recursion method has often been employed. In general, the convergence in such a method depends strongly on the properties of the eigenstates of the Hamiltonian H. In actual calculations the information on the true eigenstates is not given beforehand. Therefore, it is impossible to control the convergence in the iteration. In many cases we cannot know whether the iteration is convergent before starting calculations. Even if the iteration converges, we do not know which eigenvalues are reproduced in all of the eigenvalues. Another difficulty encountered in actual calculations is the pole problem. The $\hat{Q}$ box itself has poles at the energies which are the eigenvalues of H in the complement space (Q space). The presence of poles causes often instability in numerical calculations.

We shall show that it is indeed possible to resolve these difficulties by introducing a new vertex function, $\hat{Z}(E)$, in place of the $\hat{Q}$ box by Kuo *et al.* [12,13]. Preliminary version of the present work has been reported in Ref. [16]. Very recently Dong, Kuo, and Holt have followed the present approach and applied to the actual calculations of the shell-model effective interactions [17]. These works have shown that the present method has a possibility of providing a suitable framework with $\hat{Z}(E)$ as well as the KK approach.

The organization of the present article is as follows: In Sec. II we outline the $\hat{Q}$-box formalism and the KK method. A new vertex function operator, $\hat{Z}(E)$, is introduced and some of its mathematical properties are clarified. The algorithm of

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the calculation procedure is given by applying the secant and the Newton-Raphson methods. In Sec. III test calculations are made in order to assess the present approach. We examine whether the theoretical predictions are verified in an exactly solvable model. Concluding remarks are given in Sec. IV.

II. FORMULATION

We consider a general quantum system which is described by a Hamiltonian H. We write an eigenvalue equation with the eigenvalues $\{E_k\}$ and the eigenstates $\{|\Psi_k\rangle\}$ as

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle, \quad k = 1, 2, \ldots. \tag{1}$$

The Hamiltonian H is supposed to be composed of the unperturbed Hamiltonian H_0 and the perturbation V, i.e., $H = H_0 + V$. We decompose the entire Hilbert space into the model space (P space) and its complement (Q space) with the projection operators P and Q, respectively. Basic properties of the projection operators are $P + Q = 1$ and $PQ = QP = 0$.

We here assume that H_0 is decoupled between the P and Q spaces as

$$H_0 = PH_0P + QH_0Q. \tag{2}$$

In the present work we consider a case that the P-space states have a degenerate unperturbed energy E_0, i.e.,

$$PH_0P = E_0P. \tag{3}$$

Then the P-space eigenvalue equation is written with the effective interaction R and the eigenstate $|\phi_k\rangle$ as

$$(E_0P + R)|\phi_k\rangle = E_k|\phi_k\rangle, \quad k = 1, 2, \ldots, d, \tag{4}$$

where d is the dimension of the P space. In the above d eigenvalues E_k's should agree with d of the true eigenvalues in Eq. (1). Various solutions for R are possible, and many theoretical frameworks have been given for obtaining R. Probably the most widely applied effective interaction is given by imposing the condition that the model-space eigenstate $|\phi_k\rangle$ in Eq. (4) should agree with the P-space component of the true eigenstate $|\Psi_k\rangle$ of H, i.e., $|\phi_k\rangle = P|\Psi_k\rangle$. This restriction on $|\phi_k\rangle$ leads to the standard non-Hermitian form of R [18].

A. Solutions for effective interaction in the $\hat{Q}$-box formalism

Among many approaches to the effective interaction R we here discuss the KK formalism [12,13]. Originally the KK method is based on a diagrammatic representation of the effective interaction, which has been known as the $\hat{Q}$-box folded-diagram method originated by Kuo *et al.* [19].

For obtaining R, one first calculates the vertex function called the $\hat{Q}$ box which is defined as the sum of all the linked and nonfolded diagrams. Next one should add the folded diagrams, which can be carried out rather simply by applying the energy-derivative expression of the $\hat{Q}$ box [12,19]. Originally the KK approach was proposed to derive an effective interaction acting among a few valence particles outside the closed-shell core. However, in the present work, we consider a general quantum system and wish to reproduce d total energies of H by introducing an effective interaction. For this case the KK method can also be applied by defining the $\hat{Q}$ box in an operator form as

$$\hat{Q}(E) \equiv PVP + PVQ\frac{1}{E - QHQ}QVP, \tag{5}$$

which is a function of an energy variable E. Equation (5) is equivalent to the energy-dependent form of the effective interaction given by Bloch and Horowitz in the many-body perturbation theory [20].

With the $\hat{Q}$ box the effective interaction R can be expanded into

$$R = \hat{Q} + \hat{Q}_1\hat{Q} + \hat{Q}_1\hat{Q}_1\hat{Q} + \hat{Q}_2\hat{Q}\hat{Q} + \cdots, \tag{6}$$

where $\hat{Q} \equiv \hat{Q}(E_0)$ and $\hat{Q}_m \equiv \hat{Q}_m(E_0)$ with

$$\hat{Q}_m(E) \equiv \frac{1}{m!}\frac{d^m\hat{Q}(E)}{dE^m}, \quad m = 1, 2, \ldots. \tag{7}$$

Here E_0 is the starting energy or the degenerate unperturbed energy as given in Eq. (3).

If the series expansion in Eq. (6) converges, R is given in a formal way by

$$R = \sum_{k=1}^{d}\hat{Q}(E_k)|\phi_k\rangle\langle\tilde{\phi}_k|, \tag{8}$$

where E_k and $|\phi_k\rangle$ are given in Eq. (4), and $\langle\tilde{\phi}_k|$ is the biorthogonal state defined through the orthogonality $\langle\tilde{\phi}_k|\phi_{k'}\rangle = \delta_{kk'}$. We here note that, as seen in Eqs. (4) and (8), the derivation of the effective interaction R is equivalent to determining d eigenvalues $\{E_k\}$ and the corresponding P-space eigenstates $\{|\phi_k\rangle\}$. Using Eqs. (4) and (8), the effective interaction R is rewritten simply as

$$R = \sum_{k=1}^{d}(E_k - E_0)|\phi_k\rangle\langle\tilde{\phi}_k|, \tag{9}$$

and the model-space eigenvalue equation with the effective interaction R is expressed as

$$[E_0P + \hat{Q}(E_k)]|\phi_k\rangle = E_k|\phi_k\rangle. \tag{10}$$

From Eqs. (8) and (10) we understand that R can be given by calculating the $\hat{Q}$ box at the true eigenvalues $\{E_k\}$ of H as starting energies which are determined self-consistently.

We here show that there is another way of deriving the effective interaction R. We first note that the $\hat{Q}$ box is a function of E and resultantly the eigenvalues of $E_0P + \hat{Q}(E)$ are also functions of E. We write the eigenvalue equations in the P space for an arbitrary energy E as

$$[E_0P + \hat{Q}(E)]|\psi_m\rangle = G_m(E)|\psi_m\rangle, m = 1, 2, \ldots, d. \tag{11}$$

Since the P space is d dimensional, we have d eigenvalues denoted by $\{G_m(E); m = 1, 2, \ldots, d\}$, which we label in order of energy as $G_1(E) < G_2(E) < \cdots < G_d(E)$. It may be clear from Eqs. (10) and (11) that the eigenvalues $\{E_k\}$ in Eq. (10) can be given by solving the following equations

$$G_m(E) = E, \quad m = 1, 2, \ldots, d. \tag{12}$$

Various mathematical methods have been known to solve such equations.

We should note that a set of the equations (12) are independent of the properties of the eigenstates of H, such as P-space overlaps or energy spacings. Therefore, in principle, it is possible to reproduce the true eigenvalues $\{E_k\}$ of H more than in the usual KK method based on Eq. (10). However, as seen in Eq. (5), poles appear in the $\hat{Q}$ box when E approaches one of the eigenvalues of QHQ. The poles in $\hat{Q}(E)$ also induce the poles in $G_m(E)$ in Eq. (11). Such a situation causes instability in numerically solving Eq. (12) for $\{E_k\}$ around the pole positions.

B. Extension of the Krenciglowa-Kuo method

In order to resolve the pole problem we introduce a new vertex function of an energy variable E, which is a P-space operator defined in terms of the $\hat{Q}$ box and its energy derivative as [16]

$$\hat{Z}(E) \equiv \frac{1}{1-\hat{Q}_1(E)}[\hat{Q}(E) - \hat{Q}_1(E)(E-E_0)P]. \tag{13}$$

Hereafter we shall refer to $\hat{Z}(E)$ as the $\hat{Z}$ box. We note here that the $\hat{Z}$ box agrees, at $E = E_0$, with the first-order recursive solution in the LS method [15]. In a recent article by Dong, Kuo, and Holt [17] the definition of $\hat{Z}(E)$ is given in a more general case with a nondegenerate P-space unperturbed Hamiltonian PH_0P. In this case one should replace E_0P with PH_0P. As in Eq. (11) with the $\hat{Q}$ box, we consider an eigenvalue problem

$$[E_0P + \hat{Z}(E)]|\psi_m\rangle = F_m(E)|\psi_m\rangle, \quad m = 1, 2, \ldots, d, \tag{14}$$

where $\{F_m(E); m = 1, 2, \ldots, d\}$ are d eigenvalues which are functions of E. We here label $\{F_m(E); m = 1, 2, \ldots, d\}$ in order of energy as $F_1(E) < F_2(E) < \cdots < F_d(E)$.

The $\hat{Z}$ box and the associated functions $\{F_m(E)\}$ have the following properties:

(i) Using Eqs. (5), (8), (9), and (13), we have, for the P-space eigenstates $\{|\phi_k\rangle\}$ in Eq. (10),

$$\sum_{k=1}^{d} \hat{Z}(E_k)|\phi_k\rangle\langle\tilde{\phi}_k| = \sum_{k=1}^{d} \frac{1}{1-\hat{Q}_1(E_k)}[R - \hat{Q}_1(E_k)R]|\phi_k\rangle\langle\tilde{\phi}_k| = R. \tag{15}$$

The above fact means that, replacing $\hat{Q}(E)$ with $\hat{Z}(E)$ in Eq. (8), a new solution for the effective interaction R can be derived as

$$R_{\mathrm{EKK}} \equiv \sum_{k=1}^{d} \hat{Z}(E_k)|\phi_k\rangle\langle\tilde{\phi}_k|, \tag{16}$$

and, equivalently, Eq. (10) with the $\hat{Q}$ box is replaced with

$$[E_0P + \hat{Z}(E_k)]|\phi_k\rangle = E_k|\phi_k\rangle. \tag{17}$$

From the above relations between two approaches with $\hat{Q}(E)$ and $\hat{Z}(E)$ we may call R_{EKK} in Eq. (16) the extended Krenciglowa-Kuo (EKK) solution. In the same way as in Eq. (12), the true eigenvalues $\{E_k\}$ can be given by solving the equations

$$F_m(E) = E, \quad m = 1, 2, \ldots, d. \tag{18}$$

(ii) Using Eqs. (5), (7), and (13) we can derive a formal expression for the energy derivative of $\hat{Z}(E)$ as

$$\frac{d\hat{Z}(E)}{dE} = \frac{2}{1-\hat{Q}_1(E)}\hat{Q}_2(E)[\hat{Z}(E) - (E-E_0)P]. \tag{19}$$

In the article by Dong *et al.* [17], the above expression has also been given for a general case with the nondegenerate PH_0P. If E is one of the true eigenvalues $\{E_k\}$ satisfying Eq. (17), we see that the energy derivative of $\hat{Z}(E)$ becomes zero at $E = E_k$, namely

$$\left.\frac{d\hat{Z}(E)}{dE}\right|_{E=E_k}|\phi_k\rangle = 0, \quad k = 1, 2, \ldots, d. \tag{20}$$

As a result, we have for the energy derivative of $F_m(E)$

$$\left.\frac{dF_m(E)}{dE}\right|_{E=E_k} = 0, \quad k = 1, 2, \ldots, d. \tag{21}$$

These results for the energy derivatives have been pointed out in a previous article [16].

(iii) We discuss here some problems associated with the poles of $\hat{Q}(E)$. First we consider the eigenvalue equation for the Q-space Hamiltonian QHQ written as

$$QHQ|q\rangle = \varepsilon_q|q\rangle, \tag{22}$$

where ε_q and $|q\rangle$ are the eigenvalue and the eigenstate, respectively. It may be clear from Eq. (5) that $\hat{Q}(E)$ has a pole at $E = \varepsilon_q$. We define a P-space operator $\hat{X}_q$ with the Q-space eigenstate $|q\rangle$ in Eq. (22) as

$$\hat{X}_q \equiv PV|q\rangle\langle q|VP. \tag{23}$$

We write the eigenvalue equation for $\hat{X}_q$ with an eigenvalue x_μ as

$$\hat{X}_q|\mu\rangle = x_\mu|\mu\rangle. \tag{24}$$

From the definition of $\hat{X}_q$ in Eq. (23) we see that $\hat{X}_q$ is a Hermitian and positive semidefinite matrix, that is, $\hat{X}_q$ has positive or zero eigenvalues because of the inequality $x_\mu = |\langle\mu|V|q\rangle|^2 \geqslant 0$. We can further prove that there is only one eigenstate, denoted by $|\mu_0\rangle$, with a positive eigenvalue and that the eigenvalues of all the other eigenstates are zero. The only one positive eigenvalue of Eq. (24) is given by

$$x_{\mu_0} = \sum_{i=1}^{d} |\langle p_i|V|q\rangle|^2, \tag{25}$$

where $\{|p_i\rangle; i = 1, 2, \ldots, d\}$ are the basis-state vectors of the P space. The proof is as follows: We consider a matrix representation of $\hat{X}_q$ with the matrix element $(\hat{X}_q)_{ij} = \langle p_i|V|q\rangle\langle q|V|p_j\rangle$. Then we obtain the trace

of $\hat{X}_q$ as

$$\mathrm{Tr}\hat{X}_q = \sum_{i=1}^{d} |\langle p_i|V|q\rangle|^2. \tag{26}$$

We note that the state vector $|\mu_0\rangle$ can be written explicitly as

$$|\mu_0\rangle = \frac{[\langle p_1|V|q\rangle, \langle p_2|V|q\rangle, \ldots, \langle p_d|V|q\rangle]^T}{\sqrt{N}}, \tag{27}$$

where the symbol T means transpose of $(1 \times d)$ matrix and $\sqrt{N}$ is the normalization factor with $N \equiv \sum_{i=1}^{d} |\langle p_i|V|q\rangle|^2$. This state $|\mu_0\rangle$ becomes an eigenstate of $\hat{X}_q$ and has a positive eigenvalue as

$$\hat{X}_q|\mu_0\rangle = \left(\sum_{i=1}^{d} |\langle p_i|V|q\rangle|^2\right)|\mu_0\rangle = x_{\mu_0}|\mu_0\rangle. \tag{28}$$

The eigenvalue x_{μ_0} coincides with the trace of $\hat{X}_q$. Recalling a well-known theorem on the trace of a square matrix, we see that the trace of $\hat{X}_q$ should be equal to the sum of the eigenvalues of $\hat{X}_q$. It follows immediately that all the other eigenvalues except x_{μ_0} become zero.

(iv) Next, we prove that Eq. (17) or (18) has additional solutions other than the true eigenvalues $\{E_k\}$. We note, in the vicinity of a pole of $\hat{Q}(E)$, where $E = \varepsilon_q + \Delta$ with a small deviation Δ, that $\hat{Q}(E)$ in Eq. (5) is expressed as

$$\hat{Q}(\varepsilon_q + \Delta) = PVP + \frac{\hat{X}_q}{\Delta} + \sum_{q' \neq q} \frac{\hat{X}_{q'}}{\varepsilon_q + \Delta - \varepsilon_{q'}}. \tag{29}$$

Here we have used the definition of $\hat{X}_q$ in Eq. (23). The operations of $\hat{Q}(\varepsilon_q + \Delta)$, $\hat{Q}_1(\varepsilon_q + \Delta)$, and $\hat{Q}_2(\varepsilon_q + \Delta)$ on the state $|\mu_0\rangle$ yield in leading order, respectively

$$\hat{Q}(\varepsilon_q + \Delta)|\mu_0\rangle = \frac{x_{\mu_0}}{\Delta}|\mu_0\rangle, \tag{30}$$

$$\hat{Q}_1(\varepsilon_q + \Delta)|\mu_0\rangle = -\frac{x_{\mu_0}}{\Delta^2}|\mu_0\rangle, \tag{31}$$

$$\hat{Q}_2(\varepsilon_q + \Delta)|\mu_0\rangle = \frac{x_{\mu_0}}{\Delta^3}|\mu_0\rangle. \tag{32}$$

Using Eq. (13) and the above relations, we obtain at $E = \varepsilon_q + \Delta$

$$\begin{aligned}&[E_0 + \hat{Z}(\varepsilon_q + \Delta)]|\mu_0\rangle \\ &= \left[E_0 + \left(\frac{x_{\mu_0}}{\Delta^2}\right)^{-1}\left[\frac{x_{\mu_0}}{\Delta} + \frac{x_{\mu_0}(\varepsilon_q + \Delta - E_0)}{\Delta^2}\right]\right] \\ &= (\varepsilon_q + 2\Delta)|\mu_0\rangle.\end{aligned} \tag{33}$$

Then we have in the limit of $E \to \varepsilon_q$

$$[E_0 + \hat{Z}(\varepsilon_q)]|\mu_0\rangle = \varepsilon_q|\mu_0\rangle. \tag{34}$$

This fact means that the state $|\mu_0\rangle$ and the energy ε_q can be an additional solution to Eq. (17). This also means that the pole energy ε_q satisfies Eq. (18).

(v) We further consider the energy derivatives of $\hat{Z}(E)$ and $F_m(E)$ at the pole positions. Subtraction of Eq. (34) from Eq. (33) follows

$$\left.\frac{d\hat{Z}(E)}{dE}\right|_{E=\varepsilon_q}|\mu_0\rangle = 2|\mu_0\rangle. \tag{35}$$

We can derive the above result, in another way, by using Eqs. (19) and (34)

$$\begin{aligned}&\left.\frac{d\hat{Z}(E)}{dE}\right|_{E=\varepsilon_q+\Delta}|\mu_0\rangle \\ &\quad= \frac{2}{1 - \hat{Q}_1(\varepsilon_q + \Delta)}\hat{Q}_2(\varepsilon_q + \Delta)\Delta|\mu_0\rangle.\end{aligned} \tag{36}$$

Then, using Eqs. (31) and (32) and taking the limit of $\Delta \to 0$, we obtain

$$\begin{aligned}&\left.\frac{d\hat{Z}(E)}{dE}\right|_{E=\varepsilon_q}|\mu_0\rangle \\ &\quad= \lim_{\Delta\to 0} 2\left(\frac{x_{\mu_0}}{\Delta^2}\right)^{-1}\frac{x_{\mu_0}}{\Delta^3}\Delta|\mu_0\rangle = 2|\mu_0\rangle.\end{aligned} \tag{37}$$

As a consequence we have

$$\left.\frac{dF_m(E)}{dE}\right|_{E=\varepsilon_q} = 2. \tag{38}$$

This property of the energy derivative of $F_m(E)$ at a pole position is in marked contrast to that for a true eigenvalue in Eq. (21). These properties of the energy derivative of $F_m(E)$ given in Eqs. (21) and (38) can be used to distinguish the pole energy solutions from those of the true eigenvalues of H. It is also noted, from Eqs. (34) and (38), that the function $F_m(E)$ is a well-behaved function of E and has no singularity even at the pole energies.

C. Iteration methods for the effective interaction

Iteration methods have been employed quite often for obtaining the effective interaction or equivalently for determining the true eigenvalues of H. In the previous subsections we have given four basic equations, namely Eqs. (10) and (12) for the KK and Eqs. (17) and (18) for the EKK methods. In the KK approach Eqs. (10) and (12) lead, respectively, to the following iterative equations:

$$\left[E_0 P + \hat{Q}\left(E_k^{(n)}\right)\right]\left|\phi_k^{(n+1)}\right\rangle = E_k^{(n+1)}\left|\phi_k^{(n+1)}\right\rangle \tag{39}$$

and

$$E^{(n+1)} = G_m(E^{(n)}), \quad m = 1, 2, \ldots, d. \tag{40}$$

In the same way, two iterative equations can be derived from Eqs. (17) and (18) for the EKK method, respectively, as

$$\left[E_0 P + \hat{Z}\left(E_k^{(n)}\right)\right]\left|\phi_k^{(n+1)}\right\rangle = E_k^{(n+1)}\left|\phi_k^{(n+1)}\right\rangle \tag{41}$$

and

$$E^{(n+1)} = F_m(E^{(n)}), \quad m = 1, 2, \ldots, d. \tag{42}$$

The iterative equation (39) has long been used as a standard method in the KK approach. The convergence condition has been investigated in many of the theoretical and numerical studies [12,15,21]. From these studies it has been known that,

if the iteration converges, the KK approach in Eq. (39) derives d eigenvalues of the eigenstates of H with the largest P-space overlaps. However, it has also been known that the iteration in Eq. (39) does not always converge. Recently Takayanagi [22] has pointed out an exceptional case that the KK method does not reproduce states which have the largest P-space overlaps even if the iteration converges. Although the KK iteration method has been applied widely and has brought remarkable results in actual calculations, the rigorous condition of convergence for Eq. (39) has not yet been made clear.

The convergence condition for the iteration in Eq. (40) requires mathematically that the energy derivative of $G_m(E)$ at the solution $E = E_k$ should satisfy $|dG_m(E)/dE|_{E=E_k} < 1$. In general, this convergence condition is considered to be satisfied by certain of the true eigenvalues of H. It implies that this iteration method is restrictive for the purpose of reproducing the solutions of $\{E_k\}$ as many as possible.

The iteration in Eq. (41) leads to a new scheme of the calculations of $\{E_k\}$ and R_{EKK} in Eq. (16). As in the case of the KK iteration in Eq. (39), the convergence condition in Eq. (41) is quite complicated and has not yet been made clear. However, the iteration in Eq. (41) would be applicable in actual calculations. In the article by Dong *et al.* [17], they have employed this iteration scheme to a model problem and actual calculations of the shell-model effective interaction. They have concluded that the two iterations in Eq. (39) for the KK and Eq. (41) for the EKK methods are both suitable and efficient.

Another iterative equations in the EKK method is given in Eq. (42). The convergence condition for this iteration is given by $|dF_m(E)/dE|_{E=E_k} < 1$. It is clear from the property of the energy derivative of $F_m(E)$ in Eq. (21) that the convergence condition is satisfied for any of the true eigenvalues $\{E_k\}$. The iteration in Eq. (42) converges surely to one of $\{E_k\}$. We also note that this iteration in Eq. (42) never reaches the pole-energy solutions due to the property in Eq. (38) of the energy derivative of $F_m(E)$. We can show that the iteration in Eq. (42) is equivalent to that in the Newton-Raphson method which is often used to solve nonlinear equations. The Newton-Raphson method has been known to derive quadratic convergence, that is, the number of correct digits is doubled at each step of iteration. On the contrary, the usual methods, including the KK and the LS methods, derive single (or linear) convergence. The iteration in Eq. (42) surely guarantees faster convergence than the usual iterations given so far.

D. Graphical method for effective interaction with the $\hat{Z}$ box

We present a new method for solving Eq. (18) derived on the basis of the $\hat{Z}$ box and its associated functions $\{F_m(E)\}$. The solutions can be obtained by finding the energies of the intersections of two graphs, $y = F_m(E)$ and $y = E$. As we have already shown, the $\hat{Z}$ box has no singularities at the pole positions of the $\hat{Q}$ box. Thus, $\{F_m(E)\}$ can be considered to be well-behaved functions of E. These characteristics of the functions $\{F_m(E)\}$ enable us to employ some of the mathematically well-established methods for solving nonlinear equations.

The procedure of solving Eq. (18) in the present approach, which we call the graphical method, is given as follows: We first draw graphs of $y = F_m(E)$ for $m = 1, 2, \ldots, d$ and $y = E$. The energies at the intersections of these graphs become the solutions to $F_m(E) = E$. Furthermore, the energy derivatives of $\{F_m(E)\}$ at the intersections distinguish the pole-energy solutions $\{\varepsilon_q\}$ from those of the true eigenvalues $\{E_k\}$. As was proved in the previous subsections, the energy derivatives, denoted by $\{F'_m(E)\}$, should be $F'_m(E) = 0$ for $E = E_k$ and $F'_m(E) = 2$ for $E = \varepsilon_q$. With these simple regulations for $\{F'_m(E)\}$ we can easily specify the solutions of the true eigenvalues $\{E_k\}$.

We next figure out, from the intersections of the graphs, roughly estimated solutions for $\{F_m(E) = E\}$. Starting with these approximate solutions, we proceed to make further precise calculations for the solutions. For this purpose we employ a combined method of the secant and the Newton-Raphson methods [23]. The algorithm of this method is as follows: Let us define a function $f(E)$ as $f(E) \equiv E - F(E)$, where $F(E)$ is one of the functions $\{F_m(E)\}$. The solutions to $F_m(E) = E$ are obtained as the roots of $f(E) = 0$. Suppose that E_a and E_b be two values which bracket one of the roots and satisfy $E_a < E_b$ and $f(E_a)f(E_b) < 0$. We suppose also that $f(E)$ is a monotone function on the interval $E_a < E < E_b$. These suppositions on E_a and E_b follow that only one root exists on the interval $E_a < E < E_b$. As shown in Fig. 1, we further determine five points according to

$$e_1 = E_a, \tag{43}$$

$$e_2 = \frac{E_a f(E_b) - E_b f(E_a)}{f(E_b) - f(E_a)}, \tag{44}$$

$$e_3 = E_a - \frac{f(E_a)}{f'(E_a)}, \tag{45}$$

$$e_4 = E_b - \frac{f(E_b)}{f'(E_b)}, \tag{46}$$

$$e_5 = E_b. \tag{47}$$

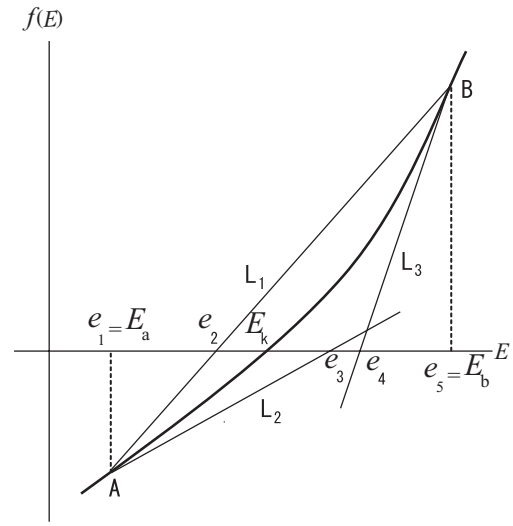

FIG. 1. Graphical representation of the modified secant method. L_1 is the straight line passing through the points A and B. L_2 and L_3 are the tangents to the function $f(E)$ at the points A and B, respectively. See text for detailed explanation.

The value e_2 in Eq. (44) is the better approximate solution in the usual secant method. The e_3 and e_4 are the approximate values in the Newton-Raphson method. We can easily select two values, e_i and e_j, among $\{e_1, e_2, \ldots, e_5\}$ such that they are neighboring on the E axis and satisfy $E_a \leqslant e_i < e_j \leqslant E_b$ and $f(e_i)f(e_j) < 0$. These conditions mean that one of the roots exists on the interval $e_i < E < e_j$. We then replace E_a and E_b as $E_a = e_i$ and $E_b = e_j$ and repeat the procedure again. This modified secant method derives surely one of the roots on the interval $E_a < E < E_b$. We also note that this method will lead to fast convergence, because we calculate approximate solutions according to the Newton-Raphson method.

We here wish to emphasize that this method is not an iteration method. The procedure in this method always derives a convergent solution to $f(E) = 0$ on the interval $E_a < E < E_b$ and never reaches any of the solutions outside the interval. Therefore, we can always control convergence and select solutions to be reproduced by selecting starting values E_a and E_b properly. Only one problem in the present method is how to choose E_a and E_b. Then the use of the graphs of $\{y = F_m(E)\}$ would be helpful. If the graphs are drawn accurately, we can determine easily these starting energies E_a and E_b.

III. TEST CALCULATIONS

In order to assess the present method we consider a model problem for which exact results can be obtained easily. The model we adopt here [21] is a slightly modified version of the one which was introduced many years ago to study the intruder state problem [24,25]. The dimensions of the entire space and the P space are four and two ($d = 2$), respectively. The degenerate unperturbed energy is taken to be $E_0 = 1$, and the interaction V is given with the coupling strength x. The relevant matrix elements are given by

$$PH_0P = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad PVP = \begin{pmatrix} 0 & 5x \\ 5x & 25x \end{pmatrix}, \quad PVQ = \begin{pmatrix} -5x & 5x \\ 5x & -8x \end{pmatrix}, \tag{48}$$

and

$$QHQ = \begin{pmatrix} 3 - 5x & x \\ x & 9 - 5x \end{pmatrix}. \tag{49}$$

We present in Table I the results of the iterative calculations, based on Eq. (40) for the KK and Eq. (42) for the EKK methods. The coupling strength x in the model Hamiltonian is taken to be $x = 0.05$. Table I shows the results for the lowest and second-lowest eigenvalues of H. We observe that the convergence in the EKK method is much faster than that in the KK method. The EKK iteration reaches convergence to 14 decimal places after three iterations. It is also impressive that the KK iteration shows linear and steady convergence. As has already been discussed in Sec. II, the iteration in the EKK method is essentially equivalent to that in the Newton-Raphson method which derives quadratic convergence. The calculation in the EKK method verifies this theoretical prediction that the number of correct digits is doubled at each iteration.

TABLE I. Convergence of the eigenvalues of the lowest-lying and second lowest-lying states obtained in the iterations $E^{(n+1)} = G_m(E^{(n)})$ and $E^{(n+1)} = F_m(E^{(n)})$ for the KK and for the EKK methods, respectively, for the model Hamiltonian with the strength $x = 0.05$. Correct digits in the KK and the EKK methods are given for n, namely the number of iterations. The starting energies $(E_1^{(1)}, E_2^{(1)})$ are taken to be (0.0, 0.0). The notation c indicates convergence to more than 15 decimal places. The exact eigenvalues here are $E_1 = 0.890\,450\,485\,886\,9942$ and $E_2 = 2.215\,680\,815\,009\,6040$.

n	Correct digits (KK)	Correct digits (EKK)
1	0.9···	0.89···
2	0.88···	0.890 450···
3	0.8904···	0.890 450 485 886 99···
4	0.890 450···	c
5	0.890 4504···	c
6	0.890 450 485···	c
7	0.890 450 4858···	c
1	2.2···	2.2···
2	2.21···	2.215 68···
3	2.215···	2.215 680 8150···
4	2.2156···	c
5	2.215 68···	c
6	2.215 680···	c
7	2.215 6808···	c
8	2.215 680 81···	c
9	2.215 680 815···	c

We depict, in Figs. 2 and 3, the dependence of the functions $\{G_m(E); m = 1, 2\}$ and $\{F_m(E); m = 1, 2\}$, respectively, on the energy variable E with the coupling strength $x = 0.2$. One observes in Fig. 2 that there are two poles in the graphs

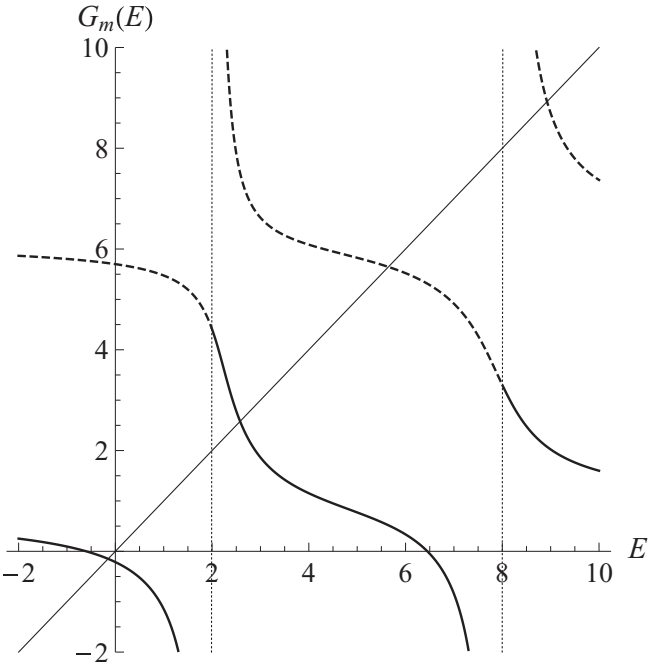

FIG. 2. Dependence of $\{G_m(E)\}$ on E with $x = 0.2$. The graphs of $y = G_1(E)$ and $y = G_2(E)$ are shown in solid and broken lines, respectively. The graph of $y = E$ is also shown.

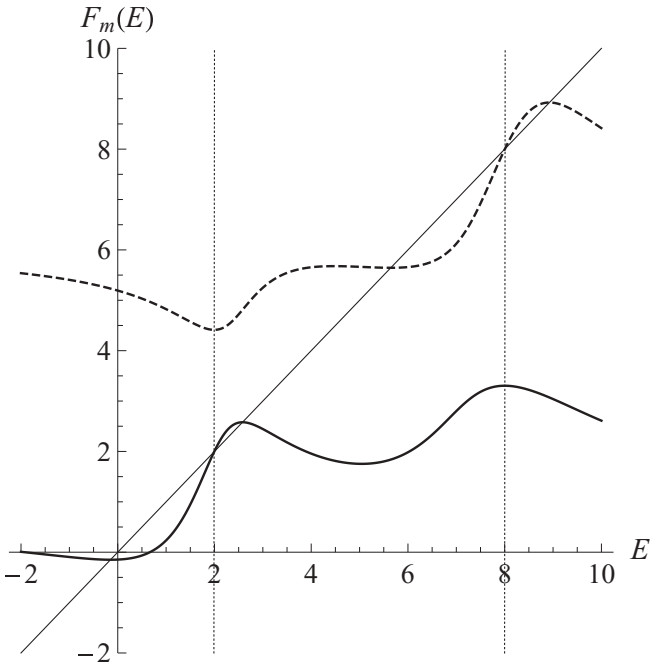

FIG. 3. Dependence of $\{F_m(E)\}$ on E with $x = 0.2$. The graphs of $y = F_1(E)$ and $y = F_2(E)$ are shown in solid and broken lines, respectively. The graph of $y = E$ is also shown.

of $\{G_m(E)\}$ associated with the $\hat{Q}$ box. On the other hand, the poles disappear in the graphs of $\{F_m(E)\}$ associated with the $\hat{Z}$ box. One sees four intersections of $y = G_m(E)$ and $y = E$, and six intersections of $y = F_m(E)$ and $y = E$ for $m = 1, 2$. Among the six intersections two of these correspond to the pole energies, the eigenvalues of QHQ. The energy derivatives $\{F'_m(E)\}$ at the intersections should be zero for the true eigenvalues of H, which are shown in Eq. (21). On the contrary the energy derivatives $\{F'_m(E)\}$ at the intersections should be two for the solutions of the pole energies. The number of the intersections in the graphs of $\{G_m(E)\}$ and $\{F_m(E)\}$ is verified as already predicted in Sec. II. The theoretical predictions on the energy derivatives $\{F'_m(E)\}$ of these functions are also verified as shown in Fig. 3.

We can obtain, from these graphs in Figs. 2 and 3, much information on the convergence conditions in some iteration methods. One observes in Fig. 2 that the energy derivatives of the first and third low-lying intersections are less than one and those of the second and fourth are larger than one. From these observations we may say that the iteration in Eq. (40) cannot reproduce the second and fourth eigenvalues of H. On the other hand, one sees from Fig. 3 that there are four intersections with zero energy derivatives. This means that the iteration in Eq. (42) in the EKK method always converges to any of the four true eigenvalues of H.

We made another numerical calculation by using the $\hat{Z}$ box and the associated function $F_m(E)$ in the modified secant method. Tables II, III, and IV show the results for the coupling strength $x = 0.05$, 0.1, and 0.2, respectively. The starting energies E_a and E_b are taken as approximate solutions for the intersections of the graphs of $\{y = F_m(E)\}$ and $y = E$. The results show that all the solutions to Eq. (18) are reproduced. They include the four true eigenvalues $\{E_1, \ldots, E_4\}$ of H and the two pole energies $\{\varepsilon_{q_1}, \varepsilon_{q_2}\}$. The values of the energy derivatives $\{F'_m(E)\}$ at the solutions were also calculated. As

TABLE II. Convergence of the solutions obtained with the graphical method for the model Hamiltonian with the strength $x = 0.05$. The E_i and $F'(E_i)$ for $1 \leqslant i \leqslant 4$ are the true eigenvalues of H and the energy derivatives of $\{F_m(E)\}$ at $E = E_i$, respectively. The ε_{q_1} and ε_{q_2} are the solutions for the pole energies. The $F'_m(\varepsilon_{q_1})$ and $F'_m(\varepsilon_{q_2})$ are the energy derivatives of $\{F_m(E)\}$ at $E = \varepsilon_{q_1}$ and ε_{q_2}, respectively. The notation c indicates convergence to more than six decimal places. The number of repeats in the modified secant method is given by n. The exact values for the solutions are also given.

n	E_1	$F'(E_1)$	E_2	$F'(E_2)$
1	0.890 462	$<10^{-6}$	2.215 995	0.00011
2	0.890 450	$<10^{-6}$	2.215 681	$<10^{-6}$
3	c	$<10^{-6}$	c	$<10^{-6}$
Exact	0.890 450	0.0	2.215 681	0.0
(E_a, E_b)	(0.8, 0.9)		(2.2, 2.3)	
n	E_3	$F'(E_3)$	E_4	$F'(E_4)$
1	2.837 465	0.413 35	8.781 060	0.041 25
2	2.860 730	0.022 42	8.781 706	0.000 14
3	2.862 158	0.000 04	8.781 708	$<10^{-6}$
4	2.862 161	$<10^{-6}$	c	$<10^{-6}$
Exact	2.862 161	0.0	8.781 708	0.0
(E_a, E_b)	(2.8, 2.9)		(8.78, 8.80)	
n	ε_{q_1}	$F'(\varepsilon_{q_1})$	ε_{q_2}	$F'(\varepsilon_{q_2})$
1	2.750 350	1.988 29	8.751 088	1.957 24
2	2.749 587	1.999 95	8.750 417	1.999 99
3	2.749 583	2.000 00	c	2.000 00
Exact	2.749 583	2.0	8.750 417	2.0
(E_a, E_b)	(2.70, 2.75)		(8.70, 8.77)	

TABLE III. Convergence of the solutions obtained with the graphical method for the model Hamiltonian with the strength $x = 0.1$.[a]

n	E_1	$F'(E_1)$	E_2	$F'(E_2)$
1	0.648 389	0.000 02	2.552 215	0.046 47
2	0.648 250	$<10^{-6}$	2.553 840	0.000 16
3	c	$<10^{-6}$	2.553 845	$<10^{-6}$
Exact	0.648 250	0.0	2.553 845	0.0
(E_a, E_b)	(0.6, 0.7)		(2.55, 2.65)	
n	E_3	$F'(E_3)$	E_4	$F'(E_4)$
1	3.649 852	0.000 05	8.647 500	0.003 92
2	3.650 111	$<10^{-6}$	8.647 794	$<10^{-6}$
3	c	$<10^{-6}$		$<10^{-6}$
Exact	3.650 111	0.0	8.647 794	0.0
(E_a, E_b)	(3.6, 3.7)		(8.63, 8.65)	
n	ε_{q_1}	$F'(\varepsilon_{q_1})$	ε_{q_2}	$F'(\varepsilon_{q_2})$
1	2.498 646	1.991 21	8.501 897	1.996 93
2	2.498 334	1.999 99	8.501 666	2.000 00
3	c	2.000 00	c	2.000 00
Exact	2.498 334	2.0	8.501 666	2.0
(E_a, E_b)	(2.48, 2.50)		(8.50, 8.52)	

[a]Notations as in Table II.

already proved in Sec. II theoretically, the energy derivative at the true eigenvalues of H should be zero and, on the other hand, two at the pole energies. These theoretical predictions are also confirmed numerically. From this difference of the derivatives of $F_m(E)$ we can easily classify the solutions into two parts, the true eigenvalues of H and the pole energies.

As a whole the convergence rates are reasonable in the cases with the coupling strength $x = 0.05$, 0.1, and 0.2. Three steps of the calculations in the modified secant method are enough for yielding the results with accuracy to six decimal places. However, the convergence depends strongly on the choice of the starting energies (E_a, E_b). When the spacing of two solutions among $\{E_k\}$ and $\{\varepsilon_q\}$ is very narrow, we need to draw graphs accurately enough to find approximate values of $\{E_a, E_b\}$ to bracket each of the solutions.

IV. CONCLUDING REMARKS

We have introduced a vertex function called the $\hat{Z}$ box, which is an operator defined in a model space and a function of an energy E. The $\hat{Z}$ box is constructed in terms of the $\hat{Q}$ box and its energy derivative originated by Kuo *et al.* We have proved that a new expression of the effective interaction can be derived by replacing the $\hat{Q}$ box by the $\hat{Z}$ box in the KK

TABLE IV. Convergence of the solutions obtained with the strength $x = 0.2$.[a]

n	E_1	$F'(E_1)$	E_2	$F'(E_2)$
1	−0.149 272	0.000 08	2.577 187	0.005 35
2	−0.149 586	$<10^{-6}$	2.579 424	$<10^{-5}$
3	c	$<10^{-6}$	2.579 425	$<10^{-6}$
Exact	−0.149 586	0.0	2.579 425	0.0
(E_a, E_b)	(−0.2, −0.1)		(2.5, 2.6)	
n	E_3	$F'(E_3)$	E_4	$F'(E_4)$
1	5.645 253	0.000 03	8.923 645	0.002 44
2	5.645 051	$<10^{-6}$	8.925 109	$<10^{-5}$
3	c	$<10^{-6}$	8.925 110	$<10^{-6}$
Exact	5.645 051	0.0	8.925 110	0.0
(E_a, E_b)	(5.6, 5.7)		(8.9, 9.0)	
n	ε_{q_1}	$F'(\varepsilon_{q_1})$	ε_{q_2}	$F'(\varepsilon_{q_2})$
1	1.993 869	1.998 86	8.007 196	1.999 21
2	1.993 341	2.000 00	8.006 659	2.000 00
3	c	2.000 00	c	2.000 00
Exact	1.993 341	2.0	8.006 659	2.0
(E_a, E_b)	(1.9, 2.0)		(8.0, 8.1)	

[a]Notations as in Table II.

method. With the $\hat{Z}$ box we have also introduced a set of scalar functions $\{F_m(E)\}$. It has been shown that the $\hat{Z}$ box and the associated functions $\{F_m(E)\}$ have the following properties:

(i) The true eigenvalues $\{E_k\}$ of the original Hamiltonian H can be given by the roots of a set of equations $\{F_m(E) = E\}$. These equations have the roots, as additional solutions, at the pole energies $\{\varepsilon_q\}$ of the $\hat{Q}$ box.
(ii) The $\hat{Z}$ box and the functions $\{F_m(E)\}$ have no singularities even at the poles of the $\hat{Q}$ box, and they are well-behaved functions of E.
(iii) The derivatives of $\{F_m(E)\}$ at the solutions for E take two values, i.e., zero at the true eigenvalues $\{E_k\}$ of H and two at the pole energies $\{\varepsilon_q\}$.

On the basis of the properties (i), (ii), and (iii), we have proposed an iteration scheme written as $E^{(n+1)} = F_m(E^{(n)})$. This iteration always converges and reproduces the true eigenvalues $\{E_k\}$ of H. Since the energy derivatives of $\{F_m(E)\}$ at the solutions for $\{E_k\}$ are always zero, this method can be understood to be equivalent to the Newton-Raphson method used to solve nonlinear equations. The Newton-Raphson iteration derives quadratic convergence. Therefore, we can expect that this new iteration leads to fast convergence. We have carried out a test calculation and confirmed the quadratic convergence.

As another method for solving a set of equations $\{F_m(E) = E\}$, we have proposed an noniterative method which we call the graphical method. The solutions of these equations can be obtained as the energies at the intersections of the graphs $\{y = F_m(E)\}$ and $y = E$. Using the property (iii) we can classify the intersections into two parts, i.e., those for the solutions of the true eigenvalues $\{E_k\}$ and of the pole energies $\{\varepsilon_q\}$. These graphs make us possible to estimate roughly the positions of the roots. With approximate solutions obtained from the graphs we proceed to make more accurate calculations of the solutions, where we have employed a modified secant method which is a combined method of the secant and the Newton-Raphson methods. This method has been shown to provide a suitable scheme for obtaining accurate results if we start with approximate energies close to the solutions.

We have made test calculations to assess the graphical method. We have confirmed numerically that the modified secant method reproduces successfully all the solutions, including the true eigenvalues $\{E_k\}$ of H and the pole energies $\{\varepsilon_q\}$. The theoretical predictions in the property (iii) on the energy derivatives of $\{F_m(E)\}$ are also verified numerically. We wish to note that the graphical method, implemented by the modified secant method, yields always convergent results, where we do not need any information on the eigenstates and/or the eigenvalues of H such as P-space overlaps and/or energy spacings.

We may conclude that the present approach, the graphical method with the vertex function $\hat{Z}(E)$, would be promising in resolving some of the difficulties in the derivation of the effective interaction.

ACKNOWLEDGMENTS

We are grateful to T. T. S. Kuo, D. Rowe, and L. Coraggio for their helpful and stimulative discussions. We also thank H. Kamada, H. Kimura, and S. Maeda for their computational advices.

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