Convergence properties of the effective interaction

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The convergence properties of two perturbative schemes to sum the so-called folded diagrams are critically reviewed in this work, with an emphasis on the intruder state problem. The methods we study are the approaches of Kuo and co-workers and Lee and Suzuki. The suitability of the two schemes for shell-model calculations is discussed.

I. INTRODUCTION

Recent works on the theory of the effective interaction for finite nuclei, have focussed on properties like hermiticity and the order-by-order convergence of the perturbative expansion for the effective interaction [1-4]. Especially, techniques to sum up subsets of diagrams to infinite order have received increased interest. Two such schemes are the summation of folded diagrams by Kuo and co-workers, exposed in ref. [5] (hereafter referred to as the FD method), and the approach proposed by Lee and Suzuki [6] (hereafter referred to as the LS method). The starting point for these iterative schemes is to define the so-called $Q$-box, which in a diagrammatic language means the sum of all valence-linked and irreducible diagrams to a given order in the interaction. The $Q$-box depends on the so-called starting energy, defined as the unperturbed energy of the interacting nucleons.

The purpose of these methods is to calculate an effective interaction $H_{\text{eff}}$ in order to reduce the full shell model eigenvalue problem, to one which is tractable within a physically selected space, the so-called model space. One then obtains a secular equation

$$PH_{\text{eff}}P|\Psi\rangle = E_P P|\Psi\rangle,$$  \hspace{1cm} (1)

acting solely within the model space, defined by the projection operator $P$, which projects out the model-space components of the true eigenfunction $|\Psi\rangle$. The quantity $E_P$ is the model-space eigenvalue, and the $d$ eigenvalues $E_P$ ($d$ being the dimension of the model space) are supposed to reproduce the corresponding exact eigenvalues $E_Q$. The degrees of freedom not represented by the model space are supposed to be taken care of by the perturbative expansion. The excluded degrees of freedom are obtained through use of the projection operator $Q$, with $P + Q = 1$ and $PQ = 0$. The corresponding eigenvalues are $E_Q$.

The above techniques have been applied extensively to light nuclei, in particular to the nuclei $^{18}$O and $^{42}$Ca where the model space is rather simple, two particles in the $sd$- or $pf$-shells, respectively. Here, however, a special problem occurs, in the literature called the intruder-state problem. In short, this means that the $P$- and $Q$-states do not separate. Experimentally, it is rather well established that the first excited $0^+$ state in both $^{18}$O and $^{42}$Ca is dominated by $Q$-state components, i.e. shell model configurations outside the $sd$- or $pf$-shell. Then a comparison between theory and experiment becomes difficult. Using the FD method to calculate $H_{\text{eff}}$, eq. (1) should reproduce the experimental levels dominated by the $P$-state configurations. For the two examples mentioned above this means that the first excited $0^+$ state in both $^{18}$O and $^{42}$Ca should not be accounted for by the theory. On the other hand the LS method, for a properly chosen starting energy, should be able to reproduce the $d$ lowest states of e.g., $^{18}$O and $^{42}$Ca, irrespectively of whether or not they are dominated by $Q$-space components. In view of this, one might expect the FD effective interaction to be more appropriate for shell-model calculations than the LS one. An important application of such an effective interaction is spectroscopic shell-model analyses of systems with more than two valence particles, and then only $P$-space degrees of freedom are considered.
In several papers, e.g., ref. [2], we have investigated the above mentioned nuclei using both the FD and the LS methods. Our results show little difference in the final energy spectra. The question then arises how one should relate the energy levels calculated by respectively the FD and LS methods to the experimental levels.

In the present paper we investigate this problem in more detail and explore the convergence properties of the FD and LS methods in the presence of so-called intruder states. In the next section we employ a simple $2 \times 2$ model to study the difference between calculations with a complete and a limited perturbation expansion. Then in section 3 we apply the FD and LS methods to the nucleus $^{18}$O, in order to test if differences seen in the exactly solvable model pertain to the realistic case as well. Of importance here is the fact that the simple $2 \times 2$ model allows us to define an exact $Q$-box, whereas in the realistic cases the $Q$-box must be approximated to a given order in the interaction. Finally, our conclusions are drawn in section 4.

II. INTRUDER STATES IN AN EXACTLY SOLVABLE MODEL

It is a well-known fact that the presence of so-called intruder states [5,7] may lead to divergence of the order-by-order pertubative expansion for $H_{\text{eff}}$.

One way to handle intruder states is that of introducing an enlarged model space which includes intruder configurations. Such calculations do however become prohibitively time-consuming for nuclei heavier than $sd$-shell nuclei. There are also other approaches which aim at overcoming the divergence of the order-by-order expansion of $H_{\text{eff}}$. One may, e.g., regroup the perturbative expansion and perform infinite partial summations to obtain convergence. Two such possibilities are represented by the summation of the folded diagrams by the FD and LS schemes discussed above. To better understand the above convergence arguments and the structure of the folded-diagram and the Lee-Suzuki methods we will first demonstrate certain properties of these methods by considering a simple $2 \times 2$ model, employed e.g. by the authors of ref. [8] in their discussion of perturbative many-body approaches. Moreover, the model can be used to demonstrate the connection between intruder states and the convergence of the perturbative expansion. Last but not least, this model allows us to define an exact $Q$-box, which in turn can be used to make statements about the convergence of the FD and LS iterative schemes.

However, first we need to repeat the equations pertinent to the FD and LS methods. The effective interaction for the FD method is given by

$$H_{\text{eff}} = H_0 + \lim_{n \to \infty} V^{(n)}_{\text{eff}},$$

with

$$V^{(n)}_{\text{eff}} = \sum_{m=0}^{\infty} Q_m \left\{ V^{(n-1)}_{\text{eff}} \right\}^m.$$  \hspace{1cm} (3)

Here we have defined $Q_m = \frac{1}{m!} \frac{d^m Q}{d \omega^m}$. The energy $\omega$ is the so-called starting energy, defined as the unperturbed energy of the interacting nucleons.

The Lee and Suzuki (LS) expansion for the effective interaction is given as [6]

$$H_{\text{eff}} = H_0 + \lim_{n \to \infty} R_n,$$

with

$$R_n = \left[ 1 - \hat{Q}_1 - \sum_{m=2}^{n-1} \hat{Q}_m \prod_{k=n-m+1}^{n-2} R_k \right]^{-1} \hat{Q}.$$  \hspace{1cm} (5)

Eqs. (3) and (4) differ not only in structure, but also in convergence properties. The convergence criterion for the method of Lee and Suzuki is related to the choice of the so-called starting energy $\omega$ only. The LS expansion converges to those eigenvalues which are closest to $\omega$, which means that we should be able even to reproduce the $Q$-space eigenvalues given an appropriate starting energy. This means that if the LS expansion converges for the $0^+_2$ state of, e.g. $^{18}$O, the structure of the exact wave function does not correspond to that of the two-particle space we have chosen. In contrast, the FD-method converges to the states dominated by the model-space components.

In order to study the importance of intruder states, we let our hamiltonian depend linearly on a strength parameter $z$. 

3
Below we will let state $P$ represent the model-space eigenvalue whereas state $Q$ represents the eigenvalue of the excluded space. The unperturbed solutions to this problem are

\[ H_0 \Phi_P = \epsilon_P \Phi_P \]  

and

\[ H_0 \Phi_Q = \epsilon_Q \Phi_Q, \]  

with $\epsilon_P < \epsilon_Q$. We label the off-diagonal matrix elements $X$, while $X_P = \langle \Phi_P | H_1 | \Phi_P \rangle$ and $X_Q = \langle \Phi_Q | H_1 | \Phi_Q \rangle$. The exact solutions given by eq. (9) are shown in fig. 1 as functions of the strength parameter $z$. Pertinent to our choice of parameters, is that at $z \geq 2/3$, the lowest eigenstate is dominated by $\Phi_P$ while the upper is $\Phi_Q$. At $z = 1$ the $\Phi_P$ mixing of the lowest eigenvalue is $1\%$ while for $z \leq 2/3$ we have a $\Phi_P$ component of more than $90\%$. The character of the eigenvectors has therefore been interchanged when passing $z = 2/3$. The value of the parameter $X$ represents the strength of the coupling between the model space and the excluded space. Thus, this simple model allows us to study how the perturbation expansion with a model space defined to consist of state $P$ only, behaves as the interaction strength $z$ increases. The order-by-order convergence in eq. (10) was discussed by the authors of ref. [8]. Here we will thence only repeat their conclusion: For small values of $z$ one obtains good convergence to the lower eigenvalue. For larger values of $z$ (i.e. $z > 2/3$), increasing orders in the perturbation expansion yield a divergent perturbation series, as expected [8]. However, it may be possible to rewrite the perturbative expansion in such a way that one sums subsets of diagrams to all orders. The hope is then that the expansion becomes convergent for appropriate infinite partial summations. This is actually the philosophy behind both the FD method and the LS method. Having defined a set of linked and irreducible valence diagrams, the so-called $\hat{Q}$-box we can define an iterative scheme to sum the contributions from folded diagrams. The $\hat{Q}$-box serves therefore as the starting point for our iterative schemes, and within the framework of our $2 \times 2$ model we can study the FD and LS methods for various approximations of the $\hat{Q}$-box. As an example, to fifth order in the parameter $z$ we have

\[ \hat{Q}_5 = z X_P + \frac{z^2 X^2}{\epsilon_P - \epsilon_Q} + \frac{z^3 X^2 X_Q}{(\epsilon_P - \epsilon_Q)^2} + \frac{z^4 X^2 X_Q^2}{(\epsilon_P - \epsilon_Q)^3} + \frac{z^5 X^2 X_Q^3}{(\epsilon_P - \epsilon_Q)^4}, \]  

and it is easy to see that a $\hat{Q}$-box of order $l + 2$ can be written as

\[ \hat{Q}_{l+2} = z X_P + \frac{z^2 X^2}{\epsilon_P - \epsilon_Q - z X_Q} \left\{ 1 - \left( \frac{z X_Q}{\epsilon_P - \epsilon_Q} \right)^{l+1} \right\}, \]  

which in the limit $l \to \infty$ gives\textsuperscript{1}\textsuperscript{2}.

\textsuperscript{1} The $\hat{Q}$-box should not be confused with the exclusion operator $Q$.

\textsuperscript{2} $l = 0$ gives a second-order $\hat{Q}$-box, $l = 1$ a third-order $\hat{Q}$-box and so forth.
\[
\dot{Q}_{\text{exact}} (\epsilon_P) = z X_P + \frac{z^2 X^2}{\epsilon_P - \epsilon_Q - z X_Q},
\]

(12)

if

\[
\left| \frac{z X_Q}{\epsilon_P - \epsilon_Q} \right| < 1.
\]

(13)

The latter equation clearly restricts the possible values of \(\epsilon_P\) for given \(X_Q\) and \(\epsilon_Q\). Actually, if we let \(\epsilon_P\) vary, our choices for \(X_Q\) and \(\epsilon_Q\) restrict \(\epsilon_P\) to \(\epsilon_P \leq 1\) and \(\epsilon_P \geq 7\), in order to have a finite \(\dot{Q}\)-box.

The exact \(\dot{Q}\)-box may be used to define the first iteration of the FD expansion as a function of the starting energy \(\omega\) as

\[
\lambda_1 = \omega + \dot{Q}_{\text{exact}} (\omega)
\]

(14)

The subsequent steps are

\[
\lambda_2 = \lambda_1 + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \dot{Q}}{d\omega^m} (\lambda_1 - \omega)^m,
\]

(15)

and

\[
\lambda_3 = \lambda_1 + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \dot{Q}}{d\omega^m} (\lambda_2 - \omega)^m.
\]

(16)

In general we have

\[
\lambda_n = \lambda_1 + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \dot{Q}}{d\omega^m} (\lambda_{n-1} - \omega)^m.
\]

(17)

If this iteration scheme converges we have, with \(\lambda = \lambda_n = \lambda_{n-1}\),

\[
\lambda = \omega + z X_P + \frac{z^2 X^2}{\lambda - \epsilon_Q - z X_Q},
\]

(18)

which is just eq. (9), so that we have obtained the true eigenvalues. In a similar way we can use the LS expansion defined in eq. (4) to sum the folded diagrams.

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**TABLE I.** The exact solutions \(E_P\) (model space) and \(E_Q\) (excluded space) of eq. (9) as functions of the strength parameter \(z\). The results obtained with the LS and FD methods with an exact \(\dot{Q}\)-box as functions of the starting energy \(\omega\) are also given.

| \(\omega\) | \(z\) | \(E_P\) | \(E_Q\) | \(F D\) | \(L S\) |
|---|---|---|---|---|---|
| 0.5 | 0.0 | 0.00 | 4.00 | 0.00 | 0.00 |
| & 0.2 | 0.60 | 3.40 | 0.60 | 0.60 |
| & 0.4 | 1.20 | 2.80 | 1.20 | 1.20 |
| & 0.6 | 1.77 | 2.23 | 1.77 | 1.77 |
| & 0.7 | 2.17 | 1.83 | 2.17 | 1.83 |
| & 0.8 | 2.43 | 1.57 | 2.43 | 1.57 |
| & 1.0 | 3.02 | 0.98 | 3.02 | 0.98 |
| 7.5 | 0.0 | 0.00 | 4.00 | 0.00 | 4.00 |
| & 0.2 | 0.60 | 3.40 | 0.60 | 3.40 |
| & 0.4 | 1.20 | 2.80 | 1.20 | 2.80 |
| & 0.6 | 1.77 | 2.23 | 1.77 | 2.23 |
| & 0.7 | 2.17 | 1.83 | 2.17 | 2.17 |
| & 0.8 | 2.43 | 1.57 | 2.43 | 2.43 |
| & 1.0 | 3.02 | 0.98 | 3.02 | 3.02 |

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\(^3\)We replace here \(\epsilon_P\) with \(\omega\).
We demonstrate the properties of the LS and FD methods with an exact \( \hat{Q} \)-box in table 1 for two starting energies, 0.5 and 7.5 (arbitrary units). Clearly, we see that with a starting energy 0.5 the LS method yields the \( Q \)-space eigenvalue at \( z \geq 2/3 \). Below \( z = 2/3 \), the LS method reproduces the \( P \)-space eigenvalue. With a starting energy of 7.5, the LS method gives the \( Q \)-space eigenvalue for \( z \leq 2/3 \), whereas the \( P \)-space eigenvalue is reproduced for \( z \geq 2/3 \). Thus, this simple model demonstrates nicely the properties of the LS scheme, i.e. it converges to those eigenvalues which are closest to the chosen starting energy, irrespectively of the structure of the wave function. From table 1 we also see that the FD method always reproduces the \( P \)-space eigenvalue. At \( z = 2/3 \), the FD scheme does not stabilize, the eigenvalue fluctuates and there is no convergence. More precisely this means that we can not go from the lower to the upper eigenvalue along the real axis \( z \). The fluctuation is intimately connected to the convergence criterion for the FD scheme. If one of the solutions contains more than 50% valence state intensity, the FD method converges to that solution. At \( z = 2/3 \), equal admixtures of \( \Phi_P \) and \( \Phi_Q \) occur in the true wave functions.

This simple example, starting with the exact \( \hat{Q} \)-box, serves to demonstrate significant differences in convergence behavior of the two methods. Of importance is the fact that with the LS scheme we are able to reproduce a \( Q \)-space state insofar we define a starting energy which is close to the actual \( Q \)-space state. However, in actual nuclear structure calculations, we are not able to define an exact \( \hat{Q} \)-box. The question we wish to bring to the attention in this work, is if an approximation of the \( \hat{Q} \)-box still gives the same difference between the LS and FD methods at \( z = 1 \). To shed light on this, we exhibit in fig. 1 results obtained with various low-order approximations to the \( \hat{Q} \)-box, recall eq. \([\text{11}]\). The starting energy for the LS and FD calculations was set equal 0.5, since we are interested in seeing if the convergence criterion for the LS method holds for an approximate \( \hat{Q} \)-box. Clearly, with a \( \hat{Q} \)-box of second order in the interaction, the difference\(^4\) between the LS and the FD method is negligible. A second-order \( \hat{Q} \)-box corresponds to setting \( X_Q = 0 \), which means that in the range of physically interesting \( z \) values \( (0 \leq z \leq 1) \) there is no intruder state, yielding an approximately straight line for the LS method. Up to fourth order in the interaction, both the LS and FD methods yield almost the same value. With a fifth-order \( \hat{Q} \)-box the FD method becomes unstable at \( z = 1 \). This can be inferred from the structure of the FD expansion, which with a fifth-order \( \hat{Q} \)-box reads

\[
\lambda_n = \epsilon_P + zX_P + \frac{z^2X^2}{\lambda_{n-1} - \epsilon_Q} + \frac{z^3X^2X_Q}{(\lambda_{n-1} - \epsilon_Q)^2} + \frac{z^4X^2X_Q^2}{(\lambda_{n-1} - \epsilon_Q)^3} + \frac{z^5X^2X_Q^3}{(\lambda_{n-1} - \epsilon_Q)^4}.
\]

The first iteration is just \( \lambda_1 = \epsilon_P + \hat{Q} \), which gives a result close to the model space eigenvalue \( \approx 3 \) at \( z = 1 \). Inserting \( \lambda_1 \) and higher iterations in the above expansion results in an FD expansion which for each iteration will fluctuate between a large value \( \lambda \) and \( \epsilon_P + X_P \). The large eigenvalue stems from the fact that the energy denominators in the higher-order terms become small. With \( X = 0.2 \) this oscillating behavior sets inn already at fifth order in the interaction, whereas if we choose the coupling between the model space and the excluded space to be \( X = 0.01 \), this divergence appears first with a \( \hat{Q} \)-box of tenth order. However, we will ultimately end up with a series which fluctuates, except for the trivial case \( X = 0 \). With the given parameters and a \( \hat{Q} \)-box of tenth or higher order in the interaction, the FD method converges only if \( z < 2/3 \). If the FD method converges, we obtain a result close to the model-space eigenvalue, and, if the coupling between the model space and the excluded space is weak, low-order perturbation theory works rather well.

\(^4\)It ought be emphasized that all results with either the FD or the LS method represent converged eigenvalues, which means that contributions from folded diagrams to high order are included.
FIG. 1. Exact solutions (solid line) and the results obtained with the FD and LS methods with various approximations to the $\hat{Q}$-box. FD-2nd and LS-2nd (dashed line) indicate that the FD and LS methods were used with a second-order $\hat{Q}$-box, while FD-4th and LS-4th are the results obtained with a fourth-order $\hat{Q}$-box. Similarly, LS-10th and LS-50th are the LS results with a tenth- and fiftieth-order $\hat{Q}$-box, respectively. A starting energy 0.5 was chosen in all calculations.

For the LS method we note that with a low-order $\hat{Q}$-box we are not able to reproduce the lowest eigenstate, even with an adequately chosen starting energy, as stated by the convergence criterion of the LS method. We actually have to go as far as to a $\hat{Q}$-box of fiftieth order before we get a result close to the lowest eigenvalue. However, if the order of the $\hat{Q}$-box is further increased (≈ 150 with the above parameters), even the LS method diverges. Thus, in summary, the general convergence properties of the LS method discussed in the introduction are demonstrated only for an exact $\hat{Q}$-box. If the $\hat{Q}$-box is approximated to a given order in the interaction, the convergence criterion cannot be applied.

The implications of these results for the more realistic cases will be discussed in the next section.

III. REALISTIC EFFECTIVE INTERACTIONS

In calculations of effective interactions for $^{18}\text{O}$, one normally chooses a model space consisting of a closed $^{16}\text{O}$ core with two nucleons in the single-particle states of the $sd$-shell. This model space consists of two-particle states only, and for $J = 0$ we have three $0^+$ states. However, from model calculations of energies and electromagnetic properties
and experimental data, the belief is that the $0^+_2$ state is predominantly of a four-particle-two-hole nature, while the ground state and the $0^+_3$ state are classified as two-particle states [9].

Before we proceed to study the convergence behavior of the folded-diagram and Lee-Suzuki expansions, let us first show how one can obtain useful information about the structure of the eigenstates from the slopes of the eigenvalues as functions of the starting energy $\omega$. Using the property $P + Q = 1$, we can rewrite the energy dependent eigenvalue problem as

$$\begin{pmatrix} PHP & PHQ \\ QHP & QHQ \end{pmatrix} \begin{pmatrix} P\Psi \\ Q\Psi \end{pmatrix} = E \begin{pmatrix} P\Psi \\ Q\Psi \end{pmatrix},$$

(19)

where $E$ is the exact eigenvalue. From eq. (19) we obtain

$$E \langle P\Psi|P\Psi \rangle = \langle P\Psi|PHP + PHQ \frac{1}{\omega - QHQ}QHP|P\Psi \rangle,$$

(20)

with $\omega = E$ and

$$\langle Q\Psi|Q\Psi \rangle = \langle P\Psi|HQ \frac{1}{(\omega - QHQ)^2}QH|P\Psi \rangle,$$

(21)

such that

$$\langle P\Psi|P\Psi \rangle = \frac{1}{1 - \frac{dE}{d\omega}|_{\omega=E}}.$$

(22)

This equation states that the slopes at the intersection between the r.h.s. of eq. (20) and the line $E = \omega$ provide information about the wave functions. The slopes $\frac{dE}{d\omega}$ should always satisfy

$$\frac{dE}{d\omega} \leq 0,$$

in order to have $\langle P\Psi|P\Psi \rangle \leq 1$. Using $H = H_0 + H_1$ we can rewrite the r.h.s. of eq. (20) as

$$PHP|\Psi \rangle = PHP|P\Psi \rangle + P\hat{Q}P|\Psi \rangle = EP|\Psi \rangle,$$

(23)

where we have introduced the $\hat{Q}$-box defined as

$$P\hat{Q}P = PH_1P + PH_1Q \frac{1}{\omega - QHQ}QH_1P.$$

(24)

How to evaluate the $\hat{Q}$-box is however an open question. Here we will expand the denominator of eq. (24) such that we obtain a perturbative expansion for the $\hat{Q}$-box which reads

$$P\hat{Q}P = PH_1P + P \left( H_1 \frac{Q}{\omega - H_0}H_1 + H_1 \frac{Q}{\omega - H_0}H_1 \frac{Q}{\omega - H_0}H_1 + \ldots \right) P.$$

(25)

The $\hat{Q}$-box is made up of non-folded diagrams which are irreducible and valence linked. A diagram is said to be irreducible if between each pair of vertices there is at least one hole state or a particle state outside the model space. In a valence-linked diagram the interactions are linked (via fermion lines) to at least one valence line. Note that a valence-linked diagram can be either connected (consisting of a single piece) or disconnected, which in the case of a two-body interaction means that we have two one-body diagrams. In the FD and LS expansions, where we include folded diagrams as well, the disconnected diagrams are found to cancel out [3].

We evaluate the $\hat{Q}$-box by including all two-body diagrams through third order in the reaction matrix $G$, as described in ref. [1]. The one-body diagrams plus the unperturbed term $H_0$ are approximated by the experimental single-particle energies. Further, since we do not evaluate diagrams with Hartree-Fock insertions, we have no disconnected diagrams through third order in the interaction in our definition of the $\hat{Q}$-box. The $G$-matrix replaces the interaction term $H_1$ through $H_1 = G - U$, $U$ being an adequately chosen auxiliary potential, and is obtained through the solution of the Bethe-Goldstone equation

$$G(\omega) = V + V \frac{\hat{Q}}{\omega - H_0}G(\omega),$$

(26)
where $V$ is the free nucleon-nucleon interaction. Note that the Pauli operator $\tilde{Q}$ may differ from the definition of $Q$ in the above perturbative expansions. Eq. (26) is solved by using the so-called double-partition scheme described in ref. [10]. For $V$, we take the parameters of the Bonn B potential as defined in table A.2 of ref. [11] with the Pauli operator $\tilde{Q}$ defined so as to prevent scattering into states with one particle in the $0^+_s$ or $0^+_p$ shells or two particles in the $1^+_s 0^+_d$ or $1^+_p 0^+_f$ shells. A harmonic oscillator single-particle basis was employed with an oscillator parameter of 1.72 fm.

FIG. 2. The eigenvalues of eq. (20) for the three $0^+$ states of $^{18}$O.

In fig. 2 we show the graphical solutions for the $0^+_1$, $0^+_2$, and $0^+_3$ states. As can be seen from fig. 2, the two lowest eigenstates exhibit negative derivatives in the region near the graphical solutions, $-12.2$ and $-8.3$ MeV for the $0^+_1$ and the $0^+_2$ states, respectively. Correspondingly, the model space overlaps of eq. (22) in the region $-20$ to $-4$ MeV for the starting energy is of the order $\approx 0.93 - 0.95$ for the $0^+_1$ state and $\approx 0.98 - 0.99$ for the $0^+_2$ state. We do not attempt to calculate the corresponding numbers near the crossing for the $0^+_3$ state, since this would require the eigenvalue to be calculated at positive starting energies, which is not possible since the $G$-matrix is calculated at negative energies only. We are therefore not able to make any statement about the wave function overlaps for this state. In our further discussion we will therefore omit this state.

For the $0^+_1$ state, the derivative becomes positive first at $-28$ MeV ($\frac{dE}{d\omega} = 0.285$), and the eigenvalue diverges as we approach the poles $\omega = QH_0Q$. However, it is interesting to see that within our approximation to the $Q$-box, the $P$-space overlap is close to one for the starting energies of interest, i.e. near the graphical solutions. This means that the
mixing from $Q$ space states is rather weak within our perturbative scheme. As discussed above, the experimental $0^+_2$ state is expected to be of four-particle-two-hole structure ($4p2h$). Although we include the second-order $4p2h$ diagram in our definition of the $\hat{Q}$-box, this contribution is not sufficient to represent the structure of the $4p2h$ correlations of the $0^+_2$ state. The $4p2h$ diagram is also the only diagram in our third-order $\hat{Q}$-box which may represent intruder state configurations. The omission of the latter diagram in our calculations does not change the qualitative aspect of the above wave function overlaps, indicating that we have a rather small $Q$-space component in conventional calculations of the effective interaction in the region of the graphical solutions. We may then summarize this to say that for a perturbative expansion up to third order in the $G$-matrix, the $Q$-space component is weak and one should identify the second eigenvalue of the model calculation with the $0^+_2$ experimental state.

From the analysis in the previous section and the above results, we expect that the differences between the FD and the LS method, i.e. when comparing the converged results, should be small in the energy domain of interest. In particular, the $P$-space overlaps for the $0^+_1$ and the $0^+_2$ should be close to unity in both schemes. In fig. 3 we plot the eigenvalues as functions of the starting energy for the FD and LS methods.

\[\text{FIG. 3. The eigenvalues derived with the FD and LS methods for the } 0^+ \text{ states of } ^{18}\text{O.}\]

\[\text{5The one-body contributions plus } H_0 \text{ are also here approximated with the experimental single-particle energies}\]
We observe that for starting energies within the range of the experimental values, the FD and LS methods show only small differences. The results here should therefore be interpreted in the same way as those exhibited in fig. 1. In that figure we showed that for low-order $\hat{Q}$-boxes, the FD and LS methods gave essentially the same results. This leads us in turn to state that the convergence criterion for the LS method applies only if we are able to define an approximately exact $\hat{Q}$-box. In realistic calculations this is however not the case, although both series converge rather rapidly, almost irrespectively of the choice of $\hat{Q}$-box. Thus, in calculations of the spectra for, e.g. $^{18}$O, we cannot choose a starting energy close to the $0^+_2$ state, in order to reproduce that state with the LS method, since the $\hat{Q}$-box does not incorporate important $Q$-space configurations. Rather, the LS and FD methods give similar results, and the second $0^+_2$ state obtained from the calculation should be identified with the experimental $0^+_3$ state, since this is believed to be predominantly a two-particle state.

Finally, an important subtlety arises. Let us assume that we are able to define an exact $\hat{Q}$-box for the two-body interaction. With an appropriately chosen starting energy, we should then be able to reproduce the intruder state in e.g. $^{18}$O employing the LS method. This interaction is then conventionally used in shell-model calculations to obtain observables of systems with more than two valence nucleons. However, for such heavier systems, the degrees of freedom of the intruder state in e.g. $^{18}$O may not be present. Thus, this two-body interaction obtained with the LS method should not be used in calculations of spectra of other sd-shell nuclei. With the LS method, we should therefore, in principle, recalculate the $n$-body interaction for the actual nucleus with $n$ valence particles. This should be contrasted to the effective interaction obtained with the FD method. The latter reproduces only those states which have the largest $P$-space overlaps. If we restrict the attention to the degrees of freedom represented by the model space, we can use this two-body interaction in heavier systems as well.

**IV. CONCLUSIONS**

We have critically reviewed the convergence properties of the folded-diagram (FD) expansion of Kuo and co-workers and the iterative scheme of Lee and Suzuki. The behavior of these perturbative expansions was first studied within the framework of an exactly solvable model. Next, we investigated the convergence properties by applying the above two methods to a test nucleus, $^{18}$O. Our conclusions are:

- The exactly solvable model allows us to define an exact $\hat{Q}$-box. With an exact $\hat{Q}$-box we were able to demonstrate that, if we choose a starting energy close to a given eigenvalue, either $P$- or $Q$-space eigenvalues, the LS expansion converges to that eigenvalue. The FD method converges always to that eigenvalue which has the largest $P$-space overlap.

- Still within the exactly solvable model, we have shown that if one chooses a $\hat{Q}$-box of low order in the interaction, the FD and LS methods give almost similar results, irrespectively of the choice of starting energy. At low orders in the interaction we are not able to reproduce the $Q$-space state with the LS method, even with an appropriately chosen starting energy. The FD method (if it converges) always gives a result close to the eigenvalue with the largest $P$-space overlap. With increasing order of the interaction, the $\hat{Q}$-box incorporates more $Q$-space degrees of freedom and the LS and FD methods give unstable results.

- In realistic calculations, like those for $^{18}$O shown here, we can only define an approximate $\hat{Q}$-box, to third order in the interaction in the present case. It is then seen that the FD and LS methods yield almost the same results, in agreement with the findings obtained from the simple model. Since the FD method converges to those states which have the largest $P$-space overlap, the structure of the LS wave function should therefore also have a large $P$-space overlap. With an approximative $\hat{Q}$-box, we can therefore not choose a starting energy close to an intruder state in order to reproduce this state with the LS method. Thus, of the two methods, the FD method is the preferable one in nuclear structure calculations since it converges to those eigenstates which have the largest $P$-space overlap, a desirable property since we in general can only employ a rather small shell-model space.

[1] M. Hjorth-Jensen, E. Osnes and H. M"uther, Ann. of Phys. 213 (1992) 102
[2] M. Hjorth-Jensen, T. Engeland, A. Holt and E. Osnes, Phys. Reports, in press
[3] D.C. Zheng, J.P. Vary and B.R. Barrett, Nucl. Phys. A560 (1993) 211
[4] K. Suzuki, R. Okamoto, P.J. Ellis, J. Hao, Z. Li and T.T.S. Kuo, Phys. Lett. B308 (1993) 1
[5] T.T.S. Kuo and E. Osnes, Folded-Diagram Theory of the Effective Interaction in Atomic Nuclei, Springer Lecture Notes in Physics, (Springer, Berlin, 1990) Vol. 364
[6] K. Suzuki and S.Y. Lee, Prog. Theor. Phys. 64, 2991 (1980)
[7] T.H. Schucan and H.A. Weidenmüller, Ann. of Phys. 73 (1972) 108; 76 (1973) 483
[8] P.J. Ellis and E. Osnes, Rev. Mod. Phys. 49 (1977) 777; P.J. Ellis and E. Osnes, Phys. Lett. B45 (1973) 425
[9] P.J. Ellis and T. Engeland, Nucl. Phys. A144 (1970) 161
[10] E.M. Krenciglowa, C.L. Kung, T.T.S. Kuo and E. Osnes, Ann. of Phys. 101, 154 (1976)
[11] R. Machleidt, Adv. Nucl. Phys. 19, 189 (1989)
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