Non-degenerate shell-model effective interactions from the Okamoto-Suzuki and Krenciglowa-Kuo iteration methods

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We present calculations of shell-model effective interactions for both degenerate and non-degenerate model spaces using the Krenciglowa-Kuo (KK) and the extended Krenciglowa-Kuo iteration method recently developed by Okamoto, Suzuki *et al.* (EKKO). The starting point is the low-momentum nucleon-nucleon interaction V_{low-k} obtained from the N^3 LO chiral two-nucleon interaction. The model spaces spanned by the sd and $sdpf$ shells are both considered. With a solvable model, we show that both the KK and EKKO methods are convenient for deriving the effective interactions for non-degenerate model spaces. The EKKO method is especially desirable in this situation since the vertex function $\hat{Z}$ -box employed therein is well behaved while the corresponding vertex function $\hat{Q}$ -box employed in the Lee-Suzuki (LS) and KK methods may have singularities. The converged shell-model effective interactions given by the EKKO and KK methods are equivalent, although the former method is considerably more efficient. The degenerate sd -shell effective interactions given by the LS method are practically identical to those from the EKKO and KK methods. Results of the sd one-shell and $sdpf$ two-shell calculations for ^{18}O , ^{18}F , ^{19}O and ^{19}F using the EKKO effective interactions are compared, and the importance of an inter-space consistency between the sd and $sdpf$ calculations is discussed.

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I. INTRODUCTION

The nuclear shell model has provided a very successful framework for describing the properties of a wide range of nuclei. This framework is basically an effective theory [1–3], corresponding to reducing the full-space nuclear many-body problem to a model-space one with effective Hamiltonian $PH_{eff}P = PH_0P + PV_{eff}P$, where H_0 is the single-particle (s.p.) Hamiltonian and P represents the projection operator for the model space which is usually chosen to be a small shell-model space such as the sd shell outside of an ^{16}O closed core. The effective interaction V_{eff} plays a central role in this nuclear shell model approach, and its choice and/or determination have been extensively studied, see e.g. [2–5]. As discussed in these references, V_{eff} may be determined using either an empirical approach where it is required to reproduce selected experimental data or a microscopic one where V_{eff} is derived from realistic nucleon-nucleon (NN) interactions using many-body methods. The folded-diagram theory [1–3] is a commonly used such method for the latter. Briefly speaking, in this theory V_{eff} is given as a folded-diagram series [1–3, 6]

$$V_{eff} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} \cdots, \quad (1)$$

where $\hat{Q}$ represents a so-called $\hat{Q}$ -box, which may be written as

$$\hat{Q}(\omega) = [PVP + PVQ \frac{1}{\omega - QHQ} QVP]_L. \quad (2)$$

Here V represents the NN interaction and ω is the so-called starting energy which will be explained later (section II). Thus from the NN interaction V we can in principle calculate the $\hat{Q}$ -box and thereby the effective interaction V_{eff} . Note that we use Q , without hat, to denote the Q -space projection operator. ($P + Q = 1$.) Note also that the $\hat{Q}$ -box is an irreducible vertex function where the intermediate states between any two vertices must belong to the Q space. As indicated by the subscript L in eq. (2), the $\hat{Q}$ -box contains valence linked diagrams only, such as the 1st- and 2nd-order $\hat{Q}$ -box diagrams for ^{18}O and ^{18}F shown in Fig. 1. The $\hat{Q}'$ -box of eq. (1) is defined as $(\hat{Q} - PVP)$, namely $\hat{Q}'$ begins with diagrams 2nd-order in V . The above folded-diagram formalism has been employed in microscopic derivations of shell model effective interactions for a wide range of nuclei [2, 3].

In the present work we would like to explore an extension of the well-known methods for computing the folded diagram series in eq. (1). For many years, the Lee-Suzuki (LS) [7, 8] iteration method was commonly used in microscopic calculations of the folded-diagram shell model effective interactions [2, 3]. This method was initially formulated for degenerate model spaces (namely PH_0P is degenerate), and was later extended to non-degenerate model spaces [9]. Here we would like to employ two different methods, the Krenciglowa-Kuo (KK) iteration method [10, 11] and the newly developed extended Krenciglowa-Kuo iteration method of Okamoto, Suzuki, Kumagai and Fujii (EKKO) [12, 13] in calculating such effective interactions for non-degenerate model spaces. The original KK method [10] was formulated for degenerate model spaces. It was later generalized to non-

degenerate model spaces [11], and the KK method used in the present work is the generalized version. Tsunoda et al. [14] have recently proposed an extended Krenciglowa-Kuo method for deriving the effective interactions for non-degenerate model spaces. A comparison of this method with the methods employed in the present work will be made (see Section II).

A special feature of the EKKO method is the use of the vertex function $\hat{Z}$ -box (to be defined in Section II) in place of the vertex function $\hat{Q}$ -box employed in the LS [7–9], KK [10, 11] and the Tsunoda-KK [14] methods. When the P - and Q -space are not adequately separated from each other, the vertex function $\hat{Q}$ -box may have singularities or be nearly singular, causing difficulty for its iterative solution. In contrast, the $\hat{Z}$ -box is by construction non-singular, thus circumventing the above singularity difficulty. As we shall also discuss in Section II, the physics given by the $\hat{Q}$ -box is preserved by the $\hat{Z}$ -box. The EKKO method was originally formulated for degenerate model spaces [12, 13], and here we shall generalize it to the case of non-degenerate model spaces. As we shall discuss later, both the EKKO and KK methods may provide a suitable framework for calculating shell-model effective interactions for large non-degenerate model spaces which may be needed for describing exotic nuclei with large neutron excess [15].

The organization of the present paper is as follows. In section II we shall first review the KK method for computing shell model effective interactions in non-degenerate model spaces and then describe how the EKKO method can be formulated to also treat the non-degenerate case. We shall also compare these two methods with the LS [7–9] and the Tsunoda-KK [14] methods.

Our results will be presented and discussed in section III. We shall first perform a sequence of model calculations comparing the EKKO, KK and LS iteration methods for degenerate and non-degenerate model spaces. The use of the EKKO and KK methods in calculating the effective interactions for non-degenerate model spaces will be emphasized. Starting from the V_{low-k} interaction [3, 16–18] derived from the chiral $N^3\text{LO}$ potential [19], the LS, KK and EKKO methods will first be used to calculate the degenerate sd one-shell effective interactions, a main purpose being to check if the results given by the commonly used LS method agree with the KK and EKKO ones. The KK and EKKO methods will then be employed to calculate the non-degenerate $sdpf$ two-shell effective interactions. The matrix elements of the above degenerate and non-degenerate interactions will be compared. As we shall demonstrate, both the EKKO and KK methods can provide a convenient framework for calculating shell-model effective interactions for large non-degenerate model spaces which may be needed for describing exotic nuclei with large neutron excess. The low-energy spectra of ^{18}O , ^{18}F , ^{19}O and ^{19}F given by these interactions will be discussed. In this section we shall also discuss the center of mass (cm) motion associ-

FIG. 1: Low-order diagrams constituting the $\hat{Q}$ -box.

ated with our sd and $sdpf$ calculations. The nuclear cm motion given by our sd one-shell calculations is assured to be in its cm ground state, but not so for our $sdpf$ two-shell calculations. The wave functions given by the latter can have spurious components corresponding to excited cm motion. Such spurious components are unphysical and, as we shall describe, can be removed by way of a projection operation. A summary and conclusion will be presented in section IV.

II. FORMALISM

In this section, we shall describe and discuss the KK and the EKKO iteration methods for computing shell model effective interactions in non-degenerate model spaces. Let us begin with a brief review of the LS iteration method where the model space is degenerate, namely $PH_0P = W_0$, where W_0 is a constant. In terms of the $\hat{Q}$ -box of Eq.(2), the effective interactions R_n are calculated iteratively by [7, 8]

$$R_1 = \hat{Q}(W_0), \quad (3)$$

$$R_2 = \frac{1}{1 - \hat{Q}_1} \hat{Q}(W_0), \quad (4)$$

and for $n > 2$

$$R_n = \frac{1}{1 - \hat{Q}_1 - \sum_{m=2}^{n-1} \hat{Q}_m \prod_{k=n-m+1}^{n-1} R_k} \hat{Q}(W_0), \quad (5)$$

where $\hat{Q}_m$ is proportional to the m th derivative of $\hat{Q}$:

$$\hat{Q}_m = \left. \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} \right|_{\omega=W_0}. \quad (6)$$

The effective interaction is given by the converged R_n , namely

$$V_{eff} = R_{n+1} = R_n. \quad (7)$$

There is a practical difficulty for the above iteration method. In actual shell-model calculations, it is usually not possible to calculate the vertex function $\hat{Q}$ -box exactly; thus it is a common practice to evaluate it with some low-order approximation and calculate the derivatives $\hat{Q}_m$ numerically. At higher orders this becomes increasingly difficult, and therefore such calculations are usually limited to low orders in the iteration. However, as we shall demonstrate in section IIIa, low-order LS iterations are often not accurate when the P - and Q -spaces are strongly coupled.

The above degenerate LS iteration method has been generalized [9] to the case where PH_0P is non-degenerate. In this situation we need not only the $\hat{Q}$ -box of eq. (2) but also a generalized $\hat{Q}$ -box defined by

$$\hat{Q}_n(\epsilon_1\epsilon_2\cdots\epsilon_{n+1}) = (-1)^n[PVQg_1^Qg_2^Q\cdots g_{n+1}^QQVP]_L. \quad (8)$$

with

$$g_i^Q \equiv \frac{1}{\epsilon_i - QHQ}. \quad (9)$$

This generalized $\hat{Q}$ -box is defined for $n \geq 1$, and ϵ_i is defined by $PH_0P\phi_i = \epsilon_i\phi_i$ where $P = \sum_{m \leq d} |\phi_m\rangle\langle\phi_m|$. The dimension of the P -space is labelled d . Note that only valence-linked diagrams are retained in $\hat{Q}_n(\epsilon_1\cdots\epsilon_{n+1})$, as indicated by the subscript L .

With the above definitions, the effective interaction given by the non-degenerate LS iteration method is given as [9]

$$\begin{aligned} R_1 &= \sum_{\alpha} \hat{Q}(\epsilon_{\alpha})P_{\alpha}, \\ R_2 &= \sum_{\alpha} \left[1 - \sum_{\beta} \hat{Q}_1(\epsilon_{\alpha\beta})P_{\beta} \right]^{-1} \hat{Q}(\epsilon_{\alpha})P_{\alpha}, \\ R_3 &= \sum_{\alpha} \left[1 - \sum_{\beta} \hat{Q}_1(\epsilon_{\alpha\beta})P_{\beta} - \sum_{\beta\gamma} \hat{Q}_2(\epsilon_{\alpha\beta\gamma})P_{\beta}R_2P_{\gamma} \right]^{-1} \\ &\quad \times \hat{Q}(\epsilon_{\alpha})P_{\alpha}, \\ &\dots \end{aligned} \quad (10)$$

with $\epsilon_{\alpha\beta} \equiv (\epsilon_{\alpha} + \epsilon_{\beta})$, $\epsilon_{\alpha\beta\gamma} \equiv (\epsilon_{\alpha} + \epsilon_{\beta} + \epsilon_{\gamma})$, $\dots$. In the above equations $P_m = |\phi_m\rangle\langle\phi_m|$. When convergent, we have $V_{eff} = R_{n+1} = R_n$. The above non-degenerate LS method can be used to calculate the effective interactions for e.g., the non-degenerate $0p$ -shell [20] or the two-shell $sdpf$ model space. But this method is rather complicated for computations, and this has hindered its application to microscopic calculations of shell-model effective interactions.

We now describe some details of the non-degenerate KK and EKKO methods. The KK iteration method was originally developed for model spaces which are degenerate [10]. A non-degenerate KK iteration method was

later formulated [11], with the effective interaction determined as follows. Let the effective interaction for the i th iteration be $V_{eff}^{(i)}$ and the corresponding eigenvalues E and eigenfunctions χ be given by

$$[PH_0P + V_{eff}^{(i)}]\chi_m^{(i)} = E_m^{(i)}\chi_m^{(i)}. \quad (11)$$

Here χ_m is the P -space projection of the full-space eigenfunction Ψ_m , namely $\chi_m = P\Psi_m$. The effective interaction for the next iteration is then

$$V_{eff}^{(i+1)} = \sum_m [PH_0P + \hat{Q}(E_m^{(i)})]|\chi_m^{(i)}\rangle\langle\tilde{\chi}_m^{(i)}| - PH_0P, \quad (12)$$

where the bi-orthogonal states are defined by

$$\langle\tilde{\chi}_m|\chi_{m'}\rangle = \delta_{m,m'}. \quad (13)$$

Note that in the above PH_0P is non-degenerate. The converged eigenvalue E_m and eigenfunction χ_m satisfy the P -space self-consistent condition

$$(E_m(\omega) - H_0)\chi_m = \hat{Q}(\omega)\chi_m, \quad \omega = E_m(\omega). \quad (14)$$

To start the iteration, we use

$$V_{eff}^{(1)} = \hat{Q}(\omega_0) \quad (15)$$

where ω_0 is a starting energy chosen to be close to PH_0P . The converged KK effective interaction is given by $V_{eff} = V_{eff}^{(n+1)} = V_{eff}^{(n)}$. When convergent, the resultant V_{eff} is independent of ω_0 , as it is the states with maximum P -space overlaps which are selected by the KK method [10]. We shall discuss this feature later in section III using a solvable model. The above non-degenerate KK method is numerically more convenient than the non-degenerate LS method.

As mentioned in Section I, Tsunoda et al. [14] recently proposed an extended KK iteration method for non-degenerate model spaces. It is useful and of interest to compare it with the generalized KK method [11] as described in Eq. (12). The Tsunoda-KK iteration method is given by [14]

$$\tilde{H}_{eff}^{(n)} = \tilde{H}_{BH}(E_x) + \sum_{k=1}^{\infty} \hat{Q}_k(E_x)[\tilde{H}_{eff}^{(n-1)}]^k, \quad (16)$$

$$\tilde{H}_{eff} = PH_0P + V_{eff} - E_x,$$

$$\tilde{H}_{BH}(E_x) = PH_0P + \hat{Q}(E_x) - E_x$$

where E_x is a parameter. We note that the above and the generalized KK method [11] as given in Eq. (12) are of different forms. The energy-independent and energy-dependent effective interactions are related by

$$\begin{aligned} (PH_0P + V_{eff})\chi_m &= E_m\chi_m \\ &= (PH_0P + \hat{Q}(E_m))\chi_m. \end{aligned} \quad (17)$$

The Tsunoda-KK formulas in Eq. (16) correspond to making an expansion of the above $\hat{Q}$ -box about E_x

$$\hat{Q}(E_m) = \hat{Q}(E_x) + \sum_{k=1}^{\infty} \hat{Q}_k(E_x)(E_m - E_x)^k. \quad (18)$$

With this expansion, Eq. (2.15) leads to

$$\tilde{H}_{eff} = \tilde{H}_{BH}(E_x) + \sum_{k=1}^{\infty} \hat{Q}_k(E_x)[\tilde{H}_{eff}]^k \quad (19)$$

in agreement with Eq. (16), which is an iterative solution of Eq. (19) or Eq. (17). It is readily seen that the KK effective interaction of Eq. (12) is also an iterative solution of Eq. (17). Thus the converged effective interactions from the Tsunoda-KK method [14] and the KK method used in the present work are equivalent. ^{#1}

We now consider the one-body effective interactions. The diagrams of Fig. 1 have both one-body (d1,d2,d3) and two-body (d4,d5,d6,d7) diagrams. When we calculate nuclei with two valence nucleons such as ^{18}O and ^{18}F , all seven diagrams are included in the $\hat{Q}$ -box. But for nuclei with one valence nucleon such as ^{17}O , we deal with the 1-body $\hat{S}$ -box which is approximated by the sum of diagrams d1, d2 and d3. The 1-body effective interaction is given by a similar KK iteration

$$S_{eff}^{(i+1)} = \sum_m [PH_0P + \hat{S}(E_m^{(i)})]|\chi_m^{(i)}\rangle\langle\tilde{\chi}_m^{(i)}| - PH_0P. \quad (20)$$

Denoting its converged value as S_{eff} , the model-space s.p. energy ϵ_m^{eff} is given by $P_m(H_0 + S_{eff})P_m$. By adding and then subtracting S_{eff} , we can rewrite Eq.(14) as

$$(E_m(\omega) - H_0^{eff})\chi_m = [\hat{Q}(\omega) - S_{eff}]\chi_m, \quad \omega = E_m(\omega), \quad (21)$$

with $H_0^{eff} = H_0 + S_{eff}$. In most shell model calculations [4, 5], one often uses the experimental s.p. energies. This treatment for the s.p. energies is in line with the above subtraction procedure, as $P(H_0 + S_{eff})P$ represents the physical s.p. energy which in principle can be extracted from experiments. In the present work we shall use the experimental s.p. energies for the model-space orbits together with the V_{eff} derived from $(\hat{Q} - S_{eff})$. A similar subtraction procedure has also been employed in

the LS calculations [2, 3] where the all-order sum of the one-body diagrams was subtracted from the calculation of the effective interaction.

In several aspects, the above KK method provides a more desirable framework for effective interaction calculations than the commonly used LS method. The KK method is more convenient for non-degenerate model spaces than the LS method, and the KK method does not require the calculation of high-order derivatives of the $\hat{Q}$ -box, which may be necessary in a converged LS calculation. The KK method has, however, a shortcoming when applied to calculations with extended model space such as the two-shell *sdpf* one. For example, certain 2nd-order diagrams for this case may diverge, resulting in an ill-defined $\hat{Q}$ -box. It is remarkable that these potential divergences can be circumvented by the recently proposed EKKO method of Okamoto *et al.* [12]. In this method, the vertex function $\hat{Z}$ -box is employed. It is related to the $\hat{Q}$ -box by

$$\hat{Z}(\omega) = \frac{1}{1 - \hat{Q}_1(\omega)}[\hat{Q}(\omega) - \hat{Q}_1(\omega)P(\omega - H_0)P], \quad (22)$$

where $\hat{Q}_1$ is the first-order derivative of the $\hat{Q}$ -box. The $\hat{Z}$ -box considered by Okamoto *et al.* [12] is for degenerate model spaces ($PH_0P = W_0$), while we consider here a more general case with non-degenerate PH_0P . An important property of the above $\hat{Z}$ -box is that it is finite when the $\hat{Q}$ -box is singular (has poles). Note that $Z(\omega)$ satisfies

$$\hat{Z}(\omega)\chi_m = \hat{Q}(\omega)\chi_m \text{ at } \omega = E_m(\omega). \quad (23)$$

The iteration method for determining the effective interaction from the $\hat{Z}$ -box is quite similar to that for the $\hat{Q}$ -box. Suppose the effective interaction for the i th iteration is $V_{eff-Z}^{(i)}$. The corresponding eigenfunction χ and eigenvalues E^Z are determined by

$$[PH_0P + V_{eff-Z}^{(i)}]\chi_m^{(i)} = E_m^{Z(i)}\chi_m^{(i)}. \quad (24)$$

The effective interaction for the next iteration is

$$V_{eff-Z}^{(i+1)} = \sum_m [PH_0P + \hat{Z}(E_m^{Z(i)})]|\chi_m^{(i)}\rangle\langle\tilde{\chi}_m^{(i)}| - PH_0P, \quad (25)$$

Although $\hat{Q}(\omega)$ and $\hat{Z}(\omega)$ are generally different, it is interesting that the converged eigenvalues E_m of $P(H_0 + V_{eff})P$ and the corresponding ones E_m^Z of $P(H_0 + V_{eff-Z})P$ are both exact eigenvalues of the full-space Hamiltonian $H = H_0 + V$, which can be seen from eqs. (14), (18) and (19). Note, however, the KK and EKKO methods may reproduce different eigenvalues of the full-space Hamiltonian H . This aspect together with some other comparisons of these methods will be discussed in section IIIa, using a simple solvable model.

For the degenerate case, Okamoto *et al.* [12] have shown that $\frac{dE_m^Z(\omega)}{d\omega} = 0$ at the self-consistent point $\omega =$

^{#1} We note that we have employed a slightly different technique to obtain the Tsunoda-KK results. In Ref. [14] Eq. (16) was obtained starting from the decoupling equation for the similarity transformed Hamiltonian $0 = P(1 - \omega)H(1 + \omega)$ where $\omega = Q\omega P$ is the wave operator. Here we start from the equivalence condition Eq. (17) between the energy-independent and energy-dependent effective interactions. We note also the effective Hamiltonian of Eq. (19) is independent of the parameter E_x when the expansion is calculated to all orders. As reported in Section III, a graphical method (where the self-consistent eigenvalues of Eq. (14) are solved graphically) for calculating the effective interaction will also be employed.

$E_m^Z(\omega)$. As outlined below, we have found that this result also holds for the case of non-degenerate PH_0P . From eq. (18), we have

$$\frac{dZ}{d\omega} = \frac{2}{1 - \hat{Q}_1} \hat{Q}_2 \frac{1}{1 - \hat{Q}_1} [\hat{Q} - \hat{Q}_1(\omega - H_0)] - \frac{2}{1 - \hat{Q}_1} \hat{Q}_2(\omega - H_0). \quad (26)$$

Then from eqs. (14) and (19) we have

$$\left[\frac{dZ(\omega)}{d\omega} \right]_{\omega=E_m^Z} |\chi_m\rangle = 0, \quad (27)$$

and

$$\left[\frac{dE_m^Z(\omega)}{d\omega} \right]_{\omega=E_m^Z} = 0. \quad (28)$$

This is a useful result; it states that at any self-consistent point the eigenvalues $E_m^Z(\omega)$ varies ‘flatly’ with ω , a feature certainly helpful to iterative calculations. In section III, we shall check this feature numerically.

III. RESULTS AND DISCUSSION

IIIa. Model calculations comparing the LS, KK and EKKO methods

In this section we shall study the above iteration methods by way of a simple matrix model, similar to the one employed in [12, 13]. We consider a 4-dimensional matrix Hamiltonian $H = H_0 + H_1$ where

$$H_0 = \begin{bmatrix} PH_0P & 0 \\ 0 & QH_0Q \end{bmatrix} \quad (29)$$

and

$$PH_0P = \begin{bmatrix} \varepsilon_{p1} & 0 \\ 0 & \varepsilon_{p2} \end{bmatrix}; \quad QH_0Q = \begin{bmatrix} \varepsilon_{q1} & 0 \\ 0 & \varepsilon_{q2} \end{bmatrix}. \quad (30)$$

The interaction Hamiltonian has a strength parameter x , namely

$$H_1 = \begin{bmatrix} PH_1P & PH_1Q \\ QH_1P & QH_1Q \end{bmatrix}, \quad (31)$$

with

$$\begin{aligned} PH_1P &= \begin{bmatrix} 0 & 5x \\ 5x & 10x \end{bmatrix}; \\ PH_1Q &= QH_1P = \begin{bmatrix} 0 & 8x \\ 8x & 0 \end{bmatrix}; \\ QH_1Q &= \begin{bmatrix} -5x & x \\ x & -5x \end{bmatrix}. \end{aligned} \quad (32)$$

As discussed in section II, both the KK and EKKO iteration methods are rather convenient for non-degenerate

model spaces. We would like to check this feature by carrying out some calculations using the above model. We consider two unperturbed Hamiltonians, given by $(\varepsilon_{p1}, \varepsilon_{p2}, \varepsilon_{q1}, \varepsilon_{q2}) = (0, 6, 4, 9)$ and $(0, 0, 4, 9)$. The PH_0P parts of them are, respectively, non-degenerate and degenerate.

In the first three entries of Table I, some results for the $PH_0P = (0, 6)$ case are presented. Here E_n are the exact eigenvalues of the full Hamiltonian, with their model-space overlaps denoted by $\langle n|P|n \rangle$. The entries E_{KK} and E_{EKKO} are the eigenvalues generated respectively by the KK and EKKO iteration methods. Not only is the above PH_0P non-degenerate but its spectrum intersects that of QH_0Q . One would expect that this PH_0P may cause difficulty for the above iteration methods. But as indicated in Table I, both the non-degenerate KK and the non-degenerate EKKO iteration methods work remarkably well. Note that the interaction used here is rather strong ($x=0.6$), and both methods still work well, converging to values of E_n which are quite far from PH_0P .

Some results for the degenerate case of $PH_0P = (0, 0)$ are listed in the last two entries of Table I. Here we have performed calculations using the degenerate LS method through 5th order iteration (i.e. in Eq.(7) we use $V_{eff} = R_5$). As shown, the results so obtained are not in good agreement with the exact results. This suggests that low-order LS iteration method may often be inadequate, and one needs higher-order iterations to obtain accurate results.

It is known that the KK iteration method converges to the states with maximum P -space overlaps [10], while the LS method converges to the states of lowest energies [7, 8]. We have found that for many cases the EKKO method also converges to states of maximum P -space overlaps. As listed in the third entry of Table I, both the KK and EKKO methods converge to states of energies $E_n = -3.51$ and 14.53 whose P -space probabilities are relatively 0.70 and 0.86 . We have also found that the EKKO and KK iteration methods can converge to different states. An example is the result shown in the last part of Table I, where the EKKO method converges to states of energy (P -space probability) -1.45 (0.87) and 0.91 (0.46), while the states of maximum P -space overlap are those with energies -1.45 and 5.25 . Note that for this case the EKKO method is clearly more accurate than the KK method.

We have noticed that for a number of cases the EKKO method converges well but not so for the KK method. This is largely because these two methods treat the singularities of the $\hat{Q}$ -box differently. To see this, let us perform a graphical solution for the $x=0.60$ case of Table I. Using the parameters of this case, we calculate and plot in Fig. 2 both $E_m^Q(\omega)$ and $E_m^Z(\omega)$ which are respectively the eigenvalues of $P[H_0 + \hat{Q}(\omega)]P$ and $P[H_0 + \hat{Z}(\omega)]P$. As discussed in section II, they have identical self-consistent solutions, namely $\omega = E_m^Q(\omega) = E_m^Z(\omega) \equiv E_m$ where E_m is the eigenvalue of the full-space Hamiltonian. Recall that $\hat{Q}$ and $\hat{Z}$ are given respectively by eqs. (2) and (18).

FIG. 2: Graphical solutions for the $\hat{Q}$ - and $\hat{Z}$ -box self-consistent equations. See text for other explanations.

As shown in the figure, the curves of E^Q and E^Z do have identical self-consistent solutions as marked by the common intersection points E_1 , E_2 , E_3 and E_4 . Note that the above two curves are distinctly different from each other, particularly in the vicinity of the poles (marked by the vertical lines through F_1 and F_2) of the $\hat{Q}$ -box. There $E^Q(\omega)$ is discontinuous, diverging oppositely before and after the pole, while $E^Z(\omega)$ remains continuous throughout. The diverging behavior of the former is due to the singularities contained in the $\hat{Q}$ -box, while the continuity of the latter is because the $\hat{Z}$ -box is free of singularities by construction. This removal of singularities clearly helps the convergence of the $\hat{Z}$ -box iteration method: The $\hat{Z}$ -box iteration proceeds along a continuous $E^Z(\omega)$ curve, while the $\hat{Q}$ -box iteration often does not converge as it may bounce back and forth across the discontinuity.

As seen from eq. (18), the $\hat{Z}$ -box method has ‘false’ solutions at $E_q^Z(\omega) = \omega = \mu_q \equiv F_q$, where μ_q are poles of the $\hat{Q}$ -box. These solutions are marked in Fig. 2 as F_1 and F_2 . These false solutions can be readily recognized and discarded. As given in Eq.(24), we have at self-consistent points $\frac{dE_q^Z}{d\omega} = 0$. As shown in Fig. 2, the slopes of E^Z do satisfy the above condition at the self-consistent points E_1 to E_4 , but not so at the false points F_1 and F_2 .

IIIb. The sd and $sdpf$ shell model effective interactions

In this subsection, we shall calculate the effective interactions for both the degenerate sd one-shell and the non-degenerate $sdpf$ two-shell cases and apply them to ^{18}O , ^{18}F , ^{19}O and ^{19}F . Before presenting our results, let us first describe some details of our calculations. The LS, KK and EKKO methods as described in section II will be employed. We first compute the low-momentum NN interaction V_{low-k} [3, 16–18] starting from the chiral N^3LO

TABLE I: Results of model calculations using the LS, KK and EKKO iteration methods. See text for other explanations.

$H_0 = (0,6,4,9)$ $x=0.10$					
E_n	-0.110705	3.328164	7.203243	8.579299	
$(n P n)$	0.991108	0.044558	0.953368	0.010966	
E_{KK}	-0.110705	7.203243			
E_{EKKO}	-0.110705	7.203242			
$x = 0.30$					
E_n	-0.974184	1.808716	8.080888	10.084581	
$(n P n)$	0.906155	0.111257	0.113523	0.869066	
E_{KK}	-0.974185	10.084580			
E_{EKKO}	-0.974185	10.084581			
$x = 0.60$					
E_n	-3.510377	-0.286183	8.265089	14.531471	
$(n P n)$	0.709531	0.189318	0.232422	0.868729	
E_{KK}	-3.510377	14.531472			
E_{EKKO}	-3.510363	14.531472			
$H_0 = (0,0,4,9)$ $x = 0.10$					
E_n	-0.296201	0.982861	3.736229	8.577111	
$(n P n)$	0.985416	0.922993	0.082811	0.008780	
E_{LS}	-0.314591	0.872176			
E_{KK}	-0.296201	0.982860			
E_{EKKO}	-0.296201	0.982860			
$x = 0.30$					
E_n	-1.448782	0.906504	5.254129	8.288149	
$(n P n)$	0.868986	0.460296	0.566014	0.104704	
E_{LS}	-1.620734	0.339561			
E_{KK}	-1.125579	5.515468			
E_{EKKO}	-1.448782	0.906504			

two-body potential [19] at a decimation scale of $\Lambda = 2.1 \text{ fm}^{-1}$. At this cutoff scale, the low-momentum interactions derived from different NN potentials [19, 21–23] are remarkably close to each other, leading to a nearly unique low-momentum interaction [18]. This V_{low-k} interaction is then used in calculating the $\hat{Q}$ -box diagrams as shown in Fig. 1. In calculating these diagrams, the hole orbits are summed over the $0s0p$ shells and particle orbits over the $0d1s1p0f$ shells. The active spaces (P -space) used for the one-shell and two-shell calculations are respectively the three orbits in the sd shell and the seven orbits in the $sdpf$ shells. The experimental s.p. energies of (0.0, 5.08, 0.87) MeV have been used, respectively, for the $(0d_{5/2}, 0d_{3/2}, 1s_{1/2})$ orbits [24]. We have employed the shell-model s.p. wave functions and energies with the harmonic oscillator constant of $\hbar\omega=14 \text{ MeV}$.

In the following, let us first report our results for the degenerate sd one-shell calculations. Here by degenerate we mean that the unperturbed s.p. energy levels for the $(0d_{5/2}, 0d_{3/2}, 1s_{1/2})$ orbits are degenerate. Our purpose here is mainly to compare the results given by the KK

FIG. 3: Energy spectrum of ^{18}O obtained from the sd -shell calculations using the LS, KK and EKKO methods. Each energy level of total angular momentum J is represented by a bar with its length linearly dependent on J . This notation has been used by Brown *et al.* [25] and will be used here from now on. See text for more explanations.

FIG. 4: Same as Fig. 3 except for ^{18}F .

and EKKO method with those given by the commonly used degenerate LS method [2, 3]. In our LS calculations a low-order iteration approximation has been employed, namely we take $V_{\text{eff}} = R_5$ (see eq. (7)). As shown in Figs. 3 and 4, the LS, KK and EKKO results for both ^{18}O and ^{18}F are in fact nearly identical to each other. A comparison of our results with experiments [24] is also presented in the figures. The agreement between our calculated energy levels with experiments is moderately satisfactory for ^{18}O , but for ^{18}F the calculated lowest (1^+ , 3^+ , 5^+) states, though of correct ordering, are all significantly higher than the experimental values. As discussed in sections II and IIIa, the LS method is known to converge to the states of the lowest energies, while the KK method to the states of maximum P -space overlaps. Thus the good agreement shown in Figs. 3 and 4 is an important indication that the states reproduced by the

FIG. 5: Comparison of the sd -shell matrix elements given by the LS (LS-eff) and EKKO (KK-eff) methods. The diagonal line indicates the equivalence of the LS and EKKO matrix elements. See text for more explanations.

model-space LS, EKKO and KK effective interaction are likely those of the lowest energies as well as maximum model-space overlaps. In Fig. 5, we compare the entire sd -shell matrix elements given by the LS and EKKO methods; it is remarkable that every individual LS matrix element is practically equal to the corresponding EKKO one. (The matrix elements given by EKKO and KK are also nearly identical.) The above good agreement indicates that the degenerate sd -shell effective interactions can be accurately calculated using a low-order (R_5) LS iteration method.

As discussed in sections II and IIIa, the EKKO or KK methods are convenient for deriving the effective interactions for non-degenerate model spaces. We first apply these methods to a relatively simple case, namely the non-degenerate sd one-shell effective interactions. Here we employ the same unperturbed s.p. spectrum as the previous degenerate sd case except that the $0d_{3/2}$ and $1s_{1/2}$ orbits are shifted upward by, respectively, 5.08 and 0.87 MeV relative to the $0d_{5/2}$, in line with the experimental s.p. energies [24]. We have found that the degenerate and non-degenerate sd EKKO effective interactions are nearly the same, and so are the energy spectra of ^{18}O , ^{18}F , ^{19}O and ^{19}F given by these two interactions. To illustrate, a comparison of the ^{19}F spectra so calculated is presented in Fig. 6. In short, the one-shell sd effective interactions given by the degenerate and non-degenerate choices for the unperturbed sd s.p. energies are nearly the same, and it is simpler to calculate them using the former choice. From now on, the above degenerate choice will be employed.

We now report our results for the non-degenerate $sdpf$ two-shell effective interactions. So far our calculations have all been carried out using the sd one-shell model space. For certain nuclei such as those with a large neutron excess, a larger model space such as the $sdpf$ one

FIG. 6: Comparison of the low-lying states of ^{19}F calculated with the degenerate (DEG) and non-degenerate (NON-DEG) sd one-shell EKKO effective interactions.

FIG. 7: Comparison of the matrix elements of the sd one-shell (1-eff) and $sdpf$ two-shell (2-eff) EKKO effective interactions. Only the matrix elements within the sd shell are shown. See text for more explanations.

may be needed. As an initial study, we shall employ in our present work an $sdpf$ model space consisting of a closed ^{16}O core with valence nucleons confined in the $sdpf$ shells.

Let us first consider ^{18}O , to illustrate the difference between the sd and $sdpf$ calculations and discuss an inter-space consistency between them. Consider the $(T = 1, J = 0)$ states of this nucleus. In the sd one-shell case, the model space is spanned by three basis states $|j^2, T = 1, J = 0\rangle$, where $j = d_{5/2}, d_{3/2}$ and $s_{1/2}$. For the $sdpf$ case, the model space is enlarged, having four additional single-particle states labeled by $j = (p_{3/2}, p_{1/2}, f_{7/2}, f_{5/2})$. The whole model space is now non-degenerate as the pf orbits are one shell above the sd ones. An important question may be asked: Should the energies of the low-lying states of ^{18}O given by the sd interactions be the same as those given by the $sdpf$ interactions? The answer is yes, as explained below.

FIG. 8: Low-lying states of ^{18}F calculated with the sd one-shell (1shell) and $sdpf$ two-shell (2shell) EKKO interactions. Two choices for the vertex function $\hat{Q}$ -box are employed. For the left-most two columns only the first-order $\hat{Q}$ -box diagrams are included, while for the middle two columns we include both the first- and second-order diagrams.

Let us denote the effective interactions for the sd and $sdpf$ spaces respectively as V_{sd} and V_{sdpf} . Since they both originate from the same full-space interaction and $\{sd\}$ is a subspace of $\{sdpf\}$, the ^{18}O energy eigenvalues given by V_{sd} should be a subset of those given by V_{sdpf} , provided that the renormalization calculations for the effective interactions are performed exactly. This inter-space consistency provides an important and necessary test of the accuracy of our renormalization calculations. The construction of model-space effective interactions is in many ways similar to the construction of an effective theory from a renormalization group (RG) evolution [18]. In RG evolution, the above inter-space consistency is also required; namely the different effective theories corresponding to different model spaces should reproduce the same low-energy physical observables. An example is the deuteron binding energy which is reproduced by the low-momentum V_{low-k} interactions at any decimation scale Λ [18].

We have calculated the $sdpf$ effective interactions using both the EKKO and KK methods, obtaining nearly identical results. In Fig. 7 we compare the matrix elements of the $sdpf$ two-shell EKKO interaction with those of the sd one-shell case. Only the matrix elements within the sd shell are shown. We find that the magnitudes of the two-shell matrix elements are noticeably weaker than the one-shell matrix elements, some differing by as much as 1 MeV. We have performed $sdpf$ shell model calculations for ^{18}O , ^{18}F , ^{19}O and ^{19}F . In such calculations, the experimental s.p. energies for the four pf orbits are needed, but their values are not well known. In the present work we have chosen to place them all at a separation of 14 MeV above the $0d_{5/2}$ orbit. (We have also used a smaller separation of 10 MeV, and as

discussed later (Fig. 11) the results given by these two choices are nearly the same.) Despite the above differences in matrix elements, the resulting spectra for ^{18}O and ^{18}F given by the one-shell and two-shell calculations are nearly equivalent to each other, as illustrated by the two middle columns of Fig. 8. In fact among the many states given by the *sdpf* calculations, it is the ones with the maximum *sd*-space overlaps which agree with the results given by the *sd*-shell calculation, which is a physically desirable result. The above results indicate that the inter-space consistency requirement is well satisfied by our one-shell and two-shell calculations of ^{18}O and ^{18}F , lending support to the accuracy of our renormalization calculations.

In our calculations we employ a low-order $\hat{Q}$ -box consisting of the 1st- and 2nd-order diagrams of Fig. 1, and we would like to point out that the 2nd-order $\hat{Q}$ -box diagrams play an essential role in fulfilling the inter-space consistency requirement. In the two leftmost columns of Fig. 8 we show the spectra of ^{18}F when only the 1st-order $\hat{Q}$ -box diagrams are included. We note that in this case (in contrast to the second-order $\hat{Q}$ -box calculation) the resulting *sd* ‘1 Shell’ and *sdpf* ‘2 Shell’ spectra are largely different, violating the above inter-space consistency requirement. Because of the difference in the model spaces, the renormalization effects for the *sd* and *sdpf* effective interactions are different. To bridge these differences, we need to include at least the 2nd-order $\hat{Q}$ -box diagrams (note that the allowed intermediate states of the 2nd-order $\hat{Q}$ -box diagrams are model-space dependent). These diagrams are not included in the above 1st-order calculations, and consequently the *sd* and *sdpf* results are different as shown by the two leftmost columns of Fig. 8, which is a strong evidence for the importance of the model-space-dependent renormalization effects.

Before reporting our results for ^{19}O and ^{19}F , let us first discuss an important difference between our *sd* and *sdpf* calculations: the nuclear center-of-mass (cm) motion is assured to be in its ground state for the former but not so for the latter. Let us denote the unperturbed state in *sd* and *sdpf* spaces respectively as

$$\begin{aligned}\Phi_{\alpha}^{sd}(s^4 p^{12}(sd)^{n_v}) &\equiv \Phi_{\alpha}^{sd}, \\ \Phi_{\alpha}^{sdpf}(s^4 p^{12}(sdpf)^{n_v}) &\equiv \Phi_{\alpha}^{sdpf},\end{aligned}\quad (33)$$

where n_v denotes the number of valence particles outside a closed ^{16}O core. α represents the quantum numbers necessary in specifying the state. Following [26–28], we consider the cm raising and lowering operators $C_{cm}^{\dagger}$ and C_{cm}

$$\begin{aligned}C_{cm}^{\dagger} &= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{Am\omega}{\hbar}}\mathbf{R} - \frac{i}{\sqrt{Am\omega\hbar}}\mathbf{P}\right] = \frac{1}{\sqrt{A}}\sum_{i=1}^A c_i^{\dagger} \\ C_{cm} &= [C_{cm}^{\dagger}]^{\dagger}\end{aligned}\quad (34)$$

where $\mathbf{R}$ and $\mathbf{P}$ are respectively the cm position and momentum. $c_i^{\dagger}$ and c_i are respectively the single nucleon raising and lowering operators.

TABLE II: Eigenfunctions of the lowest two $J^{\pi} = 1^{+}$ states of ^{18}F (fourth-from-left column of Fig. 8). The single-particle orbits are (4 = $d_{5/2}$, 5 = $d_{3/2}$, 6 = $s_{1/2}$, 7 = $f_{7/2}$, 8 = $f_{5/2}$, 9 = $p_{3/2}$, 10 = $p_{1/2}$).

j_a	j_b	$\Psi_1(j_a j_b)$	$\Psi_2(j_a j_b)$
4	4	-.582	-.539
4	5	.658	.085
5	5	.051	.098
5	6	-.148	.097
6	6	-.429	.825
7	7	.041	.010
7	8	-.110	-.007
8	8	-.006	-.012
8	9	.043	.009
9	9	.025	-.011
9	10	-.058	.029
10	10	.019	-.019

Because of Pauli blocking, we have for all α

$$C_{cm}\Phi_{\alpha}^{sd} = 0. \quad (35)$$

This implies that our *sd* calculations are free of spurious cm motion, as every Φ_{α}^{sd} is a state of ground-state cm motion. But for the *sdpf* case we have

$$C_{cm}\Phi_{\alpha}^{sdpf} \neq 0 \quad (36)$$

because C_{cm} can lower a *pf* particle to the *sd* orbits which are not fully filled. Thus our two-shell *sdpf* calculations are not free of spurious cm motion. Such spurious motion can be corrected by a projection operation as outlined in [26–28].^{#2} It will be useful to carry out such projection calculations, and we plan to do so in a future work.

We have found, however, the eigenfunctions Ψ_{α}^{sdpf} of the low-lying states given by our *sdpf* calculations are largely dominated by their *sd* components, as illustrated by the examples shown in Table 2. There we consider two low-lying $J^{\pi} = 1^{+}$ eigenfunctions of our *sdpf* calculations for ^{18}F . As seen, they are almost entirely composed of *sd* components, and consequently they are practically free of spurious cm motion. We have found that

^{#2} In so doing one first constructs, for example, the cm spurious states

$$|S_{\alpha}\rangle = C_{cm}^{\dagger}|\Phi_{\alpha}^{sd}\rangle$$

and

$$|S'_{\alpha}\rangle = C_{cm}^{\dagger}|S_{\alpha}\rangle$$

and then project them out from the shell-model Hamiltonian calculated on the Φ_{α}^{sdpf} basis. The solutions of the resulting Hamiltonian will then be free from $1\hbar\omega$ and $2\hbar\omega$ spurious cm excitations.

FIG. 9: Low-lying states of ^{19}O calculated with the sd one-shell (1 Shell) and $sdpf$ two-shell (2 Shell) EKKO interactions. The experimental results are from [24].

FIG. 10: Same as Fig. 10 except for ^{19}F .

the calculated $sdpf$ eigenfunctions of the low-lying states of ^{18}O , ^{18}F , ^{19}O and ^{19}F we have considered (as listed in the spectroscopy figures of this paper) all have similar sd dominance. For them, the corrections from the cm projection should be small. But for states with significant pf components, such corrections are expected to be important and have to be included.

Our results for the sd one-shell and $sdpf$ two-shell calculations of ^{19}O and ^{19}F are presented in Figs. 9 and 10. The one-shell and two-shell results for ^{19}O are nearly identical as shown in Fig. 9, indicating that the above inter-space consistency requirement is well satisfied here. As shown in Fig. 10, the results for ^{19}F given by the two interactions are, however, noticeably different especially in level ordering. Recall that we have employed the folded-diagram expansion of eq. (1) to calculate the effective interaction V_{eff} . For nuclei with two valence nucleons, only the 2-body $\hat{Q}$ -box diagrams such as those shown in Fig. 1 are needed for calculating V_{eff} . But for nuclei with three valence nucleons, we need in addi-

FIG. 11: A 3-body $\hat{Q}$ -box diagram for the sd one-shell effective interactions. Its external lines all belong to the sd shell, while its intermediate states between any two vertices must have at least one line belonging to the pf shell.

FIG. 12: Low-lying states of ^{19}O and ^{19}F calculated using the $sdpf$ two-shell EKKO interactions, with the pf experimental s.p. energies placed at 10 ('pf-I') and 14 MeV ('pf-II') above the $0d_{5/2}$ orbit.

tion 3-body $\hat{Q}$ -box diagrams [1]. The diagram shown in Fig. 11 is such a 3-body diagram, which should be included in the sd effective interactions for ^{19}O and ^{19}F . But we have not done so in our 'One Shell' calculations of Figs. 9 and 10. This diagram is, however, implicitly included in our 'Two Shell' calculations there. Thus the good agreement shown in Fig. 9 indicates that for ^{19}O it is adequate to include only the 2-body $\hat{Q}$ -box diagrams. But for ^{19}F the inclusion of only these 2-body diagrams is inadequate as indicated by the differences between the one-shell and two-shell results shown in Figs. 10, and in this case the 3-body diagrams as shown in Fig. 11 may be important.

As discussed earlier, in our $sdpf$ two-shell calculations the experimental s.p. energies for the four pf orbits are needed, but their values are not well known. So far we have chosen to place them at a separation of 14 MeV above the $0d_{5/2}$ orbit. We have repeated our calculations using instead a smaller separation of 10 MeV. As illustrated in Fig. 12, the low-lying states of ^{19}O obtained with the separations of 14 and 10 MeV are nearly identical. The differences between the two sets of states for ^{19}F

are also generally small, as also shown in Fig. 12. That our results are nearly independent of the above separations indicates that our *sdpf* effective interactions have a generally weak coupling between the *sd* and *fp* shells. This weak coupling is also consistent with the close similarity between the one-shell and two-shell spectra shown in Figs. 8-10.

We have seen that the non-degenerate Z-box method can be conveniently used to calculate the *sdpf* two-shell effective interactions. This method can also be used for other non-degenerate model spaces such as the *psd* space for light nuclei and the $(f_{5/2}, p_{3/2}, p_{1/2}), g_{9/2}$ space for medium-mass nuclei. It should be of much interest to apply the Z-box method to these model spaces.

IV. SUMMARY AND OUTLOOK

We have applied the iteration method of Krenciglowa and Kuo and that recently developed by Okamoto *et al.* to the microscopic derivation of the *sd* and *sdpf* shell-model effective interactions using the low-momentum nucleon-nucleon interaction derived from the chiral N^3LO two-body potential. We first considered a solvable model and found that both methods are suitable and efficient for deriving the effective interactions for non-degenerate model spaces, where the Lee-Suzuki iteration method is considerably less convenient. Even in the situation where the *P*- and *Q*-space unperturbed Hamiltonians have spectrum overlaps, the KK and EKKO methods perform remarkably well. The EKKO method has the special advantage that its vertex function $\hat{Z}$ -box is, by construction, a continuous function of the energy, while the $\hat{Q}$ -box function used in the LS and KK methods may have singularities. This feature was found to be particularly useful for the convergence of the EKKO iteration method.

Using the above two-body interaction, we first calculated the degenerate *sd* one-shell effective interactions using the LS, KK and EKKO methods. The results given by KK and EKKO were found to be identical. It is noteworthy that the LS results, calculated with a low-order (5th order) iteration, were also in very good agreement with both the KK and EKKO results, supporting the accuracy of the low-order LS method for calculating the degenerate shell-model effective interactions. For the non-degenerate shell-model effective interactions, we first considered a relatively simple case, namely a non-degenerate *sd* one-shell model space in which the $1s_{1/2}$ and $0d_{3/2}$ orbits were shifted relative to the $0d_{5/2}$ orbit according to their experimental single particle energies. In this case the results of the degenerate and non-degenerate *sd*-shell calculations were very similar, giving support to the use of the degenerate *sd* model space in subsequent calculations.

We have calculated the non-degenerate *sdpf* two-shell effective interactions using both the EKKO and KK

methods. Both methods gave identical results and were found to be suitable for such non-degenerate calculations, with the former being more efficient (faster converging). We have applied these interactions to compute the low-lying energy spectra for several nuclei with two and three valence nucleons above the ^{16}O core. A weak-coupling feature of our two-shell effective interactions was observed, namely they provide a rather weak coupling between the *sd* and *pf* shells. Consequently, the *sdpf* wavefunctions of the low-lying states (such as those considered in the figures of section III) are dominated by their *sd* components, and for them the spurious center-of-mass motion that can arise in the *sdpf* calculations should be minimal. But for the higher states of large *pf* components in their wave functions the contamination of the spurious center-of-mass motion can be significant. Such contamination should be examined and projected out. In the present calculation we have not done this, and plan to do so in a future work. Since the *sd* model space is a subspace of the *sdpf* model space, we expect the effective Hamiltonians for these two spaces to have common eigenvalues. Indeed this was largely confirmed in our calculations of ^{18}O , ^{18}F , ^{19}O and ^{19}F spectra, where it was found that the states in the *sdpf* calculations with the maximum *sd*-space overlap agreed with the results given by the *sd* calculations. The above agreement was found to be excellent for ^{19}O , though not as good for ^{19}F , which indicates that the shell-model three-nucleon force is more important in ^{19}F (where the proton-neutron interaction is involved) than in ^{19}O .

The calculated ground state energies for the above four nuclei are all higher (less bound) than the corresponding experimental values. We are studying if the inclusion of the chiral three-nucleon force may give additional binding energy. In the present work we have employed the $\hat{Q}$ -box irreducible vertex function consisting of the first- and second-order diagrams only. The inclusion of the Kirson-Babu-Brown (KBB) all-order core polarization diagrams in the $\hat{Q}$ -box may provide additional binding energy [29]. We plan to carry out further calculations with the inclusion of such all-order KBB diagrams.

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