Effective Hamiltonian in non-degenerate model space

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Abstract. We present a novel method to calculate a microscopic effective interaction in many-body systems. This method applies not only to degenerate model spaces but also to non-degenerate model spaces, and therefore allows us to construct microscopically the effective interaction in multi-major-shell model spaces. As an application of this novel method, we examine the effective interaction between valence neutrons of ^{18}O in the sd-shell (model space of single-major-shell), and in the sdf_7p_3-shell (model space of multi-major-shells). We find that the microscopic cross-shell interactions are much more attractive than have been expected by *ad hoc* methods. Our approach presents an essential step to a microscopic description of nuclei in multi-major-shells, which is crucial, e.g., to describe many of the neutron-rich nuclei.

1. Introduction

The shell model has been playing an important role in nuclear physics. In order to describe nuclear properties in a satisfactory fashion, however, we still need to improve the theory of the effective interaction, the only input of the nuclear shell model. Phenomenological effective interactions, being obtained by tuning two-body matrix elements to reproduce observed experimental data, have described many properties of nuclei successfully [1, 2, 3, 4, 5]. Microscopic effective interactions, on the other hand, have been calculated in the Kuo-Krenciglowa (KK) [6] or the Lee-Suzuki (LS) methods [7] in degenerate model spaces only; these methods cannot be applied, e.g., to a calculation of ^{18}O if we take the non-degenerate model (valence) space composed of sd and pf-shells.

It has now become clear that many unstable nuclei require two or more major-shells for their description, e.g., physics in the island of inversion cannot be explained with the single-major-shell degrees of freedom alone [3]. To date, investigations of these nuclei have been performed using phenomenological effective interactions. It is, therefore, highly desirable to establish a theory to construct the microscopic effective interaction in the multi-major-shell model spaces starting from realistic nucleon-nucleon interactions.

Recently, the KK and the LS methods have been extended so that they apply not only to the degenerate, but also to the non-degenerate model spaces [8, 9]. In this situation, we naturally adopt the extended KK (EKK) method to construct the microscopic effective interaction in multi-major-shell model spaces. We shall see that our theory is a natural extension of the well known folded diagram theory [6, 10].

In Sec.2, we briefly explain the formal theory of effective interaction and the EKK method. Then in Sec.3, we apply the EKK method to ^{18}O, and present discussions using test calculations of the effective interaction in a single major shell (sd-shell) and in two major shells (sdf_7p_3-shell). We shall see clearly that our theory has established a way to calculate the microscopic effective interaction in multi-major-shell model spaces. In Sec.5 we give a brief conclusion.

2. Formal theory of effective interaction

We consider a quantum system that is described by $H = H_0 + V$ in a Hilbert space of dimension D, where H_0 is the unperturbed Hamiltonian and V is the perturbation:

$$H|\Psi_\lambda\rangle = E_\lambda|\Psi_\lambda\rangle, \quad \lambda = 1, \cdots, D. \tag{1}$$

Because the dimension D is very large in many cases, we divide the Hilbert space of dimension D into a model space (P-space) of dimension d to describe the system and its complement (Q-space). Let us denote the projectors onto the P and Q-spaces as P and Q, respectively. We then define the effective Hamiltonian, $H_{\text{eff}} = PH_0P + V_{\text{eff}}$, in the P-space that describes P-space projections of selected d eigenstates of the full Hamiltonian H:

$$H_{\text{eff}} \ P|\Psi_i\rangle = E_i \ P|\Psi_i\rangle, \quad i = 1, \cdots, d. \tag{2}$$

We now explain how to calculate H_{eff}.

2.1. Extended Kuo-Krenciglowa (KK) method

The effective Hamiltonian H_{eff} can be obtained most simply by the similarity transformation of the Hamiltonian, $\mathcal{H} = e^{-\omega}He^{\omega}$. Here we determine $\omega = Q\omega P$ by the following decoupling equation:

$$0 = Q\mathcal{H}P = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega, \tag{3}$$

which decouples the P-space part from the rest in the transformed Schrödinger equation, and gives the desired effective Hamiltonian H_{eff} and the effective interaction V_{eff} as follows.

$$H_{\text{eff}} = P\mathcal{H}P = PHP + PVQ\omega, \quad V_{\text{eff}} = PVP + PVQ\omega. \tag{4}$$

The EKK method is devised to solve Eqs. (3) and (4) without imposing the assumption of the degenerate model space [8, 9], and gives the following iterative scheme for H_{eff}:

$$H_{\text{eff}}^{(n)} = H_{\text{BH}}(E) + \sum_{k=1}^{\infty} \hat{Q}_k(E)(H_{\text{eff}}^{(n-1)} - E)^k, \tag{5}$$

where $H_{\text{eff}}^{(n)}$ stands for H_{eff} at the nth step of iteration, and $\hat{Q}(E)$ and $\hat{Q}_k(E)$ are the $\hat{Q}$-box and its derivatives given by

$$\hat{Q}(E) = PVP + PVQ\frac{1}{E - QHQ}QVP, \quad \hat{Q}_k(E) = \frac{1}{k!}\frac{\mathrm{d}^k\hat{Q}(E)}{\mathrm{d}E^k}. \tag{6}$$

In Eq. (5), we have introduced an arbitrary parameter E that shifts the origin of the Hamiltonian. In the right hand side of Eq. (5), the first term, $H_{\text{BH}}(E) = PH_0P + \hat{Q}(E)$, is the Bloch-Horowitz Hamiltonian, and is the input of the iteration, $H_{\text{eff}}^{(1)}$. In case of convergence, $H_{\text{eff}}^{(n)} \to H_{\text{eff}}$, Eq. (5) gives H_{eff} of Eq. (4) that satisfies

$$H_{\text{eff}} = H_{\text{BH}}(E) + \frac{\mathrm{d}\hat{Q}(E)}{\mathrm{d}E}(H_{\text{eff}} - E) + \frac{1}{2!}\frac{\mathrm{d}^2\hat{Q}(E)}{\mathrm{d}E^2}(H_{\text{eff}} - E)^2 + \cdots. \tag{7}$$

Note that Eq. (7) is interpreted as a Taylor series expansion of H_{eff} around $H_{\text{BH}}(E)$, and changing E corresponds to shifting the origin of the expansion. This explains that the left hand side of Eq.(7) is independent of E, while the right hand side is seemingly dependent on E.
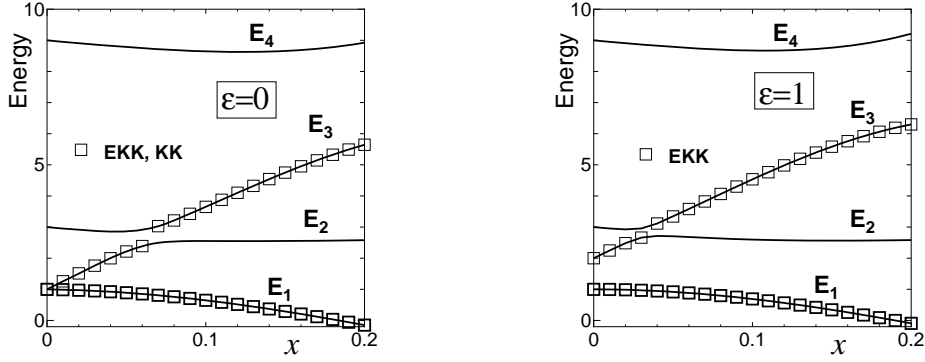
Figure 1. Open squares show eigenenergies of H_{eff} obtained by iterative methods (KK,EKK) in the degenerate (left, $\varepsilon = 0$) and the non-degenerate (right, $\varepsilon = 1$) P-spaces. Solid curves show exact eigenenergies of the Hamiltonian H as functions of the strength parameter x.

2.2. Toy model calculation

Here we carry out the EKK iterative scheme (5) using a toy model. We take a four-dimensional ($D = 4$) Hilbert space that is spanned by the basis vectors $\{|\lambda\rangle, \ \lambda = 1, 2, 3, 4\}$, and a two-dimensional ($d = 2$) P-space $\{|1\rangle, |2\rangle\}$. Our Hamiltonian in the above basis is given by

$$
H = H_0 + V = \begin{pmatrix} 1 & & & \\ & 1+\varepsilon & & \\ & & 3 & \\ & & & 9 \end{pmatrix} + x \begin{pmatrix} 0 & 5 & -5 & 5 \\ 5 & 25 & 5 & -8 \\ -5 & 5 & -5 & 1 \\ 5 & -8 & 1 & -5 \end{pmatrix}, \tag{8}
$$

where a nonzero value of ε removes the degeneracy of the P-space, and the perturbation V is proportional to a strength parameter x. By diagonalizing $H = H_0 + V$, we obtain four eigenstates which we denote as $\{|\Psi_\lambda\rangle, \ \lambda = 1, 2, 3, 4\}$ with eigenenergies $E_1 < E_2 < E_3 < E_4$.

Fig.1 shows the numerical results for the degenerate (left, $\varepsilon = 0$) and the non-degenerate (right, $\varepsilon = 1$) P-spaces. We see that that the EKK method can reproduce excellently two ($= d$) eigenstates both in the degenerate and non-degenerate P-spaces [8, 9], while the standard KK method is available in the degenerate P-space only. Fig.1 demonstrates very well that the EKK method can give microscopic H_{eff} (and V_{eff}) in non-degenerate P-spaces, which had long been beyond the scope of former theories. We are now ready to set out for microscopic shell model calculations in multi-major-shell model spaces.

3. Application to ^{18}O

Here we apply the above EKK theory of the effective interaction to ^{18}O, a simple nucleus composed of two neutrons on top of the ^{16}O core. As the P-space for ^{18}O, we take the sd-shell (degenerate case), and the sdf_7p_3-shell (non-degenerate case) composed of the sd-shell and $0f_{7/2}$ and $1p_{3/2}$ orbits. Detailed description of the theory and comprehensive study of other nuclei will be published elsewhere [11].

3.1. Many-body theory of effective interaction

In the many-body system, H_{eff} of Eq. (7) has a well defined expression in terms of the folded diagrams using the valence-linked $\hat{Q}$-box as in the standard KK theory [6, 10], because the

energy derivative of the $\hat{Q}$-box represents the folding procedure. In order to calculate H_{eff}, all that we have to know is the valence-linked $\hat{Q}$-box and its energy derivatives at the arbitrarily specified energy E [11].

3.2. scheme of calculation

Our input interaction V is the low-momentum interaction $V_{\text{low}k}$ with a sharp cutoff $\Lambda = 2.0\,\text{fm}^{-1}$, which is derived from the $\chi\text{N}^3\text{LO}$ interaction [12]. Our total Hilbert space is composed of the harmonic oscillator basis states in the lowest seven major shells. The single particle energies in the shell model diagonalization are taken from the USD interaction [1, 13].

Let us note here that the new parameter E in our EKK theory provides us with a useful test of calculation [11]; Eq. (7) shows that H_{eff} does not depend on the value of E, provided that the $\hat{Q}$-box in Eq. (7) is given exactly. Any approximation may spoil the E-independence of H_{eff}, and therefore of physical quantities described by H_{eff}. This in turn implies that E-independence of physical quantities is a signal of convergence. In this work, we have calculated the $\hat{Q}$-box diagrams up to the third order in powers of V. In Sec.3.3. we shall see that our numerical results for Eq. (7) are almost E-independent, suggesting that H_{eff} is convergent if $\hat{Q}(E)$ in Eq. (7) is calculated up to the third order in V. Note that the above useful test of convergence is possible only for the EKK method; there is no such criterion in the original KK method.

3.3. Numerical results

Here we present numerical results for ^{18}O in the degenerate sd-shell and in the non-degenerate sdf_7p_3-shell; we show (i) two-body matrix elements of the effective interaction V_{eff}, and (ii) several energy levels obtained by the shell model calculation of ^{18}O, paying special attention on their E-independence.

3.3.1. degenerate sd-shell　Fig.2 shows our numerical results in the degenerate sd-shell model space, where both of the standard KK and the EKK methods are available. To see the E-independence of the EKK results for V_{eff}, we have varied the parameter E in the range of $-5 \leq E \leq 2$ MeV in Fig. 2. Here the origin of energy is so fixed that the EKK method with $E = 0$ coincides with the KK method.

Let us start with the upper panel, where we present the monopole part of V_{eff} in the sd-shell. The dotted lines (which make a shaded band in the figure) are calculated by dropping the folded diagram contributions, i.e., by replacing V_{eff} simply by $\hat{Q}(E)$. We can see clearly that $\hat{Q}(E)$ is strongly dependent on E. Now we take into account all the folded diagram contributions in the right hand side of Eq. (7). The results are shown by solid lines for $E = -5, 0, 2$ MeV, which almost coincide with each other. This shows clearly that the folded diagrams cancel the E-dependence of $\hat{Q}(E)$ to yield the E-independent H_{eff} (and V_{eff}) in Eq. (7).

The lower panels display several energy levels of ^{18}O with respect to ^{16}O calculated by the shell model with our V_{eff}. Let us look at the results without the folded diagram contributions (left panel). They are obviously E-dependent, and are decreasing functions of E, which is explained naturally by the E-dependence of $\hat{Q}(E)$. On the other hand, the calculation with the folded diagrams (right panel) shows clearly that the results are almost independent of the parameter E, as they should.

The above observation shows that the evaluation of the $\hat{Q}$-box up to third order in V is sufficient to establish the E-independence of the right hand side of Eq. (7), and therefore of V_{eff}. This also implies that the $\hat{Q}$-box through third order gives convergent results for V_{eff}, and that we do not need to move on to the fourth order calculation of the $\hat{Q}$-box .
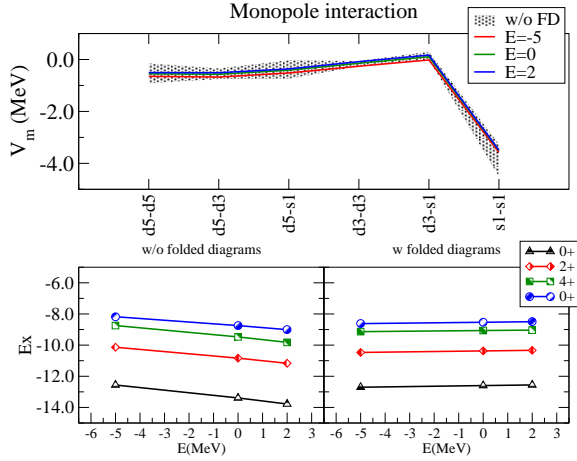
Figure 2. *E*-dependence of the EKK results in the *sd*-shell (degenerate model space). upper panel: the monopole part of $V_{\rm eff}$, ($-5 \leq E \leq 2$ MeV). lower panels: level energies of ^{18}O without (left) and with (right) folded diagram contributions. See the text.
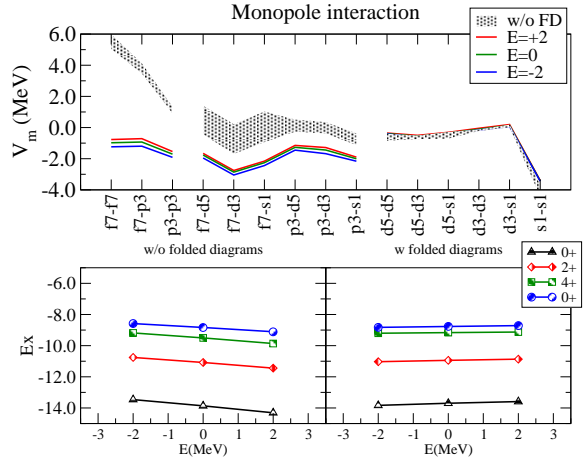
Figure 3. *E*-dependence of the EKK results in the *sdf*$_7$*p*$_3$-shell (non-degenerate model space). The range of *E* is $-2 \leq E \leq 2$ MeV. Other notation is the same as for Fig. 2

3.3.2. non-degenerate sdf$_7$p$_3$-shell Here we examine ^{18}O in the non-degenerate *P*-space, *sdf*$_7$*p*$_3$-shell, composed of the *sd*-shell and $0f_{7/2}$ and $1p_{3/2}$ orbits. In this non-degenerate model space, the standard KK method does not work, and the EKK method only is available. To date, therefore, there have been only phenomenological interactions in this model space [14].

Fig.3 shows the numerical results of the EKK method in the *sdf*$_7$*p*$_3$-shell, in the same way as Fig. 2 in the degenerate *sd*-shell. Let us first look into the monopole part of $V_{\rm eff}$. Here we have cross-shell interactions (f_7-d_5,..,p_3-s_1), in addition to the interactions within the *sd*-shell. We see that the cross-shell interaction is strongly dependent on *E* without the folded diagram contributions. This can be explained by noticing that the corresponding $\hat{Q}(E)$ has intermediate states with small energy denominators. The figure clearly shows that the folded diagram contributions cancel the above strong *E*-dependence of $\hat{Q}(E)$, to make the resultant $V_{\rm eff}$ almost independent of *E*. This observation confirms that the EKK method, implemented by the $\hat{Q}$-box through third order, is robust not only in the degenerate *sd*-shell, but also in the non-degenerate *sdf*$_7$*p*$_3$-shell.
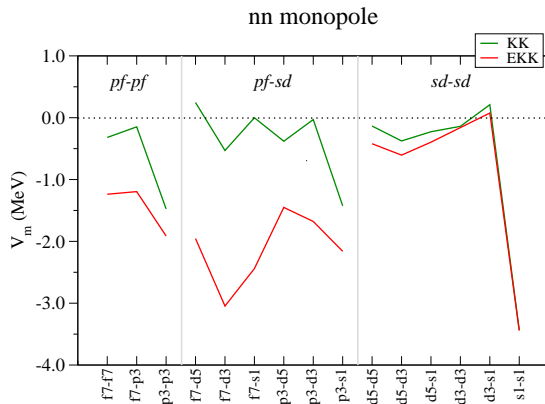
Figure 4. The monopole part of $V_{\rm eff}$ in the *sdf*$_7$*p*$_3$ model space, obtained by the EKK method (lower lines, red) and by the *ad hoc* KK method (upper lines, green).

3.3.3. comparison of KK and EKK methods   Here we compare the KK and the EKK methods in the non-degenerate sdf_7p_3-shell model space. Given the non-degenerate model space, the standard way has been to use the KK method by shifting the single particle energies by hand to make them degenerate, and by treating the energy shift as a perturbation. The resultant effective interaction is not, however, as meaningful as the EKK effective interaction, since it is an *ad hoc* interaction between orbits with artificial single particle energies. Here we show how different they are.

Fig. 4 shows the monopole part of V_{eff} in the sdf_7p_3-shell. The lower (red) lines show the results of the EKK method, and the upper (green) lines stand for the results of the KK method with the *ad hoc* modification of the unperturbed Hamiltonian. It is really striking that the cross-shell interaction (f_7-d_5,..,p_3-s_1) is much more attractive in the EKK method than in the *ad hoc* KK method. This discrepancy clearly comes from the difference in the energy denominator; excitations from the artificially degenerate sdf_7p_3-shell have larger excitation energies than from the non-degenerate sdf_7p_3-shell, to make their contributions smaller in $\hat{Q}(E)$. We expect that the strong cross-shell attraction would have a significant effect, e.g., on the shell evolution, which is one of the hottest topics in nuclear physics.

4. Conclusion

We have presented a novel many-body theory (EKK) to calculate the effective interaction V_{eff} for the shell model which is applicable not only to degenerate (single-major-shell) model spaces, but also to non-degenerate (multi-major-shell) model spaces. On the basis of our numerical results, we have clarified the followings.

First, we have shown that the EKK method works beautifully in many-body systems. In the degenerate model space, it gives the same results as the former methods. In the non-degenerate model space, which is beyond the range of the former theories, our EKK method nicely works.

Second, we have shown that our results for V_{eff} are almost E-independent, as they should, if we calculate the $\hat{Q}$-box up to third order in the perturbation theory. This in turn suggests strongly that the $\hat{Q}$-box through third order is sufficient to give convergent results for V_{eff}.

Third, we have shown that the difference is significant between the EKK method and the KK method with an *ad hoc* modification of the unperturbed Hamiltonian, especially for cross-shell interactions. This should have a large impact, e.g., on the investigation of neutron-rich nuclei where it is essential to incorporate two-major-shell degrees of freedom.

At the end, we stress that our method has established a robust way to calculate the effective interaction in non-degenerate model spaces, or in multi-major-shells, in a microscopic way. We believe that this is an indispensable step to make the nuclear shell model a reliable theory based on a microscopic effective interaction derived from realistic nucleon-nucleon interactions.

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