Extrapolation method in shell model calculations with deformed basis

Takahiro Mizusaki
Institute of Natural Sciences, Senshu University, Kawasaki, Kanagawa, 214-8580, Japan
(Dated: December 21, 2021)

Extrapolation is an intriguing and useful concept in computational physics in quantum many-body problems in condensed matter physics, nuclear structure physics and other fields. The Hilbert spaces of quantum many-body systems can be finite but essentially large or infinite. To handle such Hilbert spaces completely by numerical methods, there exist various difficulties. However if we can handle its dominant but small subspace, the contribution of the rest huge subspace can be taken into account by extrapolation. More concretely we can estimate the exact energy by extrapolation if we know a scaling property how to change energy as a function of a certain physical quantity.

In the nuclear structure physics, shell model is one of fundamental frameworks. For shell model calculations, one needs handle very huge Hilbert space. One of conventional approaches is diagonalization with spherical single particle basis states, which recently have been applicable to quite large-scale problem with dimension up to $10^{10}$. However, for further larger spaces, diagonalization is impossible. To overcome such a limitation of diagonalization, various methods have been proposed and have been developed. Among them, extrapolation methods have been developed, combined with diagonalization of the Hamiltonian matrix evaluated with spherical basis states. For instance, exponential convergence method (ECM) can predict the exact energy by assuming exponential behavior of energy as a function of the number of basis states and empirical successes of its assumption have been reported with various truncation schemes.

We have also proposed an extrapolation method in shell model calculations, combined with Lanczos diagonalization for a series of truncated spaces, where we take an advantage of a scaling property between the energy difference $\delta E$ and energy variance $\Delta E$ for a series of systematically approximated wave functions. Such a scaling property has been originally introduced in the study of Hubbard models. We have introduced this scaling property into shell model calculations. Moreover, we have shown that, for precise estimation, higher order term of expansion can be taken into consideration. Very recently this scaling property has been successfully applied to the no core shell model.

Thus two kinds of extrapolation methods have been proposed and are quite promising. However they have a common drawback that they strongly depend on the diagonalization with spherical basis states. The dimension of necessary truncated subspace heavily depends on each nucleus as the dimension of whole shell model space does.

In the present paper, we propose an extrapolation method in the shell model calculations with deformed bases, which are expected to be suited for deformation of nuclei. As our extrapolation scheme depends on only energy and energy variance, we can apply it to deformed basis. We will show that the exact energy can be extrapolated by the behavior of energy evaluated by single Slater determinant with angular momentum projection.

First we briefly summarize our extrapolation scheme. We consider a series of systematically approximated wave functions as $|\psi_1\rangle$, $|\psi_2\rangle$, $\cdots$. Here we assume that they are systematically generated and their energies becomes lower as $E_1 \geq E_2 \geq \cdots$ where $E_i$ is an energy of $|\psi_i\rangle$. Later we will discuss how to prepare them in deformed basis in detail. The approximated wave function contains large fraction of true wave function and contamination of rest wave function is small. By expanding this small value, a following relation is obtained. We define the difference $\delta E$ between the lowest energy eigenvalue of approximated wave functions and true energy eigenvalue as $\langle \hat{H} \rangle_0$ as $\delta E = \langle \hat{H} \rangle - \langle \hat{H} \rangle_0$. The energy variance $\Delta E$ of approximated wave function is also defined as $\Delta E = \langle (\hat{H})^2 \rangle - \langle \hat{H} \rangle^2$. As a first order approximation, we can show a proportionality as $\delta E \propto \Delta E \frac{\delta E}{\Delta E}$ by expanding $\delta E$ as a function of $\Delta E$. We can take into account second order effects for precise estimation. By these scaling properties, we can estimate the exact energy by taking $\Delta E \rightarrow 0$.

Next we will discuss how to prepare such systematically approximated wave functions in deformed basis. We consider an angular momentum projected deformed
wave function such as
\[ |\psi_{J,M}\rangle = \sum_K g_K P_{M,K}^J |\psi\rangle \]  
(1)

where \( P_{M,K}^J \) is angular momentum projection operator and \( g \)'s are coefficients. The wave function \( |\psi\rangle \) is a Slater determinant as \( |\psi\rangle = \prod a_\alpha^\dagger |0\rangle \) where \( |0\rangle \) is a vacuum state and \( a_\alpha^\dagger \)'s are creation operators on deformed orbit \( \alpha \) and are defined as \( a_\alpha^\dagger = \sum_i D_{\alpha,i} c_i^\dagger \). The \( c_i^\dagger \) denotes creation operator of spherical orbit \( i \) and \( D \)'s are coefficients and are determined by the following variational equation:
\[ \delta \left( \frac{\langle \psi_{J,M} | \hat{H} | \psi_{J,M} \rangle}{\langle \psi_{J,M} | \psi_{J,M} \rangle} \right) = 0. \]  
(2)

In order to solve above equation, we minimize the energy expectation value with angular momentum projected wave function concerning \( D_{\alpha,i} \). This can be achieved by gradient method where we evaluate the gradient vector in the projected energy surface and then we change the wave function along the steepest descent line. By iterating this procedure, the variation of the angular momentum projected energy is achieved. In general, obtained wave function in this procedure corresponds to local minimum in angular momentum projected energy surface. By examining several local minima, we can obtain lowest minimum in the practical calculations. Here we assume that wave function obtained in this procedure is a good approximation for the true wave function, that is, it has a large overlap to true one. In practical shell model calculations, this assumption seems to be good [19].

Under this assumption, we consider how to construct a series of systematically approximated wave functions. The wave function of lowest minimum is written by \( |\varphi_{\text{min}}\rangle \). The shell model orbits are grouped into upper and lower orbits, for instance, in the \( fp \)-shell, four orbits are grouped by \( \{ f_{7/2}/0 \} \) and \( \{ p_{3/2}, f_{7/2}, p_{1/2} \} \). By this grouping, we consider a following parameterized projected wave functions:
\[ |\varphi_{J,M}(x)\rangle = \sum_K g_K P_{M,K}^J |\varphi(x)\rangle \]  
(3)

and
\[ |\varphi(x)\rangle = \prod a_\alpha^\dagger |0\rangle \]  
(4)

where the creation operator \( a_\alpha^\dagger (x) \)'s are defined as \( a_\alpha^\dagger (x) = \sum_i D_{\alpha,i}^\text{min} x_i c_i^\dagger \). The \( D_{\alpha,i}^\text{min} \) corresponds to the one of \( |\varphi_{\text{min}}\rangle \) and \( x_i \) takes 1 or \( x \), depending on the group of \( i \). The \( g \)'s are determined at each \( x \). When the \( x \) increases or decreases from unity, the angular momentum projected energy of \( |\varphi(x)\rangle \) increases because of \( |\varphi(x = 1)\rangle = |\varphi_{\text{min}}\rangle \). In this way, we can systematically generate a series of well-approximated wave functions near the lowest minimum continuously as a function of energy. This construction is not unique and we may find other methods. However this way to construct a series of wave functions works well for \( fp \)-shell calculations as we will show later.

Note that, in general, we have no method to know whether or not a considered wave function is well-approximated to the true wave function unless information of the true state is available. Empirically an optimized projected wave function by variation after angular momentum projection is known to describe deformed state well while we can not, strictly, know the precision of its approximation. In the present method, the energy variance can give an index of precision of approximation.

For the extrapolation by these deformed bases, expectation value of \( \langle \hat{H}^2 \rangle \) is necessary. As we consider a realistic description, we use a general two-body shell model effective interaction as,
\[ \hat{H} = \sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha + \sum_{\alpha<\beta<\gamma<\delta} v_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \]  
(5)

where \( \varepsilon \)'s and \( v \)'s are single particle energies and two-body matrix elements, respectively. Then \( \hat{H}^2 \) includes one-body, two-body, three-body and four-body terms. For instance, normal ordered form of four body term is shown by
\[ \hat{H}_4 = \sum_{i<j<k<l, \alpha<\beta<\gamma<\delta} \tilde{v}_{ijkl\alpha\beta\gamma\delta} c_i^\dagger c_j^\dagger c_k c_l c_\gamma c_\delta c_\alpha \]  
(6)

where \( \tilde{v} \) can be given by summing up relevant \( v \)'s and is totally antisymmetric for \( i, j, k, l \) and for \( \alpha, \beta, \gamma, \delta \). Expectation value of this operator by angular momentum projected state can be carried out by Wick’s theorem.

We define generalized one-body density matrix as
\[ \rho_{\beta\alpha} = \frac{\langle \varphi | c_\alpha^\dagger c_\beta | \psi \rangle}{\langle \varphi | \psi \rangle} \]  
(7)

where \( |\varphi\rangle \) and \( |\psi\rangle \) are deformed Slater determinants. For angular momentum projection, density matrices between different wave functions are necessary. By this one-body density matrix, we can define two-body density matrix as
\[ \rho_{\alpha\beta\gamma\delta} = \frac{\langle \varphi | c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta | \psi \rangle}{\langle \varphi | \psi \rangle} = \rho_{\gamma\alpha} \rho_{\delta\beta} - \rho_{\delta\alpha} \rho_{\gamma\beta}. \]  
(8)

By the two-body density matrix, we can show the expectation value of the four-body term \( \hat{H}_4 \) which can be given by six terms of product of two two-body density matrices. As we consider proton-neutron system and isospin projection is not introduced, two-protons and two-neutrons creation and annihilation part \( c_\pi^\dagger c_\pi^\dagger c_\nu^\dagger c_\nu^\dagger c_\rho^\dagger c_\rho^\dagger c_\sigma^\dagger c_\sigma^\dagger \), which is a dominant part of the \( \langle \hat{H}^2 \rangle \) calculation, needs only one product of two two-body density matrices. Then such a normal ordered form of the \( \hat{H}^2 \) operator is most efficient for numerical calculation.

Next we consider how to reduce computational time by taking an advantage of time-reversal symmetry. By
solving eq. (2) for $J = 0$ ground state, we can obtain the wave function with time-reversal symmetry. For such a case, it is known that an integral domain for angular momentum projection can be reduced. The projected matrix element of the Hamiltonian $H_{KK'}^{j}$ is defined by

$$H_{KK'}^{j} = \langle \psi | \hat{H} \hat{P}_K^{j} | \psi \rangle,$$

which is evaluated by a following integral:

$$
H_{KK'}^{j} = \frac{2j+1}{\pi} \int_0^\pi d\alpha \int_0^{\pi/2} d\beta \int_0^{2\pi} d\gamma W_{KK'}^{j}(\Omega).
$$

The $\Omega$ stands for the Euler’s angles. The $W_{KK'}^{j}(\Omega)$ is a sum of relevant product of the Wigner’s D-function and rotated matrix element $\langle \psi | \hat{H} \hat{R}(\Omega) | \psi \rangle$ where $\hat{R}(\Omega)$ is a rotating operator. Detailed form is written in Ref. 21, for instance. Due to the reduced integral domain and relations of rotated matrix element concerning Euler’s angles, computational time reduces $1/8$ shorter.

Furthermore, to reduce amount of computation, as a series of systematically approximated wave functions for the extrapolation of excited states, we use the same series of ground state. In this case, we can use the same rotated matrix elements for $(\hat{H}^2)$ calculation. Therefore we can simultaneously obtain extrapolations of several low-lying states in addition to the one of the ground state.

![FIG. 1: Extrapolations of two kinds of extrapolation method are shown for the ground and first excited states of $^{60}$Zn with the FPD6 interaction 10. The open circles are shown for energies and energy variances of $t = 3 \sim 5$ truncated spaces. Their extrapolations are shown by dashed lines. The filled squares and filled diamonds are energies and energy variances of deformed states with angular momentum projection for groupings (i) and (ii), respectively. The angular momentum projected energies and energy variances for $J = 0$ and 2 from the Hartree Fock wave function are shown by open diamonds and are indicated by the word VBP. The energy of variation after angular momentum projection for $J = 0$ state is labeled by the word VAP.](image)

In order to test the present extrapolation method, we take an example of $^{60}$Zn in the $fp$ shell model space, the dimension of which Hilbert space is largest in the $fp$ shell model space and is $2,292,604,744$ in $M = 0$ space. We use the FPD6 effective interaction 10. To test the present extrapolation, the exact ground state energy is needed. The exact ground state energy of this nucleus may be obtained by the state-of-the-art Lanczos shell model diagonalization if we take quite long computational time. However here we use extrapolation method which we have proposed in Refs. 12, 13. The extrapolation method also use the scaling property of energy and energy variance while we combined it to Lanczos shell model diagonalization. By the minimum number $t$ of the holes in the $f_{7/2}$ orbit, we can systematically define the truncation spaces as $\oplus f^{(16-t)}_{7/2} r^{4+t} (r = p_{3/2}, f_{5/2}, p_{1/2}).$ Truncation spaces are labeled by $t$. As the $t$ increases, its truncation space becomes larger and the lowest energy state $|\varphi_{t}\rangle$ of such a truncated space becomes a better approximation to the true state.

In Fig. 1, we use the truncation spaces with $t = 3, 4$ and 5. The dimensions of truncated shell model spaces are 4794006, 31077402 and 133553398 respectively. For each space, we diagonalize the shell model Hamiltonian matrix and obtain the approximated wave functions of the true ground state. Then we evaluate the matrix element of $\hat{H}^2$. The extrapolation is shown in Fig. 1. For the diagonalization in truncated spaces, we use the shell model code MSHELL 21.

As deformed basis, Hartree-Fock energy is primarily important and is -243.03 MeV for $^{60}$Zn. First step of improvement of wave function is the angular momentum projection. The angular momentum projected energies for $J = 0$ and 2 states from the Hartree Fock wave function are shown in Fig. 1. Angular momentum projection improves energy and we can explicitly handle angular momentum quantum numbers. This approach is known to be the VBP (variation before projection). Next step is a variation after angular momentum projection. We can determine the minimum energy in the angular momentum projected energy surface for $J = 0$. This energy is also shown in Fig. 1. By these energies and energy variances, we may extrapolate the true energy. In this case, this extrapolation is not so bad. However, relation between these two wave functions is not clear and extrapolation from only two data is not reliable.

For extrapolation, a series of systematically approximated wave functions is important. To construct such a series, four $fp$ shell orbits are grouped in following two ways: (i) $\{f_{7/2}, p_{3/2}\}$ and $\{f_{5/2}, p_{1/2}\}$ and (ii) $\{f_{7/2}\}$ and $\{p_{3/2}, f_{5/2}, p_{1/2}\}$. For these groupings, we change $x$ parameter in $|\varphi(x)\rangle$. The dependence of $x$ in $a_{x}^{t}(x)$ is simple, but for the angular momentum projected energy, the dependence of $x$ is no more simple and is non-linear. However by rescaling the energy as a function of energy variance, we can obtain a simple scaling again. In Fig. 1, we take $x = 1.0, 0.8, 0.75, 0.7, 0.65$ and 0.6 for grouping (i) and $x = 1.0, 0.8, 0.7, 0.6,$ and 0.5 for grouping (ii). These data of energy to the energy variance for ground
and excited states are well-aligned and we can find fine proportionality, by which we can make sure extrapolation. The energies of the present extrapolation method agree with those of the previous method within 0.1 MeV. In the respect of the computational amount, previous extrapolation with spherical basis \[\text{12, 13} \] needs four days while this new approach needs less than half day in this calculation. Therefore the present extrapolation method is superior to the previous one.

In the present method, we solve eq. \[\text{2}\] for \( J = 0 \) ground state while extrapolations are carried out for several low-lying states from the series of wave functions for \( J = 0 \) state. This method has an advantage for drastically reducing computational time. However for higher spin states, the approximation may become worse. Therefore, we test what extent the extrapolation works well for several low-lying yrast states by this approach. Here we take \(^{48}\text{Cr}\) as an example. For comparison, we can give exact energies for yrast states by Lanczos diagonalization. In the left panel of Fig. 2, we show the exact level scheme. In the right panel, the energies as a function of energy variances for \( x = 1.0, 1.1, 1.2 \) and 1.3 are plotted. For \( fp \) shell orbits are grouped in a following way: \( \{f_{7/2}\} \) and \( \{p_{3/2}, f_{5/2}, p_{1/2}\} \). Because \( x = 1.0 \) corresponds to the minimum energy, energies with \( x > 1 \) are higher than minimum energy. By this construction, for a series of wave functions \( x \geq 1 \) (\( x \leq 1 \)), excitation from the \( f_{7/2} \) orbit to other upper three orbits increases (decreases). As more excitation is needed, in general, to generate high spin states, we consider a series for \( x \geq 1 \).

In Fig. 2, the extrapolated energies agree with the exact ones within 0.1 MeV, which means that a series of wave functions for \( J = 0 \) state works for other low-lying states. However, minimum of variance for higher spin state increases. This means deterioration of approximation, while such deterioration is somewhat compensated by the extrapolation procedure. Thus the present approach works well for low spin yrast states.

For higher spin, deterioration of approximation is evident. This point is expected to be improved by optimizing a deformed wave function for each spin, which needs longer computational time. Moreover, here we show energies for \( J \leq 8 \) states while this nucleus is known to have a backbending \[\text{22}. \] For such a large change of structure in wave functions as a function of spin, such an optimization becomes necessary.

Finally we discuss an advantage of the present extrapolation method to other extrapolation methods. In an open-shell nuclei, deformed states often appear due to residual interaction. To describe deformed states by spherical bases, we need almost entire spherical bases. Consequently truncation is not so effective and the convergence of energy as a function of the number of spherical basis state becomes very slow. According to the ECM\[\text{8}, \] necessary number of spherical basis state increases exponentially as we need more precise energy. On the other hand, it is evident that deformed basis can handle deformed solution more naturally. In the present paper, we use always one Slater determinant. This fact is in sharp contrast with other extrapolation methods and becomes a distinct advantage for larger shell model problems, where a physically relevant truncation by spherical basis becomes severely difficult. Another merit of the present method is to handle all nucleus in the considered model space within almost the same amount of computation. In extrapolation methods based on the spherical shell model, as the number of valence nucleons reaches half of degeneracy of orbits, amount of computation rapidly increases. Therefore feasibility of the present method is wider than other extrapolation methods. Moreover the present method has a close link to mean-field or projected mean-field theory. It is also an advantage that physical interpretations of the obtained results based on mean-field is easy.

In summary, we have proposed an extrapolation method in shell model calculations by deformed wave functions with angular momentum projection. Our extrapolation technique relies on a scaling property between energy and energy variance of a series of systematically approximated wave functions. To apply it to shell model calculations, a key issue is how to construct such a series. In our previous papers \[\text{12, 13} \], we consider physically relevant truncation subspaces and we solve shell model problem within these subspaces by Lanczos method. Then we obtain such a series and apply the extrapolation technique. On the other hand, in the present paper, we consider a deformed wave functions with angular momentum projection. By variation-after-projection, we can solve shell model problem under a restriction of single Slater determinant with angular momentum pro-
jection. This wave function often becomes a relevant approximation to the true state, especially when nucleus is deformed. We have shown that a series of approximated wave functions can be generated by changing their structure systematically. To evaluate the energy variances by such an angular momentum projected Slater determinant, the Wick’s theorem is used. As we do not use isospin projection for proton-neutron systems, most time consuming part of $\langle H^2 \rangle$ calculations is rather simplified. Time reversal symmetry is also useful to reduce the numerical calculations concerning angular momentum projection. By these developments, we have shown that the extrapolation method with deformed basis works well.

In the present paper, for minimizing necessary amount of computation, we introduced several restrictions. However, for more precise extrapolation and description of excited states with the same quantum numbers, we can introduce a diagonalization with several optimized Slater determinants and optimization of deformed bases for each spin. Such important extensions will be able to be realized with a help of parallel computation.

As applications of the present method, $fpg$ shell is important, whose orbits are $p_{3/2}$, $f_{5/2}$, $p_{3/2}$ and $g_{9/2}$. The ground state of $A \sim 80$ nuclei is determined by a subtle competition between oblate and prolate deformed states and occupation of the $g_{9/2}$ orbit is essential, which means that relevant truncation spaces become quite huge. On the other hand, deformed states can be well-approximated by well-optimized Slater determinant with angular momentum projection. The present extrapolation method can handle such a subtle competition. Moreover, the present extrapolation may also apply to the study of fractional quantum Hall effect formulated on the Haldane sphere [24]. Such studies are being in progress.

This work was supported in part by Grant-in-Aid for Specially Promoted Research (13002001) from the Ministry of Education, Science and Culture. This work was also supported by the Grant-in-Aid of the Promotion and Mutual Aid Corporation for Private Universities of Japan at 2003 and 2004.

[1] E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, J. Retamosa, A. P. Zuker, Phys. Rev. C59 2033 (1999).
[2] S. E. Koonin, D. J. Dean, and K. Langanke, Phys. Repts. 577, 1 (1996).
[3] J. Dukelsky, S. Pittel, Phys. Rev. C63 061303 (2001); J. Dukelsky, S. Pittel, S. S. Dimitrova, M. V. Stoitsov, Phys. Rev. C65, 054319 (2002).
[4] A. Petrovici, Nucl. Phys. A704, 144c (2002).
[5] M. Honma, T. Mizusaki and T. Otsuka, Phys. Rev. Lett. 75, 1284 (1995).
[6] T. Otsuka, M. Honma, T. Mizusaki, N. Shimizu, and Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001).
[7] E. Caurier, F. Nowacki, A. P. Zuker, G. Martinez-Pinedo, A. Poves, and J. Retamosa, Nucl. Phys. A654, 747c (1999).
[8] M. Horoi, A. Volya and V. Zelevinsky, Phys. Rev. Lett. 82, 2064 (1999); M. Horoi, B. A. Brown and V. Zelevinsky, Phys. Rev. C65, 027303 (2002).
[9] T. Papenbrock, D. J. Dean, Phys. Rev. C67, 051303 (2003); T. Papenbrock, A. Juodagalvis, D. J. Dean, Phys. Rev. C69 024312 (2004).
[10] F. Andreozzi, A. Porrino, J. Phys. G27 845 (2001).
[11] H. Zhan, A. Nogga, B. R. Barrett, J. P. Vary, P. Navratil, Phys. Rev. C69 034302 (2004).
[12] T. Mizusaki and M. Imada, Phys. Rev. C65, 064319 (2002).
[13] T. Mizusaki and M. Imada, Phys. Rev. C67, 041301(R) (2003).
[14] M. Imada and T. Kashima, J. Phys. Soc. Jpn. 69, 2723 (2000).
[15] E. Caurier et al., Phys. Rev. Lett. 75, 2466 (1995).
[16] [23] A. Poves and A. P. Zuker, Phys. Repts. 70, 235 (1981).
[17] M. Honma, T. Mizusaki and T. Otsuka, Phys. Rev. Lett. 77, 3315 (1996).
[18] For instance, P. Ring and P. Schuck, The Nuclear Many-Body Problem, (Springer-Verlag, New York, Heidelberg, Berlin, 1980).
[19] M. Honma, B. A. Brown, T. Mizusaki and T. Otsuka, Nucl. Phys. A704, 134c (2002).
[20] K. Enami, K. Tanabe, and N. Yoshinaga, Phys. Rev. C59 135 (1999).
[21] M. Honma, B. A. Brown, T. Mizusaki and T. Otsuka, Nucl. Phys. A704, 134c (2002).
[22] E. Caurier et al., Phys. Rev. Lett. 75, 2466 (1995).
[23] A. Poves and A. P. Zuker, Phys. Repts. 70, 235 (1981).
[24] M. Onoda, T. Mizusaki, T. Otsuka, H. Aoki, Phys. Rev. Lett. 84, 3942 (2000).