A common many-body approach in shell model and
Hubbard model

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Abstract. Recently proposed two methods such as Quantum Monte Carlo Diagonalization
method in nuclear structure physics and path-integral renormalization group method in
condensed matter physics have a similarity as quantum many-body approach, especially in
description beyond mean-field approximation. As these two methods have been developed
in different fields, there are significant differences as quantum-number projection technique
in former method and extrapolation technique in latter method. As these techniques are
independent of details of considered system, these can be applied to other fields. In this paper,
we discuss how to apply such extrapolation technique to shell model calculations and discuss
how to apply quantum-number projection to path-integral renormalization group method.

1. Introduction
Quantum many-body approaches to go beyond mean-field approximation are crucially important
for every branch of physics. There are wide varieties for considered systems, such as, atomic
nuclei, strongly correlated electrons on a lattice, atom, molecule and so on. There are, however,
many common approaches. For instance, exact diagonalization and Quantum Monte Carlo
methods are often used. For one-dimensional system, Density Matrix Renormalization Group
(DMRG) method is quite powerful. Especially in nuclear shell model, Quantum Monte Carlo
Diagonalization (QMCD) method [1] has been proposed and developed, which has widened the
scope of nuclear shell model calculations [2]. Recently similar method appears in condensed
matter physics, which is called path-integral renormalization group (PIRG) method [3, 4].

The QMCD method and PIRG method have some similarities. They are a general method
to give optimum basis sets for quantum many-body system by utilizing auxiliary-field path-
integral representation of imaginary time evolution operator. However they have differences,
which are originated in each field. In the QMCD, quantum-number projection is utilized to
handle symmetry property of wave function. For nuclei, angular momentum has a primal
significance and is indispensable for its analysis. Therefore at early stage of development of
the QMCD method, quantum-number projection is introduced [5]. On the other hand, in the
PIRG, extrapolation technique is crucially important. For example, in the Hubbard models, at
fixed filling factor, we have to consider larger and larger lattices to know a property of infinite
system. As the system size becomes larger, it is difficult to obtain precisely approximated energy
by manageable number of basis. By extrapolation based on quantum mechanics, exact energy
can be obtained as we will discuss later.

As these methods are independent of details of considered system, we can apply them to
other systems. I applied quantum-number projection to strongly correlated electron systems,
combined with the PIRG method [6]. I also applied extrapolation to nuclear shell model [7, 8, 9]. Such an exchange of these many-body techniques is quite fruitful in both fields. In the present paper, these two common techniques in shell model and Hubbard model are discussed.

2. Extrapolation technique for nuclear shell model

2.1. Extrapolation technique for spherical basis

In shell model calculations, extrapolation is a natural idea but proposed extrapolations [10, 11, 12, 13] up to now are empirical and are lack of mathematical reason. For instance, in Fig. 1, shell model calculations of $^{48}$Cr in full $fp$ shell with KB3 interaction [14] are presented. The sub-shell gap of $N = 28$ or $Z = 28$ is utilized, by truncating the whole shell model space by particle-hole excitations from $f_{7/2}$ to upper three orbits. As the number of particle-hole excitations increases, truncated space becomes bigger. In Fig. 1(A), ground state energies are plotted as a function of basis dimension. From variational principle, these energies are upper-bound of the exact ground state energy, while there is no universal pattern of energy as a function of dimension.

We consider an extrapolation method based on the the scaling property between energy difference $\delta E$ and energy variance $\Delta E$, which has been proposed in Ref. [3, 15]. This method is successful in the study of Hubbard models and recently it is also successfully applied to shell model calculations [7, 8]. We consider approximated wave function contains large fraction of exact wave function and small fraction of rest components. The energy difference $\delta E$ between the lowest energy eigenvalue $\langle \hat{H} \rangle$ of approximated wave functions and exact energy eigenvalue $\langle \hat{H} \rangle_0$ is given by $\delta E = \langle \hat{H} \rangle - \langle \hat{H} \rangle_0$. The energy variance $\Delta E$ of approximated wave function is also defined as $\Delta E = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{\langle \hat{H} \rangle^2}$. By expanding $\delta E$ and $\Delta E$ in terms of this small value, we can show a proportionality as

$$\delta E \propto \Delta E. \quad (1)$$

We prepare series of wave functions $\{ |\psi_\alpha \rangle \}$ in a systematic way, and we evaluate the energy $E_\alpha$ and energy variance $\Delta E_\alpha$. By extrapolating $E_\alpha$ into $\Delta E_\alpha \to 0$, we can estimate accurate ground-state energy.

In Fig. 1(B), we plot energy as a function of energy variance. By extrapolating into zero energy variance, we can find exact energy. As we pointed out in Ref. [8], if we consider more precise energy eigenvalue, the second order effect can be taken into account. In Fig. 2, we show the extrapolation for $^{60}$Zn, of which shell model dimension in $M$-scheme is almost 2 billion. Its complete shell model calculation is quite difficult, while its truncated shell model calculations are still feasible. These shell model energies are plotted as a function of energy variance. Energies are approximately aligned while there seems a slight deviation. We can take into account this deviation by second order extrapolation formula [8].

2.2. Extrapolation technique for deformed basis

For bigger shell model space, truncation spaces are also bigger. No feasible truncation scheme for spherical shell model diagonalization might be taken. For such a case, deformed basis is a natural choice. In general, well-optimized angular momentum projected wave function can give a nice description. Such wave functions in deformed basis are prepared as follows. An angular momentum projected deformed wave function is defined as

$$|\psi_{J,M} \rangle = \sum_K g_K P_{MK}^J |\psi \rangle \quad (2)$$

where $P_{MK}^J$ is angular momentum projection operator and $g$'s are coefficients. The wave function $|\psi \rangle$ is a Slater determinant as $|\psi \rangle = \prod \alpha \prod |a_\alpha^\dagger |0 \rangle$ 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
Figure 1. (A) Ground state energies are plotted as a function of basis dimensions for $^{48}$Cr with KB3 interaction [14]. (B) The same energies are plotted as a function of energy variance.

Figure 2. Ground and first excited state energies are shown as a function of energy variance for $^{60}$Zn with FPD6 interaction [16]. Two kinds of extrapolations are shown.

creation operator of spherical orbit $i$ and $D$’s are coefficients and are determined by the following variation-after-projection (VAP) equation:

$$\delta \left\{ \frac{\langle \psi_{J,M} | \hat{H} | \psi_{J,M} \rangle}{\langle \psi_{J,M} | \psi_{J,M} \rangle} \right\} = 0.$$  \hspace{1cm} (3)

In order to solve above VAP equation, we minimize the energy expectation value with angular momentum projected wave function concerning $D_{\alpha,i}$. This can be achieved by gradient method. Here we assume that wave function obtained in this procedure is a good approximation for the exact wave function, that is, it has a large overlap to exact one. In practical shell model calculations, this assumption seems to be good [17].

A series of systematically approximated wave functions are constructed as follows. 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 $\{ f_{7/2} \}$ and $\{ p_{3/2}, f_{5/2}, p_{1/2} \}$. By this grouping, we consider a following parameterized projected wave functions:

$$| \varphi_{J,M} (x) \rangle = \sum_K g_K P^J_M | \varphi (x) \rangle$$  \hspace{1cm} (4)

and

$$| \varphi (x) \rangle = \prod \alpha a^\dagger_{\alpha} (x) | 0 \rangle$$  \hspace{1cm} (5)

where the creation operator $a^\dagger_{\alpha} (x)$’s are defined as $a^\dagger_{\alpha} (x) = \sum_i D_{\alpha,i}^{(\text{min})} x_i c^\dagger_i$. 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 $| \varphi (x = 1) \rangle = | \varphi_{\text{min}} \rangle$. Thus we can systematically generate a
series of well-approximated wave functions near the lowest minimum continuously as a function of energy.

In Fig. 2, we show extrapolation for deformed basis. The VAP energy is lowest for each spin by definition. As we change parameter $x$ from unity, its energy systematically becomes higher and energy variance becomes larger. As these energies are well-aligned in energy - energy variance plane, we can estimate exact energy by extrapolation. This approach is to obtain yrast states. For non-yrast states or detailed description of yrast states, an extension with multi-Slater determinants with angular momentum projection is necessary and such a study is in progress.

3. PIRG method with quantum-number projection

Here we discuss the condensed matter problem by taking the PIRG method and Hubbard models. The Hubbard model on two-dimensional square lattice is defined as $H = H_t + H_t' + H_U$ where $H_t = -\sum_{\langle ij\rangle\sigma} t (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.})$, $H_t' = -\sum_{\langle kl\rangle\sigma} t' (c_{k\sigma}^\dagger c_{l\sigma} + \text{H.c.})$ and $H_U = \sum_i U (n_{i\uparrow} - \frac{1}{2}) \cdot (n_{i\downarrow} - \frac{1}{2})$. Here $i$, $j$ represent lattice points and $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is a creation (annihilation) operator of an electron with spin $\sigma$ on the $i$-th site. The summation over $\langle ij\rangle$ is for the nearest neighbor pairs and that over $\langle kl\rangle$ is for the next-nearest neighbor pairs. We impose the periodic boundary condition. In Hubbard model, we consider dynamics of many electrons on a lattice, while its basic formulation has some similarities to nuclear shell model.

We briefly explain the PIRG method [3, 4]. The ground state $|\psi_g\rangle$ can be obtained by applying the projector $e^{-\tau H}$ to an arbitrary state $|\phi_{\text{initial}}\rangle$ which is not orthogonal to the exact ground state as $|\psi_g\rangle = e^{-\tau H} |\phi_{\text{initial}}\rangle$. (6)

Based on this basic relation, the PIRG gives the optimum basis sets composed of $L$ Slater determinants as $|\psi^{(L)}\rangle = \sum_{\alpha=1}^L c_{\alpha} |\phi^{(L)}_{\alpha}\rangle$, (7)

where $c_{\alpha}$’s are amplitudes of $|\phi^{(L)}_{\alpha}\rangle$. Operation of the ground-state projection can give optimal $c_{\alpha}$’s and $|\phi^{(L)}_{\alpha}\rangle$’s, while this operation increases the number of Slater determinants. To keep manageable number of Slater determinants in actual computation, we restrict number of Slater determinants by selecting variationally better ones. Therefore this procedure can give us only an upper limit of exact energy. To know exact energy, the extrapolation technique based on the scaling property of energy and energy variance has been developed as we already discussed.

In Fig. 3, we show how well the extrapolation works in the Hubbard model. In the left figure, we plot the energies per site as a function of basis dimension $L$ ($L = 32, 64, 128, 256$). The $L = 1$ corresponds to HF by definition. Because there is no definite trend for convergence pattern, we cannot extrapolate ground state energy as a function of $L$. On the other hand, we plot the energies per site as a function of energy variance. The energies per site are well aligned as shown in the right figure. From the proportionality between energy and energy variance, we can get sure extrapolated value. Its extrapolated value is almost the same as the QMC value [18].

The basic formulation of the PIRG method is quite similar to that of the QMCD method [1]. The PIRG method, however, has extrapolation technique, which is essential difference. As shown in the previous section, this extrapolation technique works well also in shell model calculations. On the other hand, the QMCD method has angular momentum projection, which the PIRG method does not have. Then I introduce symmetry projection technique of nuclear structure physics into the PIRG method.

In the Hubbard-type models, symmetries such as spin and momentum have a significant role in the low-energy states. As shell model calculations, we can classify low-energy eigenstates
Figure 3. Ground-state energies per site are shown as a function of basis dimension $L$ (left) or energy variance (right) for the PIRG and QP-PIRG in the Hubbard model with $6 \times 6$ half-filled lattice. The parameters are at $t = 1$, $t' = 0$ and $U = 4$. HF energy is shown by open circle. The ground-state energy of Monte Carlo calculation is also shown by open diamond at zero variance with the statistical error bar [18].

and can elucidate the nature of low-energy phenomena like excitation spectra and spectroscopic properties. Therefore quantum-number projection concerning spin and momentum can be useful and we have developed an extended PIRG method, which is called QP-PIRG [6]. In this method, we start from a fact that the ground-state projector $e^{-\tau H}$ to $|\psi\rangle$ can be applied to lower the energy even within symmetry-imposed restricted space. To realize this, we consider the PIRG with quantum-number projection. However, as a partial sum over the Stratonovich auxiliary variable destroys the symmetry in an elementary PIRG procedure of the projection $\exp(-\Delta \tau H)|\psi\rangle$, we need to perform the quantum-number projection as $P \exp(-\Delta \tau H)|\psi\rangle$ to restore the symmetry. Moreover, for Hubbard models, as a quantum-number projection, we use a combination of the momentum and the spin-parity projection. This is not a complete method for spin symmetry. Then to restore the spin symmetry perfectly, after the QP-PIRG procedure above, we again perform the full spin projection. These concrete procedures are fully discussed in Ref. [6].

In Fig. 3, we show the results of QP-PIRG. In the left panel, QP-PIRG clearly gives better energies within fewer $L$. For $L \sim 140$, projected energies are already well within the error bar of the QMC energy. The right panel shows that QP-PIRG wave functions give smaller energy variances compared to those of PIRG. This example shows that a combination of PIRG with quantum-number projection makes an essential progress.

4. Summary
We presented a common approach both for shell model calculations and Hubbard models. There is a basic similarity as a method to handle quantum many-body system between the Quantum Monte Carlo Diagonalization (QMCD) method [1] in shell model calculations and the path-integral renormalization group (PIRG) method [3] in condensed matter physics. However, both methods have been developed in different fields and there are several significant differences.

One difference is an extrapolation technique based on scaling between energy difference and energy variance. Compared to the empirical extrapolations, this extrapolation is non-empirical and can be derived from quantum mechanics. This method has been developed in the study of
Hubbard models, while recently it could be successfully applied to shell model calculations in two ways. One is shell model calculations with spherical bases [7, 8], the other is with deformed bases [9]. It is shown that this extrapolation non-empirically can give us exact shell model energies.

Other difference is a symmetry projection technique, which the QMCD and other nuclear structure physics use as an angular momentum or number projection. In the Hubbard models, we consider many electrons on lattices. The relevant symmetries are total spin, total momentum and some other geometrical symmetries. These symmetries can be also taken into account by projection methods. Total spin can be projected out by projection, which is known to be axially symmetric angular momentum projection. Total momentum can be also projected out. These projections can be implemented into the PIRG method and it is shown that this extension of the PIRG method extensively widens its scope for precision of energy and description of excited states. By this extended PIRG, we are investigating the Hubbard models with geometrical frustration which are expected to have a new and exotic non-magnetic insulator phase.

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