Extrapolation method in shell model calculations with a deformed basis

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Related papers:
Extrapolation method for shell model calculations: PRC65(2002) 064319, Takahiro Mizusaki and Masatoshi Imada
Extrapolation method in shell model calculations with a deformed basis: PRC70 044316 (2004)  Takahiro Mizusaki
Introduction

- Shell model calculations
  - Two important issues
  - How to solve it!
  - How to prepare effective interaction!

- Conventional Lanczos shell model
  - Typically $10^8$ M-scheme dimension with usual PC

![Shell model dimension vs year](image)
Various methods for shell model calculations

- **Diagonalization by optimum bases** for shell model calculations
  - QMCD
  - VAMPIR
  - GCM
  - Lanczos method with truncated shell model spaces
  - Projected shell model
- **Others**
  - SVM for few body
  - AMD for cluster physics
- **In principle, these are approximations.**
- Common drawback in algorithm to ensure the exact energy
- We can check the convergence as a function of the number of basis states, at most.

Alternative methods

- **Monte Carlo method**
  - SMMC for ground state
  - Spectroscopic MC for yrast
  - *Exact* energy is obtained with stochastic error
  - Sign problem
- **DMRG**
- **Empirical extrapolation**
  - Exponential convergence
  - ECM and similar methods
- **Non-empirical extrapolation**
  - **Extrapolation by energy variance**
    - Spherical basis version
    - Deformed basis version
Clever truncation scheme

What are most important bases? (in the view of variational principle)

Optimized spherical basis
  Wave function factorization
  Truncation by stochastic criterion (a part of ECM)
Optimized deformed basis
  QMCD, VAMPIR, GCM, …

In general, deformed basis is a better approximation than spherical basis.

To obtain exact energy, we need an extrapolation method.

Energy mountain as a metaphor
Empirical extrapolation

- An **empirical extrapolation** based on the number (t) of particle-hole excitations works to some extent. (NP. A704 223c-231c Nowacki)
- The fp shell is somewhat special. As N=Z=28 is subshell, truncation specially works well.

1. Energy convergence (in MeV) of the first two states in {eq}^{56}\text{Ni} \text{ with the neutron excitations (FPD6 interaction).} \)
Empirical but more systematic extrapolation

- Truncated energy approaches true one exponentially.
- Exponential fitting
  - Exponential growth can be right but we do not like exponential growth of Hilbert space.
  - Mathematically speaking, there is no proof of exponential behavior as a function of basis dimension.
- Another applications of ECM
  - Wave function factorization (Papenbrock and his collaborators)
  - Correlated proton-neutron basis calc. (Andorezzi and Porrino)
  - Exponentially large truncation spaces are also needed for tracing exponentially growth of whole shell model space.

http://mocha.phys.washington.edu/~int_talk/WorkShops/ACD02/
Exponential convergence of wave function factorization
PRC69,024312 (2004)

- Wave function factorization is a clever optimization.
- Exponential convergence works well.

$^{56}$Ni: Full dimension $10^9$
This method reduces dimension effectively like $10^9 \rightarrow 10^6$.
The rest contribution can be estimated by EC assumption.

**FIG. 9:** Ground-state energy $E$ versus the dimension $d$ of the eigenvalue problem relative to the $m$-scheme dimension $d_{\text{max}} \approx 1.09 \times 10^9$ for $^{56}$Ni. The data points are from the $m$-scheme factorization, and the dashed line is an exponential fit to the data. Inset: Similar plot for $^{60}$Fe ($d_{\text{max}} \approx 110 \times 10^6$).
**Extrapolation by energy variance**

**Proposed extrapolation**

*Energy differences $\Delta E$ of truncated wave functions are proportional to their energy variances $\delta E$*

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INT 2002, March
http://mocha.phys.washington.edu/~int_talk/WorkShops/ACD02/People/Mizusaki_T/
Proof

Definition of energy difference and energy variance

\[ \mathcal{\delta}E = \langle H \rangle - \langle H \rangle_0 \quad \Delta E = \langle H^2 \rangle - \langle H \rangle_0^2 \]

Decomposition of wave function

\[ |\psi\rangle = c|\psi_0\rangle + d|\psi_r\rangle \quad |\psi_r\rangle = \sum_{n \neq 0} c_n |\psi_n\rangle \quad c^2 + d^2 = 1 \quad \sum_{n \neq 0} c_n^2 = 1 \]

Definition of moments

\[ D_j = \sum_{n \neq 0} \frac{c_n^2 (E_n - E_0)^j}{E_0^j} \]

Exact relations between \( \delta E \) and \( \Delta E \)

\[ \mathcal{\delta}E = d^2 D_1 E_0 \quad \Delta E = d^2 D_2 E_0^2 - \left( d^2 \right)^2 \left( D_1 E_0 \right)^2 \]

Formal solution

\[ \mathcal{\delta}E = \frac{1}{2A} \left[ 1 - \sqrt{1 - 4A^2 \Delta E} \right] \quad A = \frac{D_1}{D_2 E_0} \]
Series expansion of $\delta E$

$$\delta E = A\Delta E + A^3\Delta E^2 + \ldots$$

Series expansion of $A$

$$A = A_0 + A_1\Delta E + \ldots$$

Second order extrapolation formula

$$\varphi_E = \varphi^0_E + (\varphi^0_3 + \varphi^1)\varphi_E + \ldots$$
Schematic view of extrapolation by energy variance

- Number of basis states depends on the way of representations, while energy and energy variance are independent.
- Therefore this method can work for deformed basis!
Advantage and disadvantage of deformed basis

- **Optimized angular momentum projected deformed basis** is a best basis function, which can give a nice description even with one basis.
- We can obtain such a basis for larger model spaces in comparison with spherical basis.
- However, **evaluation of <H^2> matrix element is not computationally easy.**
• Optimized a.m.proj. deformed wave func. gives good description.
• We can generate worse wave functions by changing its structure systematically, but they are still useful.
• Afterwards we extrapolate the true energy from them.
• Therefore, we always use single basis. (computational advantage)
Variation after projection for deformed basis

- Projected deformed basis
  \[ P_{MK}^J |\psi\rangle = \prod a_{\alpha}^\dagger |0\rangle \quad a_{\alpha}^\dagger = \sum_i D_{\alpha,i} c_i^\dagger \]
- Variation after projection is a good approximation.
  \[ \delta \left\{ \frac{\langle \psi | H P^J | \psi \rangle}{\langle \psi | P^J | \psi \rangle} \right\} = 0 \]
- This variation problem is numerically solved by gradient method.
- Here, time-reversal symmetry and no isospin projection are assumed.
  - Block form of density matrix
    \[ \rho_{\alpha\beta} = \frac{\langle \psi' | c_\beta^\dagger c_\alpha | \psi \rangle}{\langle \psi' | \psi \rangle} = \begin{pmatrix} \rho_{\alpha\beta}^{\pi} & 0 & 0 & 0 \\ 0 & \rho_{\alpha\beta}^{\pi} & 0 & 0 \\ 0 & 0 & \rho_{\alpha\beta}^{\gamma} & 0 \\ 0 & 0 & 0 & \rho_{\alpha\beta}^{\gamma} \end{pmatrix} \]
  - Computational amount of angular momentum projection is reduced.
- \( <H^2> \): four-body interaction, Wick’s theorem
Angular momentum projection
Integral domain is 1/8 reduced by time-reversal symmetry.

\[ P_{KK'}^J = \frac{2J+1}{8\pi^2} \int_0^\pi d\alpha \int_0^{\pi/2} d\beta \int_0^{2\pi} d\gamma R(\Omega) D_{K,K'}^J(\Omega) \]

\[ H_{KK'}^J = \langle \psi | HP_{KK'}^J | \psi \rangle \]

For \( J>0 \) state, we simultaneously obtain their extrapolation by projecting from the same wave function onto different angular momentum states. \( J=0 \) … VAP with time reversal symmetry \( J>0 \) … VBP. Otherwise, time-reversal symmetry is broken. Computation becomes harder.

How to generate a series of wave functions

- Structure of VAP wave function can be varied in a following way.

\[ |\psi(x)\rangle = \prod a_\alpha^\dagger (x) |0\rangle \quad a_\alpha^\dagger (x) = \sum_i D_{\alpha,i}^{(\text{min})} x_i c_i^\dagger \]

For instance,
- \( x_i=1 \) for lower orbits
- \( x_i=x \) for upper orbits \[ |\psi(x=1)\rangle = |\psi_{\text{min}}\rangle \]
Test of this approach for $^{48}\text{Cr}$ --- 2 Million problem ---

- $^{48}\text{Cr}$
- fp shell
- KB3 interaction
- $2 \times 10^6$ dimension for M=0 state
Test for 2 billion problem

- $^{60}$Zn
- fp shell
- fpd6 interaction
- $2 \times 10^9$ dimension for $M=0$ state
- Two extrapolations based on the spherical basis and deformed basis

Exact energy $\rightarrow$ How to evaluate $<H^2>$

For low spin yrast states of $N$, $Z$ even-even nuclei, its evaluation is relatively easy.

For other cases, its evaluation is computationally difficult but, in principle, possible.
fpg shell model

- Shell model space: f5/2,p3/2,p1/2,g9/2
- Maximum dimension is 13.1 billion. (N=Z=39)
- Competition between oblate and prolate deformed bands
- Oblate – Prolate shape coexistence
Extrapolation of 11 billion problem

- $^{80}\text{Zr}$
- 11,090,052,440 for $M=0$
- Isospin invariant Pairing + QQ interaction
  - The number of parameters is few. In this test, we set them tentatively.
- Complete diagonalization is impossible.
- Even truncated shell model is also very difficult.

Occupation numbers for proton and neutron respectively

- Prolate: $2.96$  $4.01$  $0.97$  $4.05$
- Oblate: $2.35$  $3.37$  $0.39$  $5.90$

by VAP wave function for $J=0$

Truncation is not so easy for spherical shell model.
• The present extrapolation can solve this problem, including oblate-prolate shape coexistence.
• One Xeon 2.6GHz within 1 days
• Different slope of extrapolation for oblate and prolate states
Relation to strongly correlated electron system on a lattice

- Hubbard model with geometrical frustration is a current topic.
  - Sign problem for QMC calculation
  - New method: Path Integral Renormalization group method
  - Sign problem free
  - It is like QMCD+ extrapolation
- I apply the extrapolation technique to nuclear shell model.
  - Complex two-body interaction in nuclear shell model
  - $<H^2>$ needs further development.

- I also apply the quantum number projection technique to Hubbard model.
  - I first introduce the optimization with spin and momentum projection into Hubbard model, which works quite well.
  - PIRG + quantum number projection is a nice combination
  - PRB 69, 125110 (2004)
  - Collaboration with condensed matter physicists (Imada group).
Summary

• Based on the variationally optimized angular momentum projected Slater determinant, I develop an extrapolation method.
  – For even-even nuclei, computation is rather simple.
  – This method can give exact energy of huge shell model problem, for instance, 11 billion problem.
  – This method is also shown to be useful to handle shape coexistence.

• Next study is to evaluate high spin states and non-yrast states efficiently.