A new approach for large-scale shell-model calculations and large-scale complex scaling calculations

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Sep. (2014)
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Reference
1 Introduction: basic issue

New diagonalization method on two kinds of nuclear structure calculations

For shell model calculations, we solve energy of low-lying states. Eigen-energies are real.

Hamiltonian matrix is real symmetric.

Lanczos iteration
initial vector \( |\phi_0\rangle \)

\[ |\phi_0\rangle, H|\phi_0\rangle, H^2|\phi_0\rangle, \cdots \]

Diagonalization by Krylov subspace
Lanczos method is useful for low-lying states for large-scale shell model calculations.

For complex-scaling calculations, we solve resonance states. Eigen-energies are complex.

Hamiltonian matrix is complex symmetric, but is not Hermitian.
no good method for large-scale calculations
obstacle for many-body resonance study

New diagonalization method!
SS method
1. Introduction: outcome of my talk

large-scale shell model calculations

SS method has **almost the same performance** as Lanczos method for large-scale shell-model calculations.

SS method is **superior** in the calculations with isospin symmetry breaking.

large-scale complex scaling calculations

There is no good diagonalization method.

SS method becomes a unique diagonalization method.

**We found, the SS method can easily solve especially resonance states!!**

Up to now, max 50,000 with super computer

Hereafter, 200,000 and more with single PC!!

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2. SS method: eigenvalues from moments

SS method = Sakurai - Sugiura method


We define the following moments as

\[ \mu_p = \frac{1}{2\pi i} \int_{\Gamma} \langle\psi| \frac{(z - \varepsilon)^p}{z - H} |\phi\rangle \, dz, \]

\[ H |\varphi_i\rangle = e_i |\varphi_i\rangle \]

\[ |\psi\rangle = \sum c_i |\varphi_i\rangle \]

\[ |\phi\rangle = \sum d_i |\varphi_i\rangle \]

Formally moments can be rewritten.

\[ \mu_p = \sum_{k \in \Gamma} (e_k - \varepsilon)^p c_k d_k. \]

By expanding the complete sets, we can rewrite the moment above.

We would like to extract \( e_k \)!
2. SS method: eigenvalues from the Hankel Matrix

For simplicity, let us consider the 2x2 case with \(a_k = e_k - \varepsilon\) and \(b_k = c_k d_k\).

\[
N = \begin{pmatrix} \mu_0, & \mu_1 \\ \mu_1, & \mu_2 \end{pmatrix} = \begin{pmatrix} b_1 + b_2, & a_1 b_1 + a_2 b_2 \\ a_1 b_1 + a_2 b_2, & a_1^2 b_1 + a_2^2 b_2 \end{pmatrix} = \begin{pmatrix} 1, & 1 \\ a_1, & a_2 \end{pmatrix} \begin{pmatrix} b_1, & 0 \\ 0, & b_2 \end{pmatrix} \begin{pmatrix} 1, & a_1 \\ a_1, & a_2 \end{pmatrix}
\]

\[
V D V^T
\]

\[
M = \begin{pmatrix} \mu_1, & \mu_2 \\ \mu_2, & \mu_3 \end{pmatrix} = \begin{pmatrix} a_1 b_1 + a_2 b_2, & a_1^2 b_1 + a_2^2 b_2 \\ a_1^2 b_1 + a_2^2 b_2, & a_1^3 b_1 + a_2^3 b_2 \end{pmatrix} = \begin{pmatrix} 1, & 1 \\ a_1, & a_2 \end{pmatrix} \begin{pmatrix} b_1, & 0 \\ 0, & b_2 \end{pmatrix} \begin{pmatrix} a_1, & 0 \\ 0, & a_2 \end{pmatrix} \begin{pmatrix} 1, & a_1 \\ a_1, & a_2 \end{pmatrix}
\]

\[
V D \Lambda V^T
\]

Therefore,

\[
M - \lambda N = V D (\Lambda - \lambda I) V^T
\]

Then, \(\lambda = a_k\) is an eigenvalue of \(M x = \lambda N x\).

This relation holds for any dimension then by diagonalizing \(M x = \lambda N x\) we can obtain energy eigenvalues.
2. SS method: Hankel matrix

To extract $e_k$, we solve the following small-scale generalized eigenvalue problem with the Hankel matrices.

$$\mu_p = \frac{1}{2\pi i} \int_\Gamma \langle \psi | \frac{(z - \varepsilon)^p}{z - H} | \phi \rangle dz,$$

$$M = \begin{pmatrix}
\mu_1, & \mu_2, & \cdots & \mu_n \\
\mu_2, & \mu_3, & \cdots & \mu_{n+1} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_n, & \mu_{n+1}, & \cdots & \mu_{2n-1}
\end{pmatrix} \quad N = \begin{pmatrix}
\mu_0, & \mu_1, & \cdots & \mu_{n-1} \\
\mu_1, & \mu_2, & \cdots & \mu_n \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{n-1}, & \mu_n, & \cdots & \mu_{2n-2}
\end{pmatrix}$$

$$M x = \lambda N x \quad \lambda = e_k - \varepsilon$$

**basic strategy**

- small-scale generalized eigenvalue problem
- moments
- target eigenvalues
2. SS method: how to evaluate the moments and COCG method

In respective problems, we have to evaluate the moments by the numerical integrations as

\[ \mu_p \sim \frac{1}{N_0} \sum_{k=0}^{N_0-1} \left| \frac{\langle \psi | (z_k - \epsilon)^{p+1} | \phi \rangle}{z_k - H} \right| \]

The numerical integration along Cauchy’s contour is carried out by discretization. \( N_0 \): number of mesh points

\[ z_k = \epsilon + r e^{i \frac{2\pi}{N_0}(k+\frac{1}{2})} \]

Denominator needs to solve linear equations.

\[ | \phi \rangle = (z - H | \chi \rangle \]

\[ \langle \psi | \frac{1}{z - H} | \phi \rangle = \langle \psi | \chi \rangle \]

This linear equations can be solved by the COCG (Complex Orthogonal Conjugate Gradient) method, which is an iteration method with Krylov subspace as will be explained in the next slide.
2. SS method: Krylov subspace and shifted COCG method

How to solve linear equation \( Ax = b \)

where \( A \) is complex and symmetric.

For \( x_k, r_k, p_k \) vectors,

Initial conditions: \( \alpha_0 = 1, \beta_0 = 0, x_0 = 0 \) and \( r_0 = b \)

Iteration:

\[
\begin{align*}
x_{k+1} &= x_k + \alpha_k p_k \\
r_{k+1} &= r_k - \alpha_k A p_k \\
p_{k+1} &= r_{k+1} + \beta_k p_k,
\end{align*}
\]

where

\[
\begin{align*}
\alpha_k &= r_k^T r_k / p_k^T A p_k \\
\beta_k &= r_{k+1}^T r_{k+1} / r_k^T r_k
\end{align*}
\]

Iteration generates the Krylov subspace \( \text{span}\{b, Ab, A^2 b, \cdots\} \)

Shifted linear equations: \( (A - \sigma I) x^\sigma = b \),

without matrix-vector calculations,

\[
\begin{align*}
r_k^\sigma &= \frac{1}{\pi_k^\sigma} r_k; \\
\pi_{k+1}^\sigma &= (1 + \alpha_k \sigma) \pi_k^\sigma + \frac{\alpha_k \beta_k}{\alpha_{k-1}} (\pi_k^\sigma - \pi_{k-1}^\sigma), \\
\alpha_k^\sigma &= \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \alpha_k, \\
\beta_k^\sigma &= \left(\frac{\pi_k^\sigma}{\pi_{k+1}^\sigma}\right)^2 \beta_k.
\end{align*}
\]

It is easy to solve it!

\( \text{span}\{b, (A - \sigma I) b, (A - \sigma I)^2 b, \cdots\} \) is the same as \( \text{span}\{b, Ab, A^2 b, \cdots\} \)


2. SS method: summary

1) We choose Cauchy’s contour and initial wave functions.

\[ \mu_p = \frac{1}{2\pi i} \int_{\Gamma} \langle \psi \rangle \frac{(z - \epsilon)^p}{z - H} |\phi\rangle \, dz, \]

2) We compute moment by numerical integration with shifted COCG method.

\[ \mu_p \sim \frac{1}{N_0} \sum_{k=0}^{N_0-1} \langle \psi \rangle \frac{(z_k - \epsilon)^{p+1}}{z_k - H} |\phi\rangle \]

3) We make Hankel matrices.

\[ M = \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_n \\ \mu_2 & \mu_3 & \cdots & \mu_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} \end{pmatrix} \quad N = \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{pmatrix} \]

4) We solve the small-size generalized eigen-value problem.

\[ Mx = \lambda Nx \]

\[ \lambda = e_k - \epsilon \]
3. Example of the SS method: benchmark test in pf-shell model calculations

As a benchmark test, we take $^{48}\text{Cr}$ with pf shell. Yrast states can be easily solved (M-scheme, 2M dim).

![Diagram showing benchmark test](image)

We solve off-yrast states with different size of circles.

We solve off-yrast states with $J=0$.

\[ \mu_p = \frac{1}{2\pi i} \int_{\Gamma} \langle \psi | \frac{z - \epsilon)^p}{z - H} | \phi \rangle dz, \]

**total angular momentum**

Although we use M-scheme for large-scale shell model calculations, total angular momentum can be easily handled if we use the wave functions with good total angular momentum.
As a benchmark test, we take \( ^{56}\text{Ni} \) with pf shell. Three \( 0^+ \) can be easily solved (M-scheme, 1 billion dim) by PC.

Convergence pattern of Lanczos method for three \( 0^+ \) states

![Lanczos step](image)

0\(_1\)

0\(_2\)

0\(_3\)

Energy [MeV]

0 50 100

Lanczos step

At every step of COCG calculations, we evaluate wave function and then we evaluate the energy.

Large-scale Shell Model codes in the world

- Strasbourg codes: \( 10^{10} \) dim for PC cluster
- MSU codes: \( 10^{10} \) dim for PC cluster
- Oslo code: \( 10^{10} \) dim for super computer
- IOWA code: \( 10^{10} \) dim for super computer
- MSHELL: several \( 10^9 \) dim only for PC
- KSHELL: beyond \( 10^{10} \) dim for super computer

Convergence patterns of Lanczos and SS method for two \( 0^+ \) states

![Convergence patterns](image)

(a) \( 0_1 \)

(b) \( 0_2 \)

Filled circles: Lanczos method

Open circles: SS method
3. Example of the SS method: large-scale pf-shell calculations

Technique for off-yrast states in SS method

In Lanczos method, off-yrast states needs too much computations because there is no good way to use wave function obtained in smaller truncated subspace.

In SS method, wave function obtained in smaller truncated subspace can be used through the moment expression.

\[
\mu_p = \frac{1}{2\pi i} \int \langle \psi | \frac{(z - \epsilon)^p}{z - H} | \phi \rangle dz.
\]
3. Convergence property of Lanczos and SS methods

**Lanczos method**

- initial vector  \( |\phi_0\rangle \)
- Lanczos iteration
  \[ |\phi_0\rangle, H|\phi_0\rangle, H^2|\phi_0\rangle, \cdots \]
- Diagonalization by Krylov subspace
- Lower energies are converged faster.
- Higher energies are converged slower.
- This is quite natural and ordinary.

**SS method**

- initial vector  \( |\phi_0\rangle \)
- Iteration in COCG
  \[ |\chi_0\rangle, (z - H)|\chi_0\rangle, (z - H)^2|\chi_0\rangle, \cdots \]
- Iteration number depends on \( z \).

![Graph showing convergence property](image)

- low level density area: fast convergence
- high level density area: slow convergence

This nature is quite important in complex-scaling calculations.
5. Complex scaling calculations with the SS method: Cluster orbital shell model

Cluster Orbital shell model + Complex scaling method \rightarrow resonance spectroscopy

**Cluster orbital shell model (COSM)**

Cluster orbital

\[ r^l e^{-\left(\frac{r}{r_n}\right)^2} Y_{lm}(\hat{r}) \]

\( r_n \): a geometrical progression

**Cluster orbital basis with angular momentum J**

\[ |\phi_k(J)\rangle \quad \text{non-orthogonal basis} \]

**Hamiltonian and Norm kernel**

\[ H_{k',k}^{\theta,J} = \langle \phi_{k'}(J) | H^\theta | \phi_k(J) \rangle \]

\[ N_{k',k}^{J} = \langle \phi_{k'}(J) | \phi_k(J) \rangle \]

W. f. can be determined by solving

\[ H_{k',k}^{\theta,J} x_k^\theta = \varepsilon_k^\theta N_{k',k}^{J} x_k^\theta \]

**Cluster orbital w. f. with angular momentum J**

\[ |\Psi_{\theta}^{J}\rangle = \sum x_k^\theta |\phi_k(J)\rangle \]

scaling angle

Taken from Phys. Rev. C85 034338 (2012).
5. Complex scaling calculations with the SS method: What is complex scaling

Complex scaling + Cluster orbital shell model + SS method

We consider orthogonalized basis function. \(|\tilde{\phi}_k(J)\rangle\)

We solve the following eigenvalue problem as

$$\tilde{H}_{k',k}^{\theta,J}\tilde{x}_k^{\theta} = \varepsilon_k^{\theta}\tilde{x}_k^{\theta}$$

Hamiltonian matrix in terms of orthogonal basis complex and symmetric (non-hermitian)

Complex scaling method

Hamiltonian

$$H = \sum_{i=1}^{N_v+1} t_i - T_G + \sum_{i=1}^{N_v} V_{i,i}^{pp} + \sum_{i<j}^{N_v} V_{ij}^{pp}$$

$$= \sum_{i=1}^{N_v} \left[ \frac{p_i^2}{2\mu} + V_i^{op} \right] + \sum_{i<j}^{N_v} \left[ \frac{p_i \cdot p_j}{4m} + V_{ij}^{pp} \right]$$

Complex Scaling \(r_i \rightarrow r_i e^{i\theta}\)

Complex Scaled Hamiltonian \(H \rightarrow H^{\theta}\)

Taken from Phys. Rev. C85 034338 (2012).

where \(t_i\) and \(T_G\) are the kinetic energies of each particle (\(p\) and \(^4\text{He}\)) and of the center of mass of the total system, respectively. The operator \(\vec{p}_i\) is the relative momentum between \(p\) and \(^4\text{He}\). The reduced mass \(\mu = 4m/5\) using a nucleon mass \(m\). The \(^4\text{He}-p\) interaction \(V^{\alpha p}\) is given by the microscopic KKNN potential [27, 34] for the nuclear part, in which the tensor correlation of \(^4\text{He}\) is renormalized on the basis of the resonating group method in the \(^4\text{He}+N\) scattering. For the Coulomb part, we use the folded Coulomb potential using the density of \(^4\text{He}\) having the \((0s)^4\) configuration. We use the Minnesota potential [35] as the nuclear part of \(V^{pp}\) in addition to the Coulomb interaction. These interactions reproduce the low-energy scattering of the \(^4\text{He}-N\) and the \(N-N\) systems, respectively.
5. Complex scaling calculations with the SS method: Continuum and resonance states

**Eigenvalue distribution as a function of scaling angle by taking \(^7\text{He}\) for example**

![Diagram showing eigenvalue distribution with scaling angle](image)

**Continuum states**

Various continuum states are aligned along straight lines with \(2\theta\).

**Resonance states**

Resonance states do not move against the scaling angle.

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Taken from Phys. Rev. C76 054309 (2007)
5. Complex scaling calculations with the SS method: Eigenvalue distribution on complex plane

Eigenvalue distribution of $^8$C by direct diagonalization

by Zgeev in the LAPACK

dimension : 22582

scaling angle : $20^\circ$

In the SS method, we solve the following linear equation by the COCG method.

$$|\phi\rangle = (z - \hat{H})|\chi\rangle$$

general and gross structure of eigenvalue distribution for complex scaling calculation

**eigenvalue distribution = continuum energy region + its boundary**

SS method: high density : difficult to solve  low density : easy to solve

because the number of needed iteration (dim. of Krylov subspace) depends on the eigenvalue distribution according to the shell model study.
5. Complex scaling calculations with the SS method: isolation and search of resonance pole

Resonance pole can be isolated by taking relevant scaling angle.

Level density around resonance pole becomes very low. Therefore, it is quite easy to solve resonance state by SS method.

We can search resonance pole with less numerical effort by shift algorithm.

By moving Cauchy’s contour, we can search resonance pole. With shifted COCG, many contour integrals can be carried out by a COCG calculation at single position $z$. 
5. Complex scaling calculations with the SS method: verification of resonance pole

SS method can easily solve eigenvalue and eigenstate of low level density.

SS method can not guarantee whether obtained state is resonance or not, even although its possibility is large.

Direct diagonalization gives no information!

Resonance or not $\rightarrow$ Move it as a function of scaling angle

$$\mu_p = \frac{1}{2\pi i} \int_{\Gamma} \langle \psi | \frac{(z - \epsilon)^p}{z - H} | \phi \rangle dz,$$

A variation of wave function is expected not to be so large if we change the scaling angle slightly.

Setting a wave function in the moment by that calculated at a certain nearby scaling angle, convergence is expected to become fast.

In a direct diagonalization method, all the energies should be calculated from scratch at each scaling angle.
5. Complex scaling calculations with the SS method: numerical test

Numerical test in the case of $^8$C

1) First we solve this problem at the scaling angle $21^\circ$ and obtain several candidates for the resonance state.
2) Next we solve the eigenvalue problem at $18^\circ$, starting from these candidate wave functions at $21^\circ$.
3) We repeat this procedure up to $3^\circ$.

As the scaling angle decreases, energies labelled by B, C, D and E continuously move as an arc, which shows that these states are continuum ones. On the other hand, energies labelled by A do not substantially move, which shows that they stand for resonance states.

We can easily obtain candidates of resonance energy and can verify whether these candidates are resonance or not.

In this example, dimension is 203545 with single PC. This huge complex-scaled COSM calculation has never been carried out before!

By this approach, we could remove obstacle of the current limitation in complex scaling calculation.

$\longrightarrow$ study of many-body resonances
6. Summary, Perspective and Collaborators

Summary

1) We have successfully applied the SS method to nuclear shell model calculations.
2) We also have successfully applied the SS method to obtain many-body resonance calculations with complex scaling calculations.

Perspective

1) The SS method plays a unique role especially for large-scale complex-scaling calculation.
2) Many-body resonance calculations become possible by complex-scaled COSM with the SS method.

Collaborators

SS method for shell model calculations: K. Kaneko, M. Honma, T. Sakurai
SS method for complex scaling calculations: T. Myo, K. Kato