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

Nordita, Stockholm
Sep. (2014)
Takahiro Mizusaki
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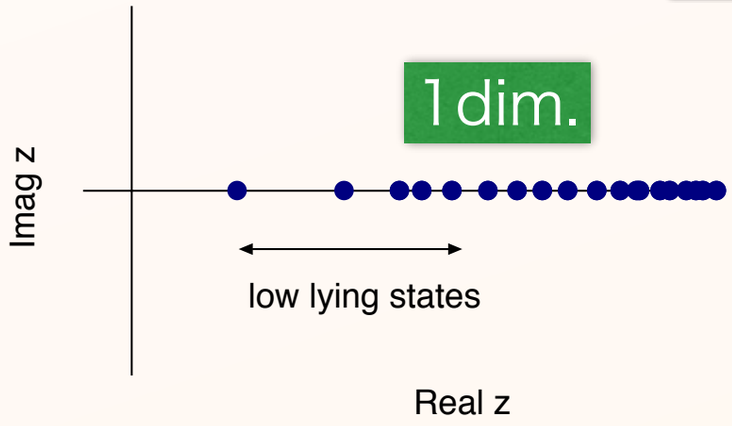
Reference
[1]T. Mizusaki, K. Kaneko, M. Honma, T. Sakurai, Phys. Rev. C82 024310 (2010).
[2] T. Mizusaki, Bulletin of the Institute of Natural Sciences, Senshu Univ. No.43, p23-40 (2012) in Japanese.
[3] T.Mizusaki, T.Myo, K.Kato, Prog. Theor. Exp. Phys. (2014) 091D01.

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.

bound state



Hamiltonian matrix is real symmetric.

Lanczos iteration

initial vector $|\phi_0\rangle$

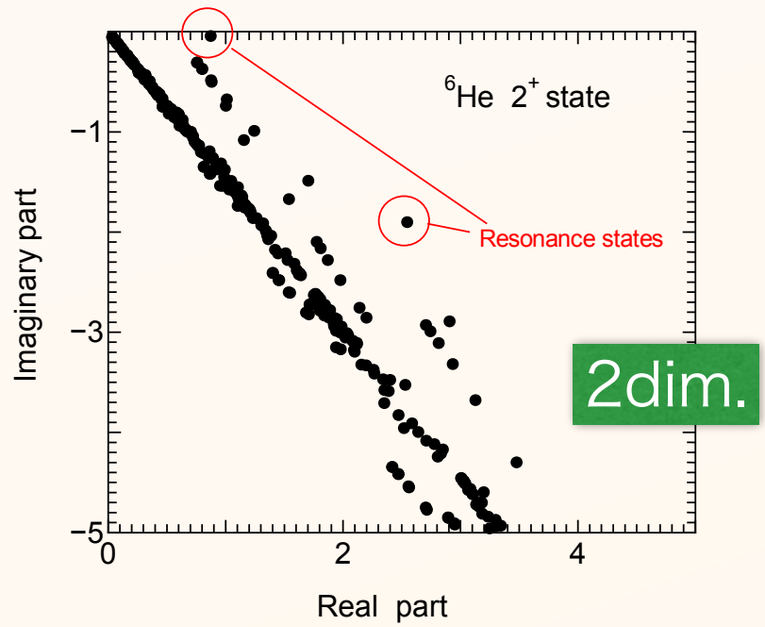
$$|\phi_0\rangle, H|\phi_0\rangle, H^2|\phi_0\rangle, \cdots$$

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.

weakly bound and unbound state



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.

Computational Challenges

large-scale complex scaling calculations

There is no good diagonalization method.

↓

SS method becomes a unique diagonalization method.

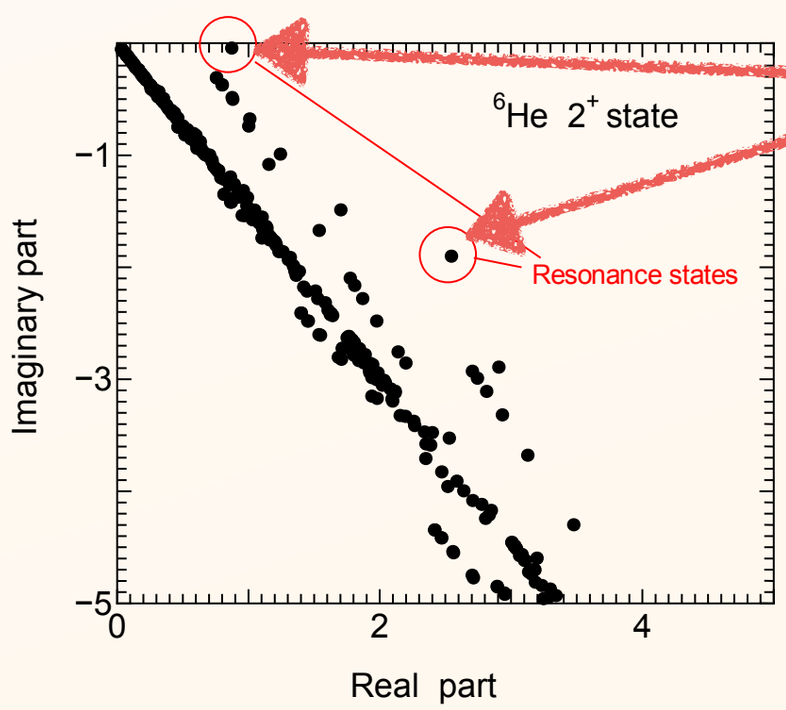
We found, the SS method can easily solve especially resonance states!!

Up to now, max 50,000 with super computer

↓

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

Breakthorugh !!



2. SS method: eigenvalues from moments

SS method = **S**akurai - **S**ugiura method

T. Sakurai and H. Sugiura, J. Comput. Appl. Math. 159, 119 (2003).

We define the following **moments** as

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

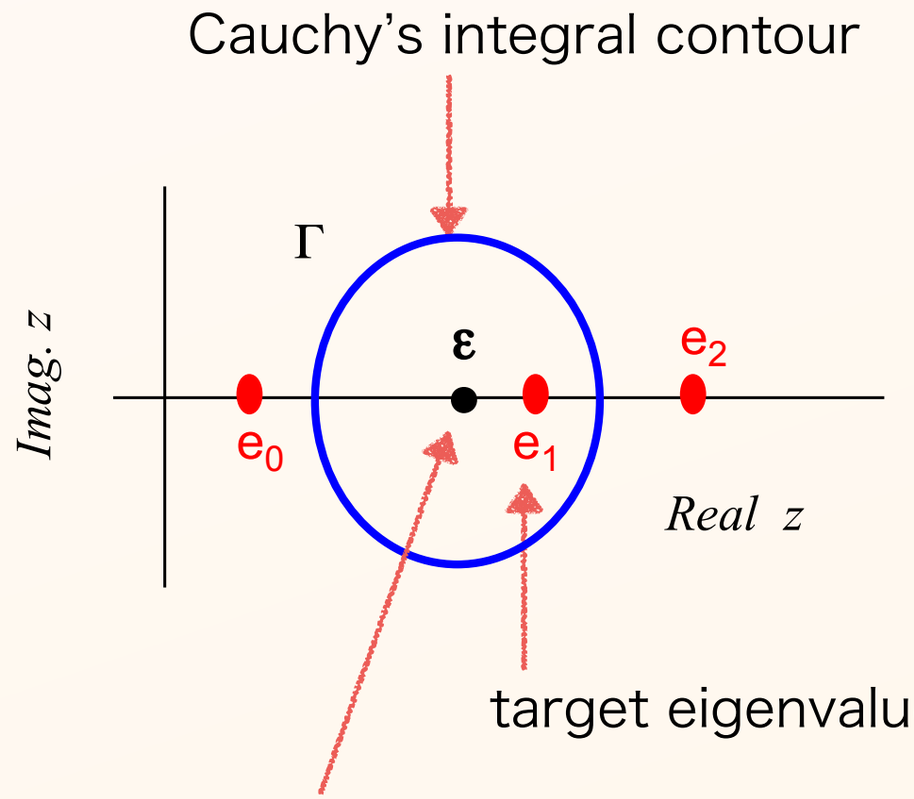
$$H|\varphi_i\rangle = e_i|\varphi_i\rangle$$
$$|\psi\rangle = \sum c_i|\varphi_i\rangle$$
$$|\phi\rangle = \sum d_i|\varphi_i\rangle$$

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 $b_k = c_k d_k$

$$N = \begin{pmatrix} \mu_0, & \mu_1 \\ \mu_1, & \mu_2 \end{pmatrix}$$

$$= \begin{pmatrix} b_1 + b_2, & a_1 b_1 + a_2 b_2 \\ a_1 b_1 + a_2 b_2, & a_1^2 b_1 + a_2^2 b_2 \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} 1, & 1 \\ a_1, & a_2 \end{pmatrix}}_{V} \underbrace{\begin{pmatrix} b_1, & 0 \\ 0, & b_2 \end{pmatrix}}_{D} \underbrace{\begin{pmatrix} 1, & a_1 \\ 1, & a_2 \end{pmatrix}}_{V^T}$$

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

$$a_k = e_k - \varepsilon$$
$$b_k = c_k d_k$$

$$M = \begin{pmatrix} \mu_1, & \mu_2 \\ \mu_2, & \mu_3 \end{pmatrix}$$

$$= \begin{pmatrix} a_1 b_1 + a_2 b_2, & a_1^2 b_1 + a_2^2 b_2 \\ a_1^2 b_1 + a_2^2 b_2, & a_1^3 b_1 + a_2^3 b_2 \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} 1, & 1 \\ a_1, & a_2 \end{pmatrix}}_{V} \underbrace{\begin{pmatrix} b_1, & 0 \\ 0, & b_2 \end{pmatrix}}_{D} \underbrace{\begin{pmatrix} a_1, & 0 \\ 0, & a_2 \end{pmatrix}}_{\Lambda} \underbrace{\begin{pmatrix} 1, & a_1 \\ 1, & a_2 \end{pmatrix}}_{V^T}$$

factorization of Hankel matrix

Therefore,

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

Then, $\lambda = a_k$ is an eigenvalue of $Mx = \lambda N x$

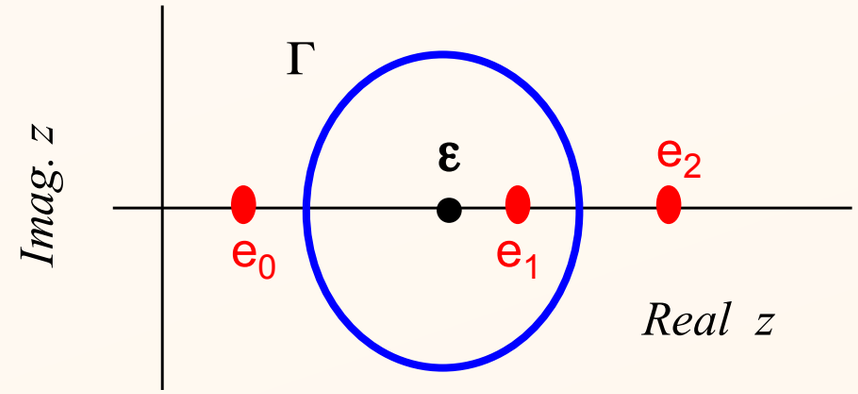
This relation holds for any dimension then by diagonalizing $Mx = \lambda N x$
we can obtain energy eigenvalues.

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

moments

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

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



$$Mx = \lambda Nx \quad \rightarrow \quad \lambda = e_k - \varepsilon$$

basic strategy

small-scale generalized eigenvalue problem

moments → target eigenvalues

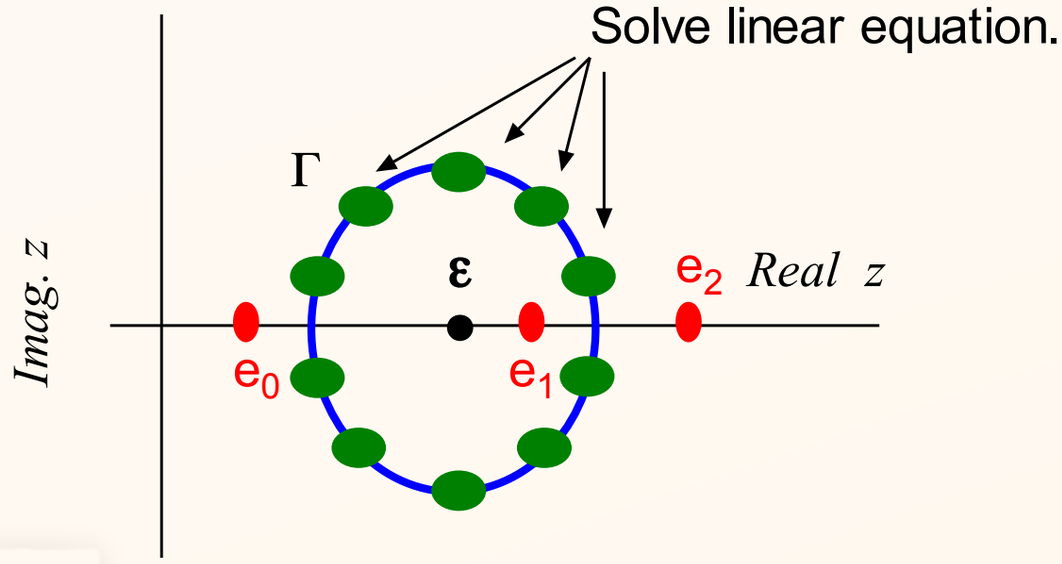
In respective problems, we have to evaluate the moments by the numerical integrations as

The numerical integration along Cauchy's contour is carried out by discretization.

N_0: number of mesh points

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

$$z_k = \varepsilon + re^{i\frac{2\pi}{N_0}(k+\frac{1}{2})}.$$



Denominator needs to solve linear equations.

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

$$\rightarrow \quad \langle\psi|\frac{1}{z-H}|\phi\rangle = \langle\psi|\chi\rangle.$$

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.

How to solve linear equation $Ax = b$ where A is complex and symmetric.

→ Complex Orthogonal Conjugate Gradient (COCG) method

For x_k, r_k, p_k vectors,

COCG method

H. A. van der Vorst and J. B. M. Melissen, IEEE Trans. Magn.26, 706 (1990).

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

Iteration :

$$x_{k+1} = x_k + \alpha_k p_k$$
$$r_{k+1} = r_k - \alpha_k A p_k$$
$$p_{k+1} = r_{k+1} + \beta_k p_k,$$

where

$$\alpha_k = r_k^T r_k / p_k^T A p_k$$
$$\beta_k = r_{k+1}^T r_{k+1} / r_k^T r_k$$

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

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

without matrix-vector calculations,

shift algorithms

R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, and T. Fujiwara, Phys. Rev. B 73, 165108 (2006).

$$r_k^\sigma = \frac{1}{\pi_k^\sigma} r_k;$$

$$\pi_{k+1}^\sigma = (1 + \alpha_k \sigma)\pi_k^\sigma + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}(\pi_k^\sigma - \pi_{k-1}^\sigma),$$
$$\alpha_k^\sigma = \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma}\alpha_k,$$
$$\beta_k^\sigma = \left(\frac{\pi_k^\sigma}{\pi_{k+1}^\sigma}\right)^2 \beta_k.$$

It is easy to solve it !

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

2. SS method: summary

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

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

↓

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

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

↓

3) We make Hankel matrices.

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

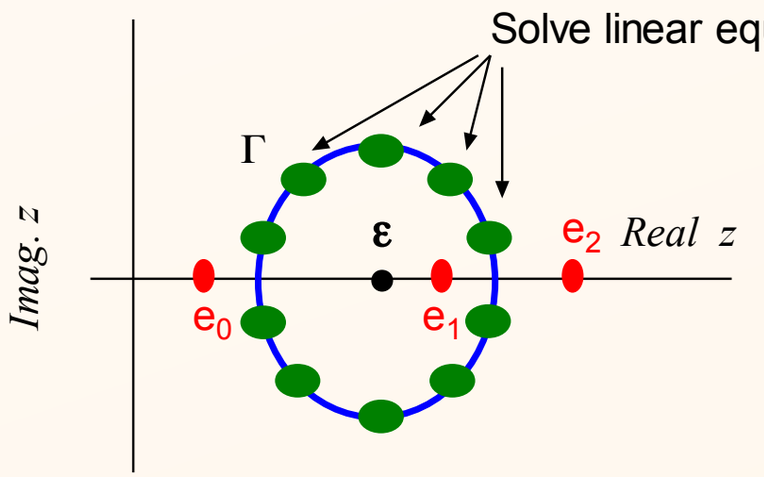
↓

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

$$Mx = \lambda N x$$

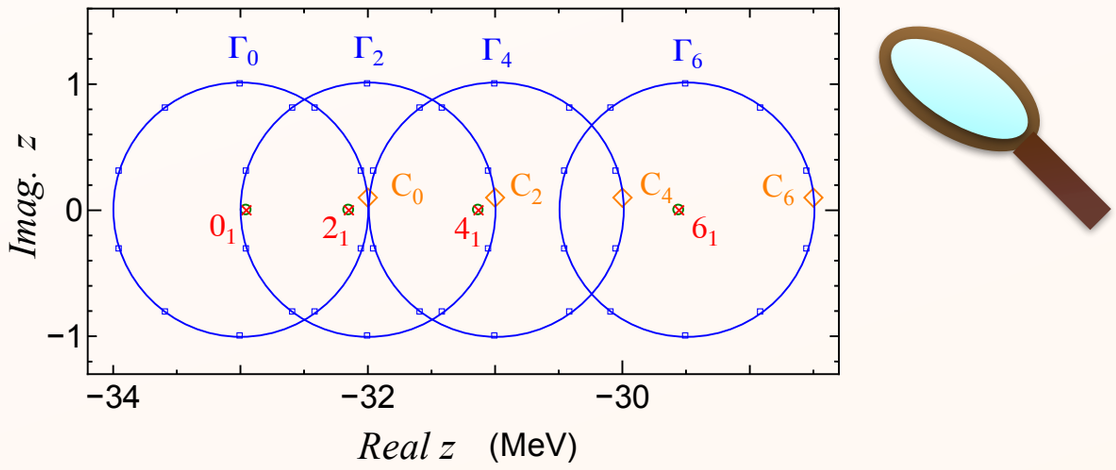
↓

$$\lambda = e_k - \varepsilon$$



3. Example of the SS method : benchmark test in pf-shell model calculations

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



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

total angular momentum

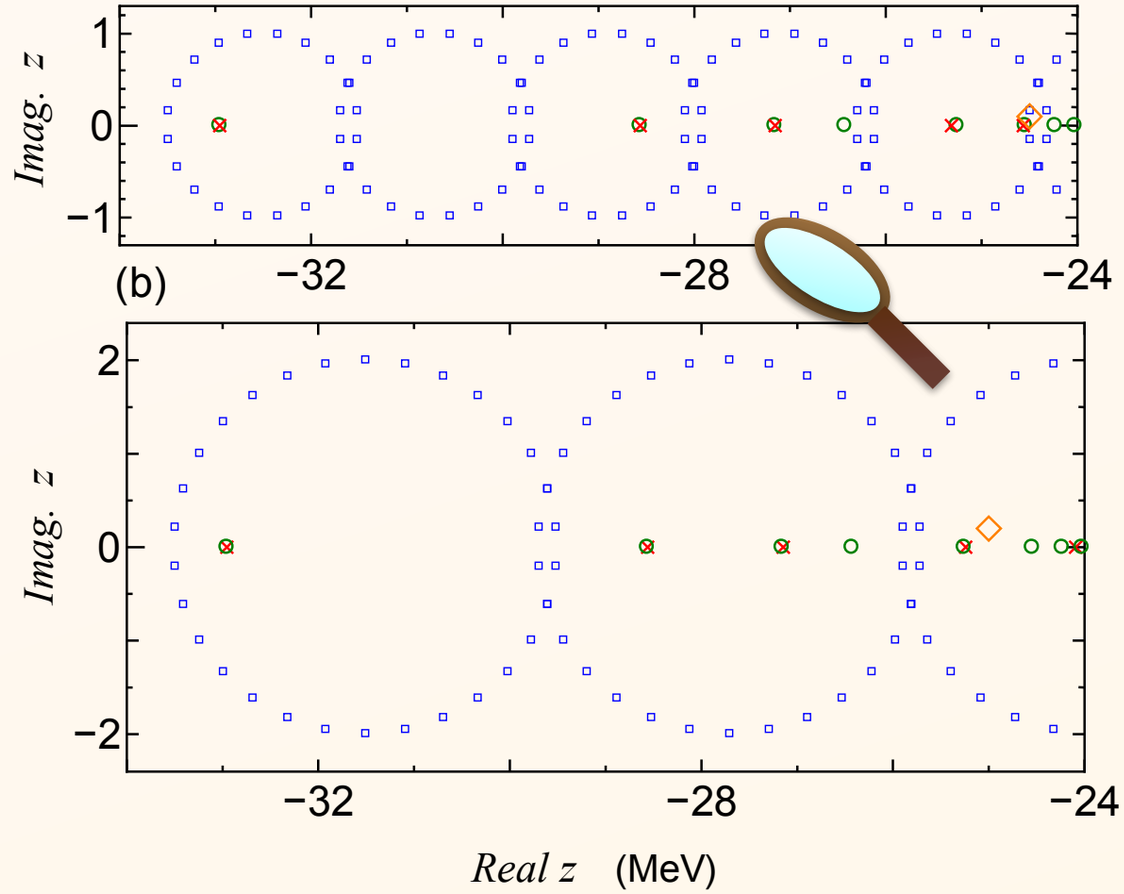
Although we use M-scheme for large-scale shell model calculations, total angular momentum can be easily handled if we use the wave functions with good total angular momentum.

Benchmark test

Test for off-yrast states with J=0

We solve off-yrast states
with different size of circles

(a)



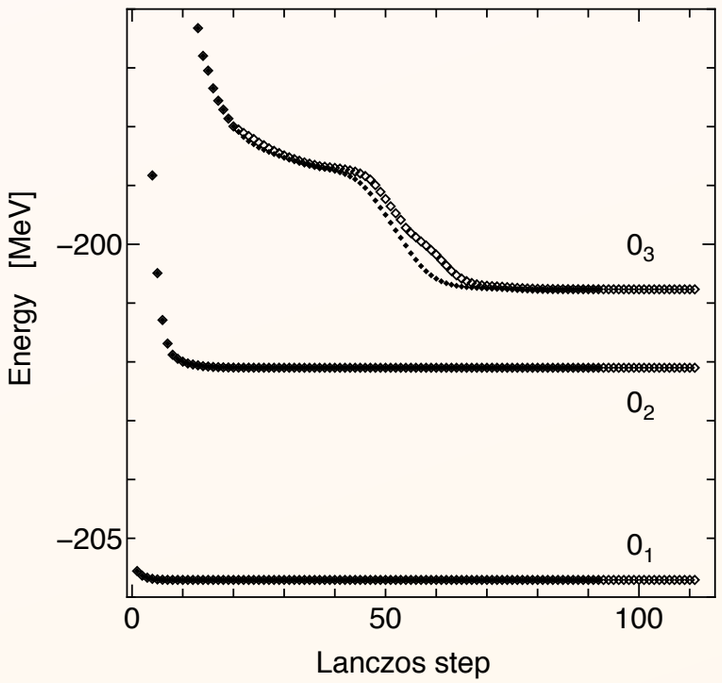
3. Example of the SS method : large-scale pf-shell calculations

As a benchmark test, we take ^{56}Ni with pf shell. Three 0+ can be easily solved (M-scheme, 1 billion dim) by PC.

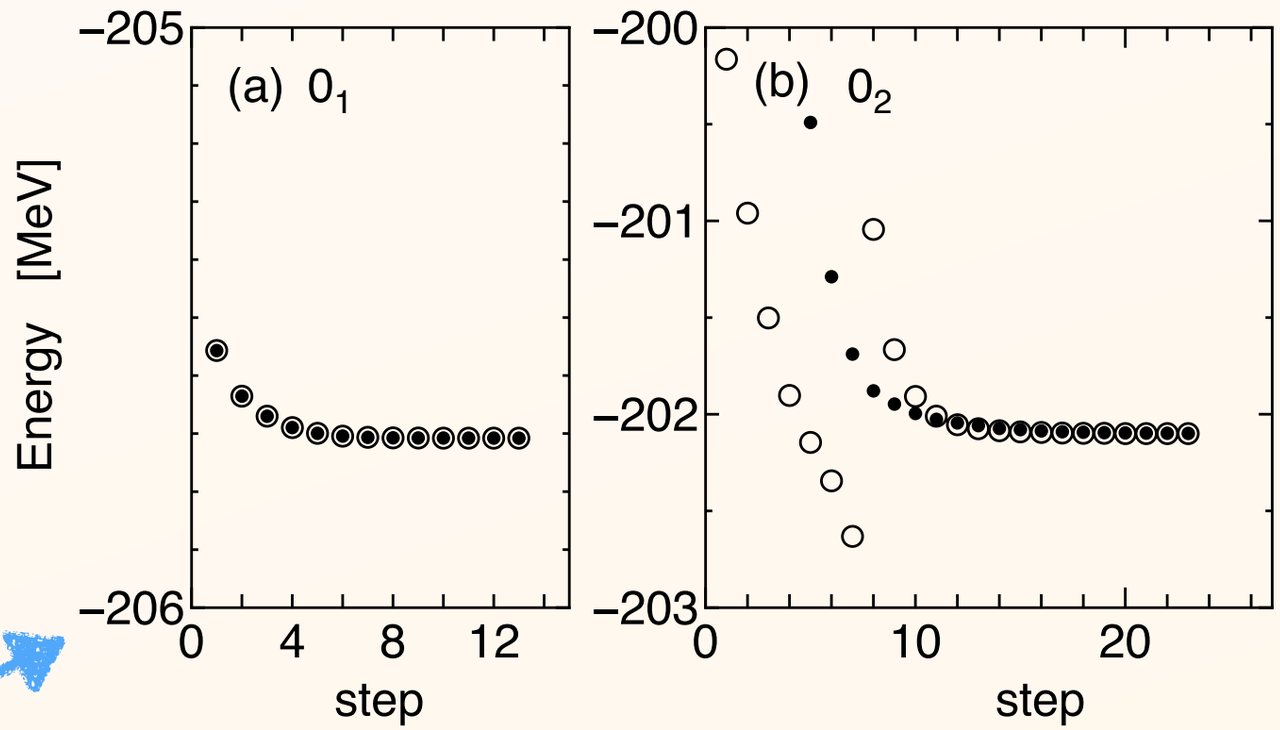
Large-scale Shell Model codes in the world

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 K

Convergence pattern of Lanczos method for three 0^+ states



convergence patterns of Lanczos and SS method for two 0^+ states



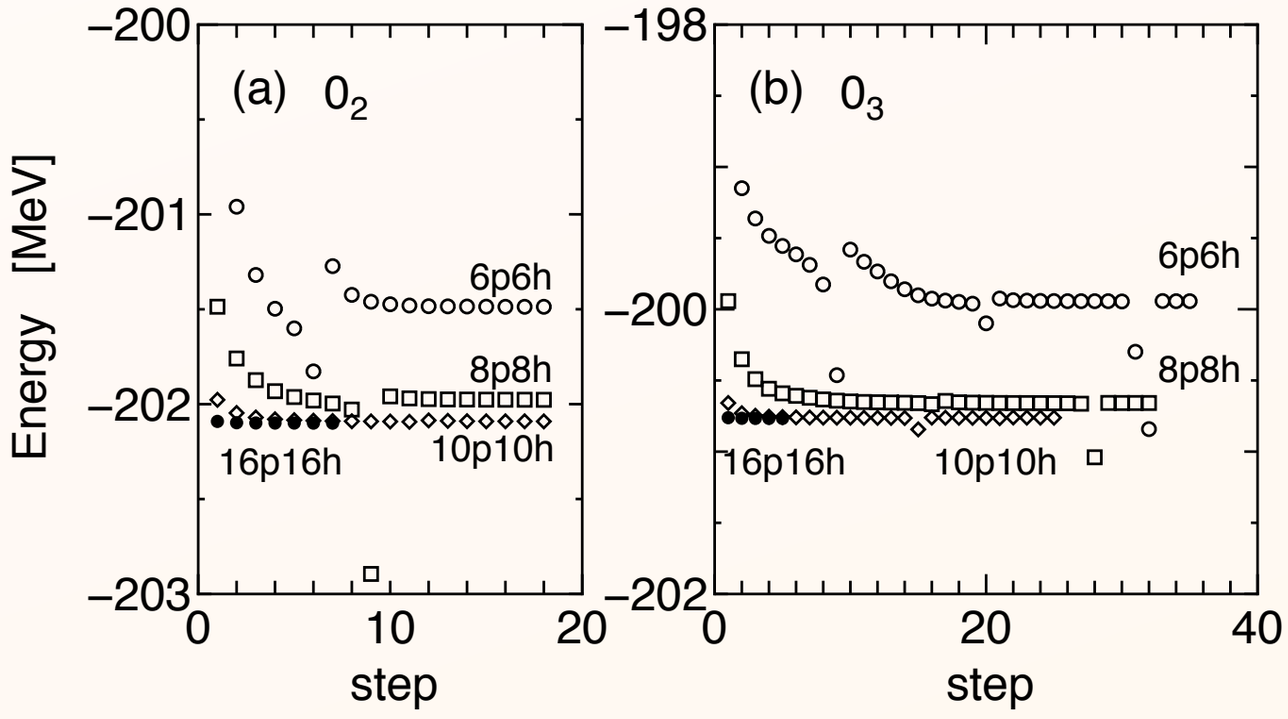
Filled circles : Lanczos method

open circles : SS method

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

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.

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

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.

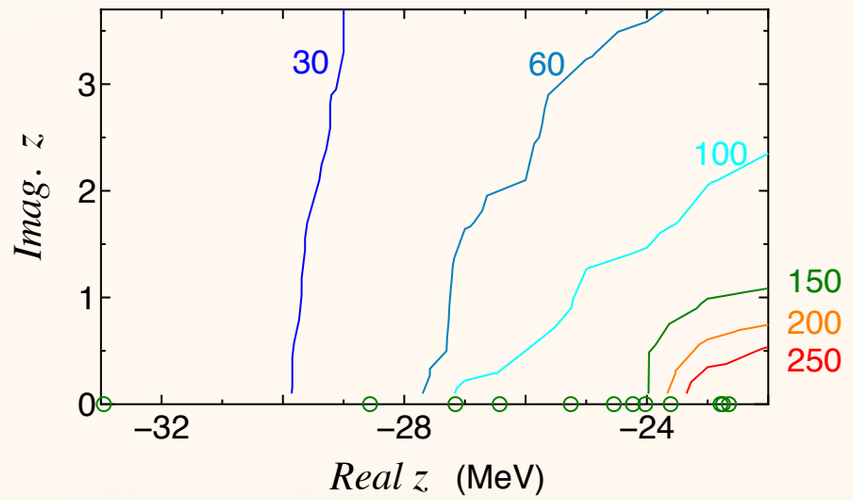
SS method

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.



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** → **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

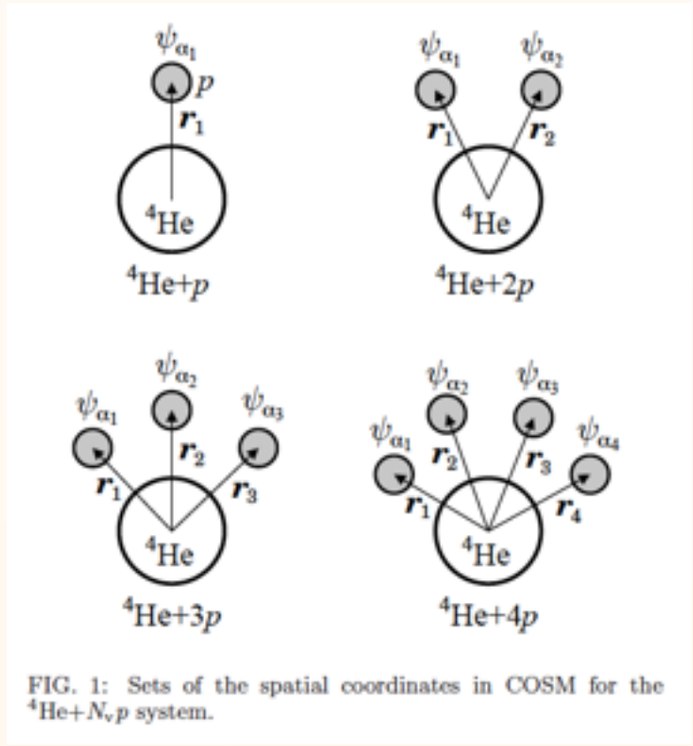


FIG. 1: Sets of the spatial coordinates in COSM for the ^{4}He+$N_v p$ system.

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

Cluster orbital basis with angular momentum J

$|\phi_k(J)\rangle$ non-orthogonal basis

Hamiltonian and Norm kernel

$$H^{\theta,J}_{k',k} = \langle\phi_{k'}(J)|H^\theta|\phi_k(J)\rangle$$

$$N^J_{k',k} = \langle\phi_{k'}(J)|\phi_k(J)\rangle$$

W. f. can be determined by solving

$$H^{\theta,J}_{k',k} x^\theta_k = \varepsilon^\theta_k N^J_{k',k} x^\theta_k$$

Cluster orbital w. f. with angular momentum J

$$|\Psi^J_\theta\rangle = \sum_k x^\theta_k |\phi_k(J)\rangle$$

scaling angle

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

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

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

Complex scaling method

Hamiltonian

$$\begin{aligned} H &= \sum_{i=1}^{N_v+1} t_i - T_G + \sum_{i=1}^{N_v} V_i^{\alpha p} + \sum_{i<j}^{N_v} V_{ij}^{pp} \\ &= \sum_{i=1}^{N_v}\left[\frac{\vec{p}_i^{\,2}}{2\mu} + V_i^{\alpha p}\right] + \sum_{i<j}^{N_v}\left[\frac{\vec{p}_i\cdot\vec{p}_j}{4m} + V_{ij}^{pp}\right] \end{aligned}$$

Complex Scaling $r_i \to r_i e^{i\theta}$

Complex Scaled Hamiltonian

$$H \to H^{\theta}$$

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

where t_i and T_G are the kinetic energies of each particle (p and ^{4}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}He. The reduced mass μ is $4m/5$ using a nucleon mass m. The ^{4}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}He is renormalized on the basis of the resonating group method in the ^{4}He+N scattering. For the Coulomb part, we use the folded Coulomb potential using the density of ^{4}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}He-N and the N-N systems, respectively.

Eigenvalue distribution as a function of scaling angle by taking ^{7}He for example

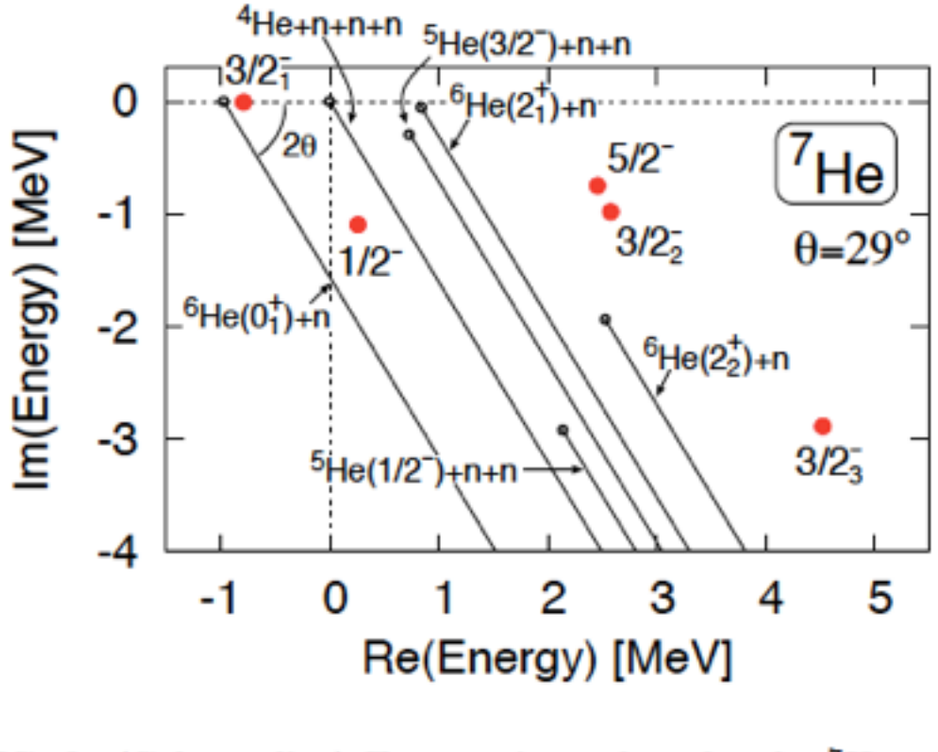


FIG. 3: (Color online) Energy eigenvalues for the ^{7}He resonances (solid circles) in the complex energy plane. The continuum states rotated down by 2θ are schematically displayed with the cut lines.

Taken from Phys. Rev. C76 054309 (2007)

continuum states

Various continuum states are aligned along straight lines with 2θ.

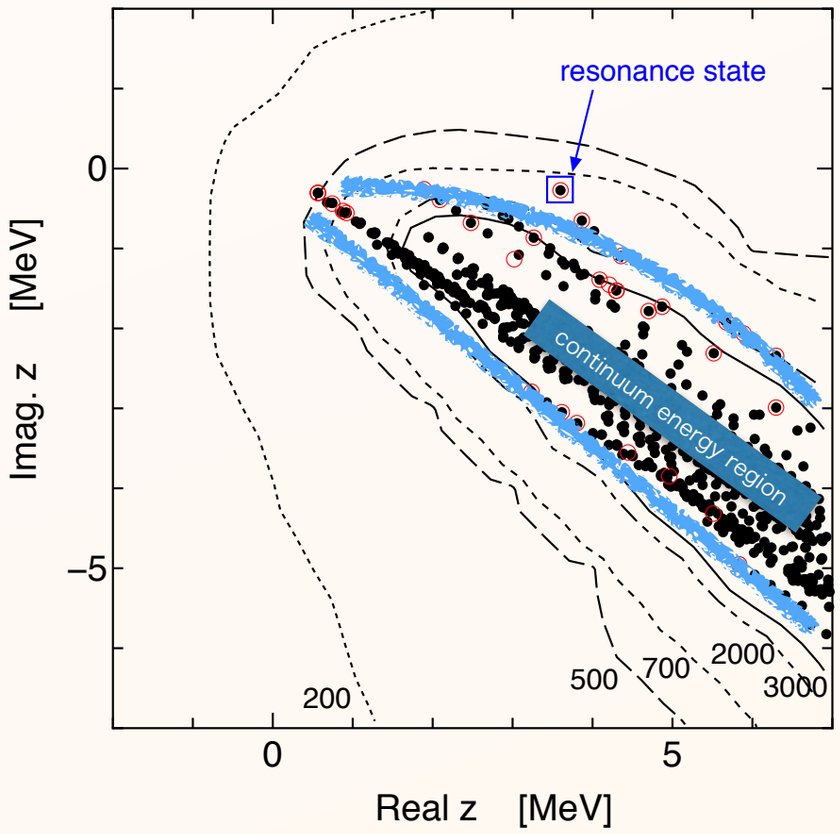
Resonance states

Resonance states do not move against the scaling angle.

CSM, we obtain all the energy eigenvalues E of bound and unbound states on a complex energy plane, governed by the ABC-theorem[23]. In this theorem, it is proved that the boundary condition of the Gamow resonances is transformed to the damping behavior at the asymptotic region. This condition enables us to use the same theoretical method to obtain the many-body resonances as that for the bound states. For a finite value of θ, the Riemann branch cuts are rotated down by 2θ, and continuum states such as of the ^{6}He+n ^{5}He+$2n$ and ^{4}He+$3n$ channels are obtained on these cuts with the 2θ dependence (See Fig. 3). On the contrary, bound states and resonances are discrete and obtained independently of θ. Hence they are located separately from the many-body continuum spectra on the complex energy plane.

Taken from Phys. Rev. C76 054309 (2007)

Eigenvalue distribution of ^{8}C by direct diagonalization



by Zgeev in the LAPACK

dimension : 22582

scaling angle : 20°

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

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

general and gross structure of eigenvalue distribution for complex scaling calculation

eigenvalue distribution = continuum energy region + its boundary

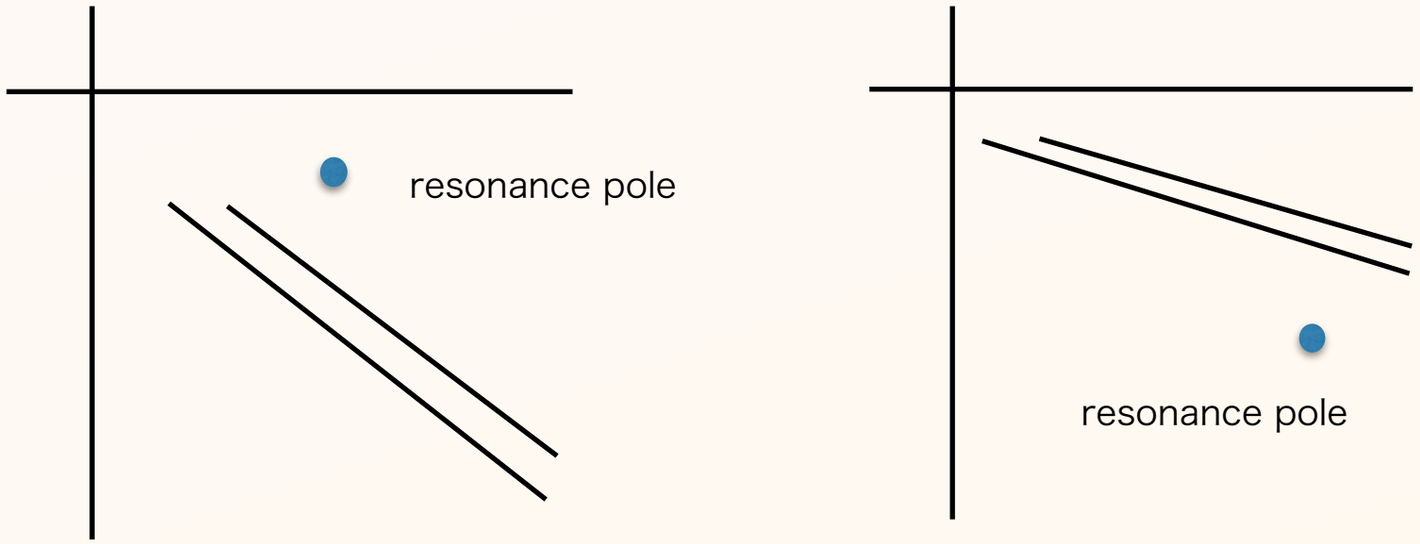
SS method: high density : difficult to solve low density : easy to solve

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

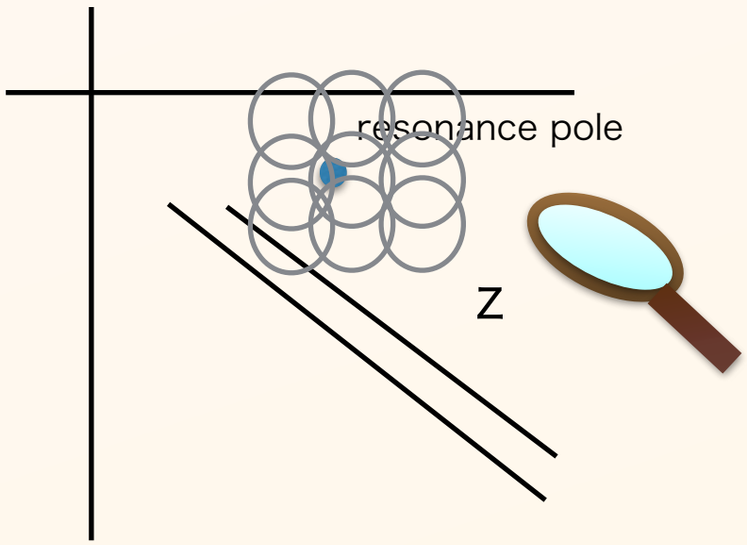
Resonance pole can be isolated by taking relevant scaling angle.

→ 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.



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.

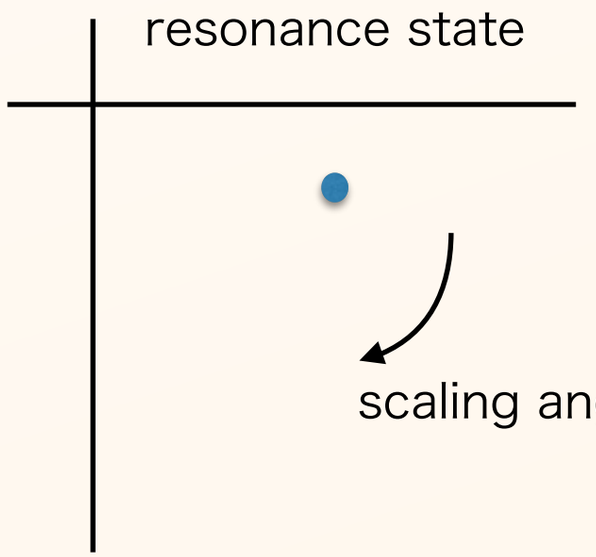
Direct diagonalization gives no information!

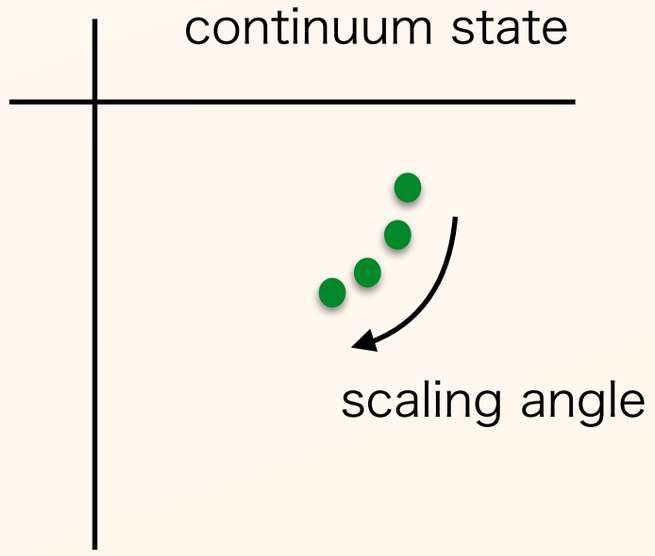
Resonance or not —> Move it as a function of scaling angle

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

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

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





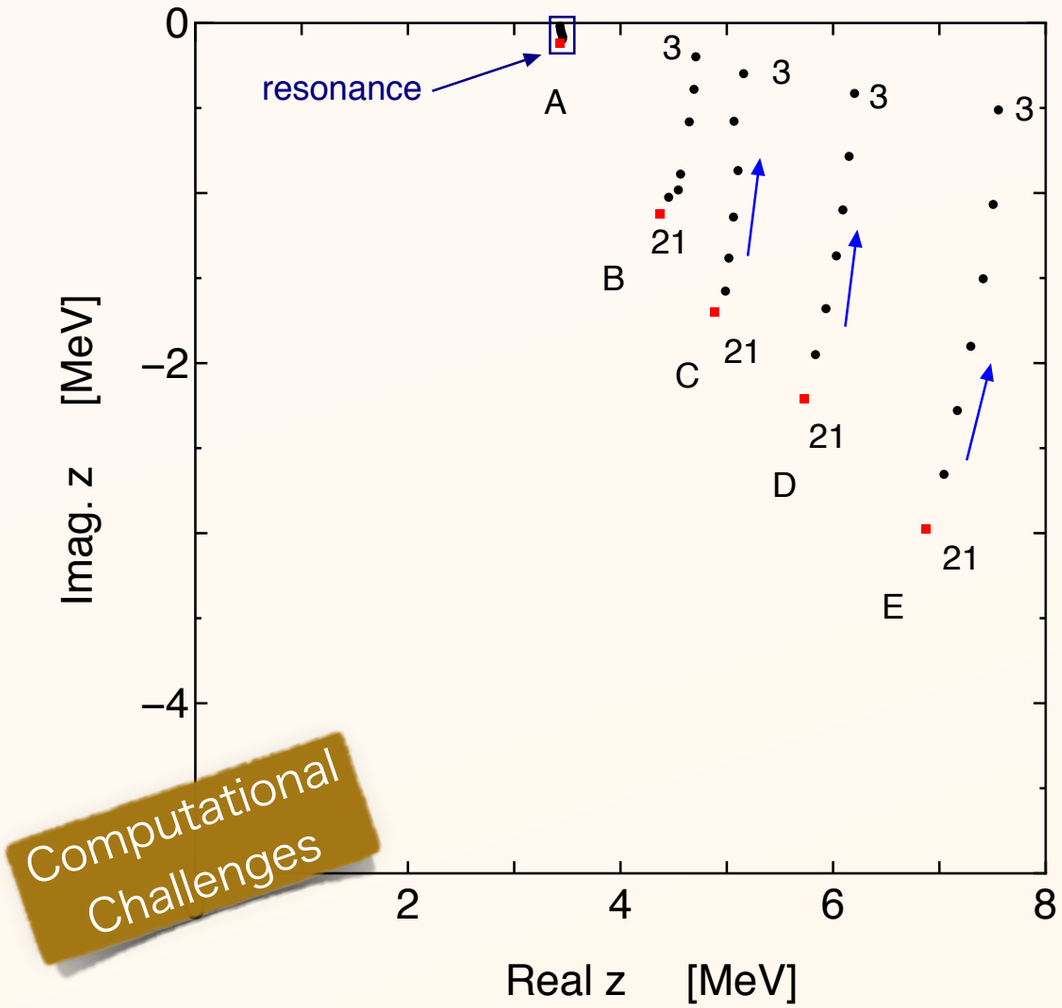
In a direct diagonalization method, all the energies should be calculated from scratch at each scaling angle.

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° and obtain several candidates for the resonance state.
2) Next we solve the eigenvalue problem at 18°, starting from these candidate wave functions at 21°.
3) We repeat this procedure up to 3°.

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.



Computational Challenges

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!

Breakthrough!

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

—> study of many-body resonances

6. Summary, Perspective and Collaborators

Summary

1) We have successfully applied the SS method to nuclear shell model calculations.
1-1) The SS method is useful as the same as the Lanczos method for large-scale shell model calculations.
1-2) The SS method can utilize the truncation scheme well especially for off-yrast states.
1-3) The SS method plays a unique role for isospin-symmetry-breaking problem (though I skipped this issue.)
2) We also have successfully applied the SS method to obtain many-body resonance calculations with complex scaling calculations.
2-1) The SS method plays a unique role for large-scale many-body resonance calculations.
2-2) We can obtain candidates of resonance states effectively thank to eigenvalue distribution on the complex plane.
2-3) We can find resonance states among their candidates effectively thank to the moment expression.

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