Cluster Structures Described by Randomly-Selected Multiple Slater Determinants

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Introduction

- Various theories have been developed to describe excited states.
  - Shell model
  - Mean-field theory
    - RPA, GCM
  - Cluster model, AMD

- We propose a new framework based on mean-field theory.
  - Prepare Slater determinants by some stochastic method
    $\{\Phi^i\} \quad (i = 1, \cdots, N)$
  - Angular momentum projection and configuration mixing.
    $$\{h^{J\pm} - E n^{J\pm}\} g = 0$$
    $$\left\{ \begin{matrix} h^{J\pm}_{iKi'K'} \\ n^{J\pm}_{iKi'K'} \end{matrix} \right\} = \langle \Phi^i | \left\{ \begin{matrix} \widehat{H} \\ 1 \end{matrix} \right\} P^J_{KK'} P^{\pm} | \Phi^{i'} \rangle$$

How to prepare the Slater determinants?

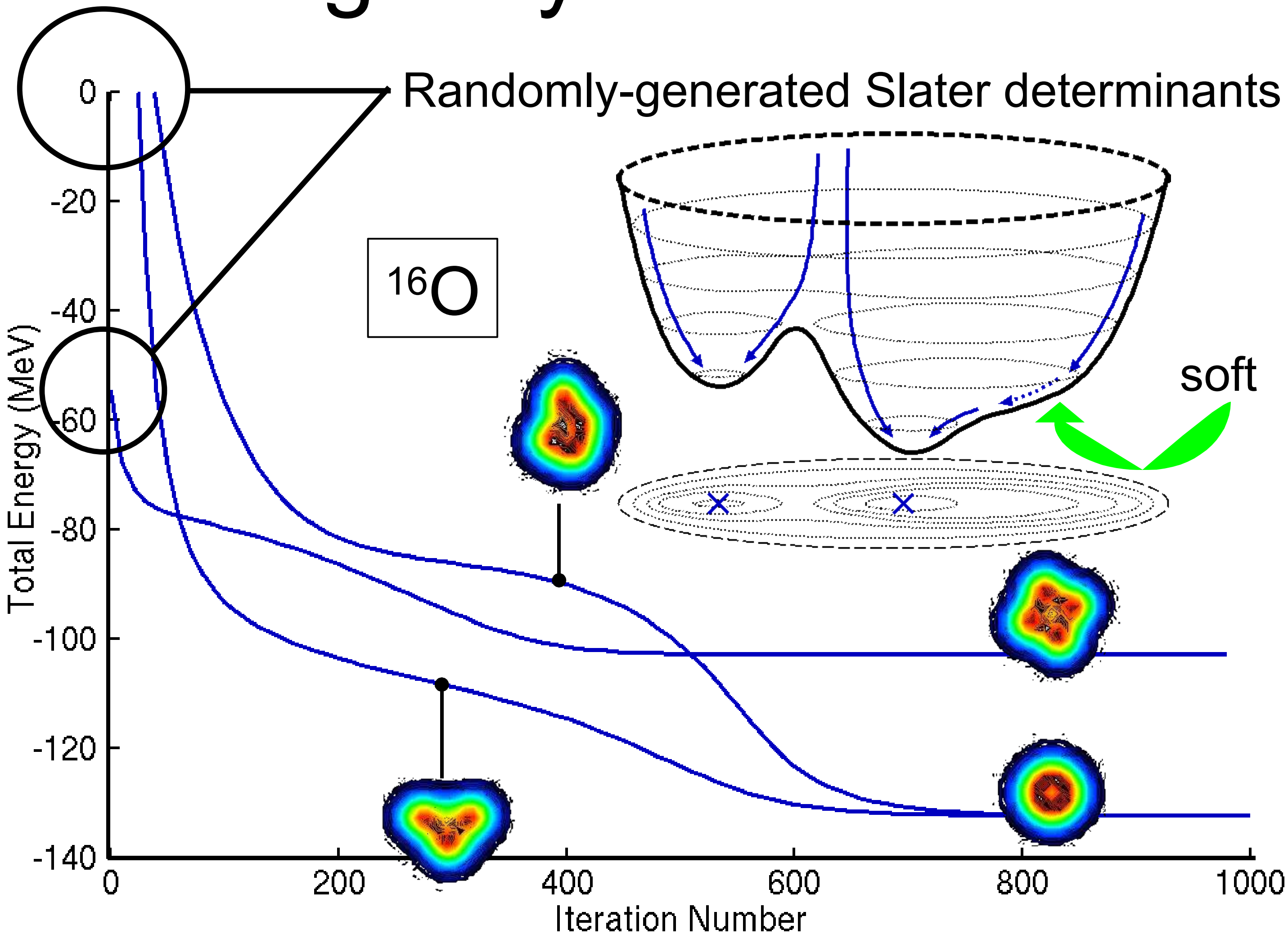
Superposition of randomly-selected Slater determinants

- Description of various low-lying excitations.
  - Without assuming nuclear shape.
  - Superposition of multiple Slater determinants.

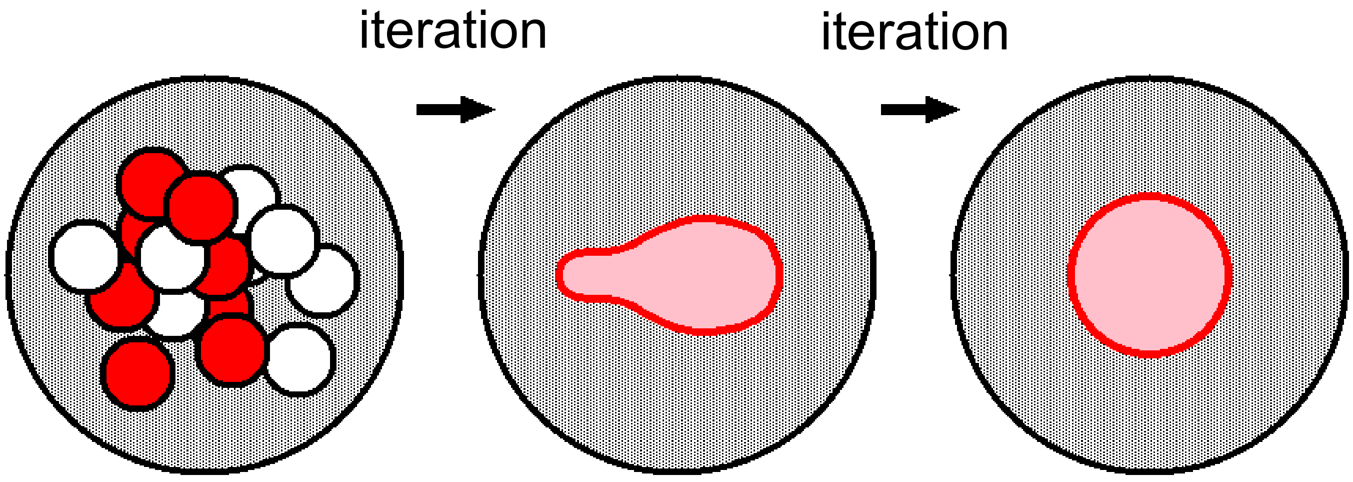
- We propose a new stochastic approach.
  - Slater determinants are randomly-generated and are cooled by “imaginary-time method”.

- We examine the accuracy of our method by using BKN force in the calculation of light nuclei.

Many paths created by imaginary-time method



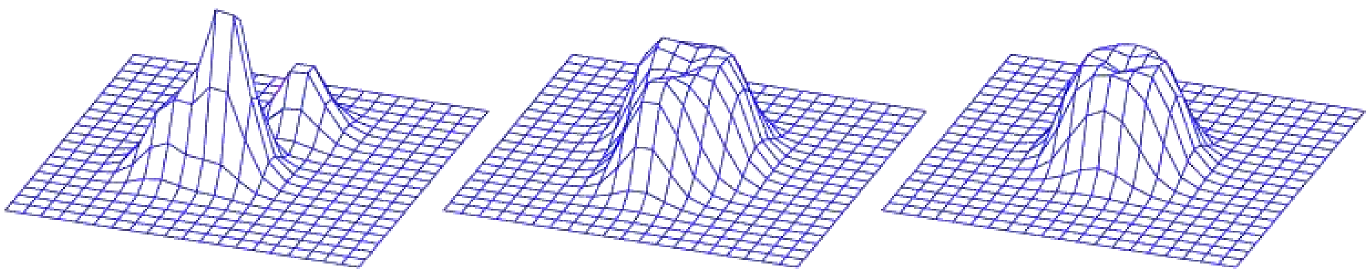
Initial Slater determinants



- Gaussian single-particle wave functions are distributed.
- Positions of the Gaussian-centers are determined by random numbers.

3D-mesh representation

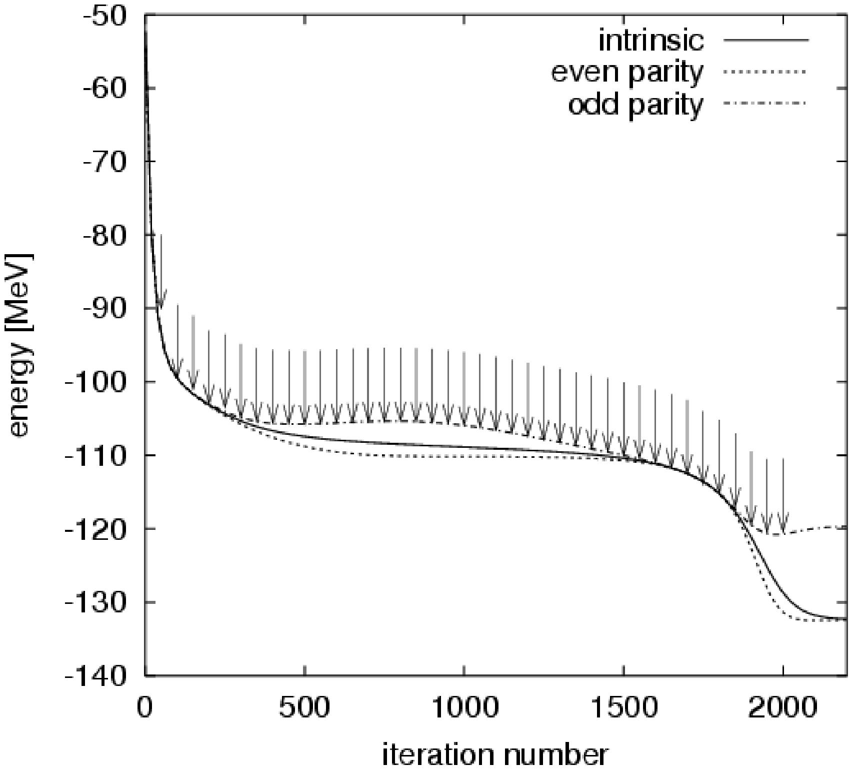
3D-mesh representation is applied to deal with largely deformed shape.



Initial state - - - - - - - - - - - - - - -→ **HF state**

How to select Slater det

- An imaginary-time calculation is continued until 2000 step.
  - 40 checkpoints in an imaginary-time calculation.
- Basis set should be linearly independent.

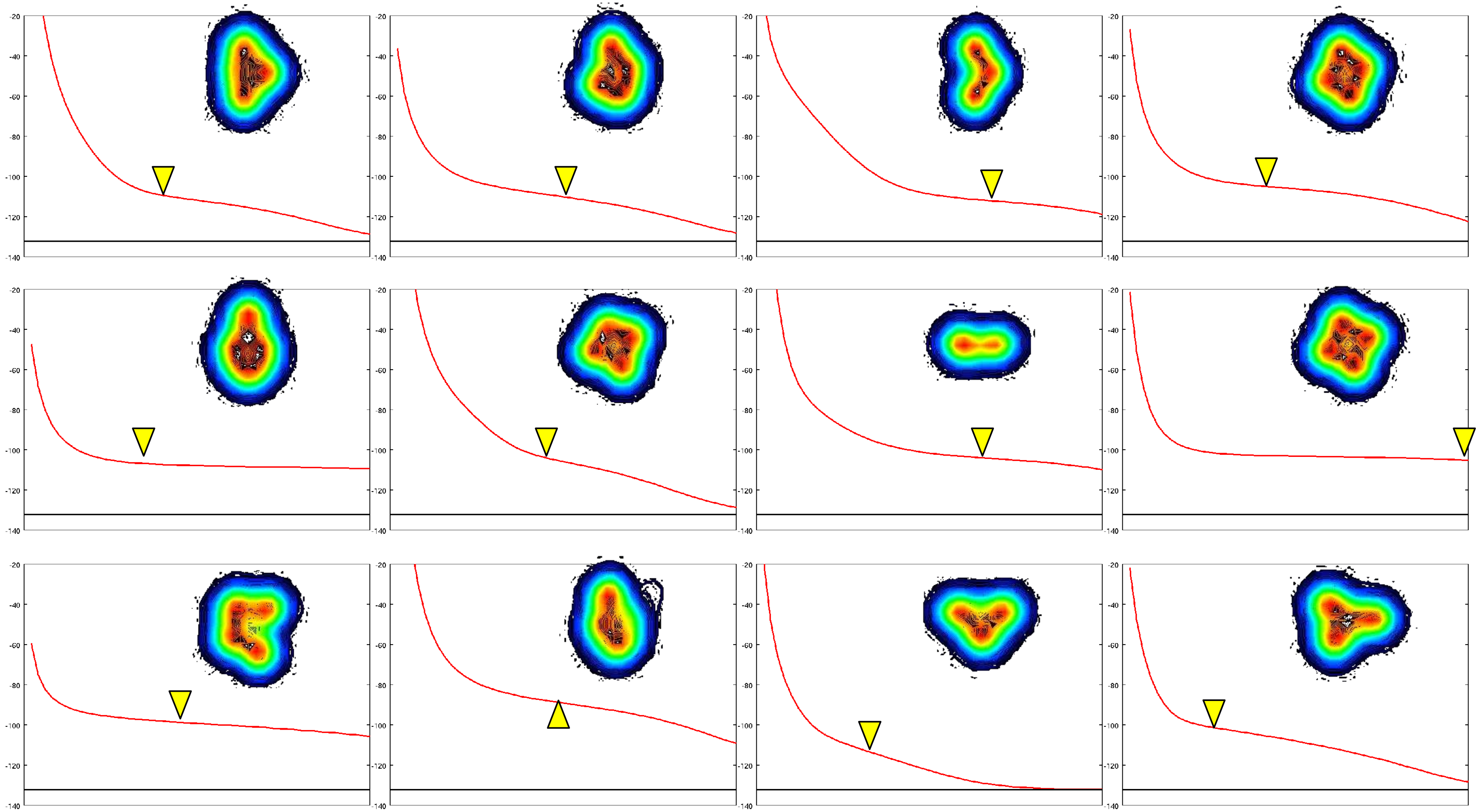


We exclude a state $|\Phi\rangle$ if this does not satisfy the condition

$$\langle \Phi^{(\pm)} | \Phi^{i(\pm)} \rangle < 0.7$$

for any of already selected Slater determinants $\{|\Phi^{i}\rangle\}$.

Many configurations included in the calculation in ^{16}O



Local minima and soft modes automatically appear.

Configuration Mixing

- Parity and angular momentum projection

$$|\Phi^i\rangle \to P^J_{MK} P^{\pm} |\Phi^i\rangle \qquad (i = 1, 2, \cdots 50)$$

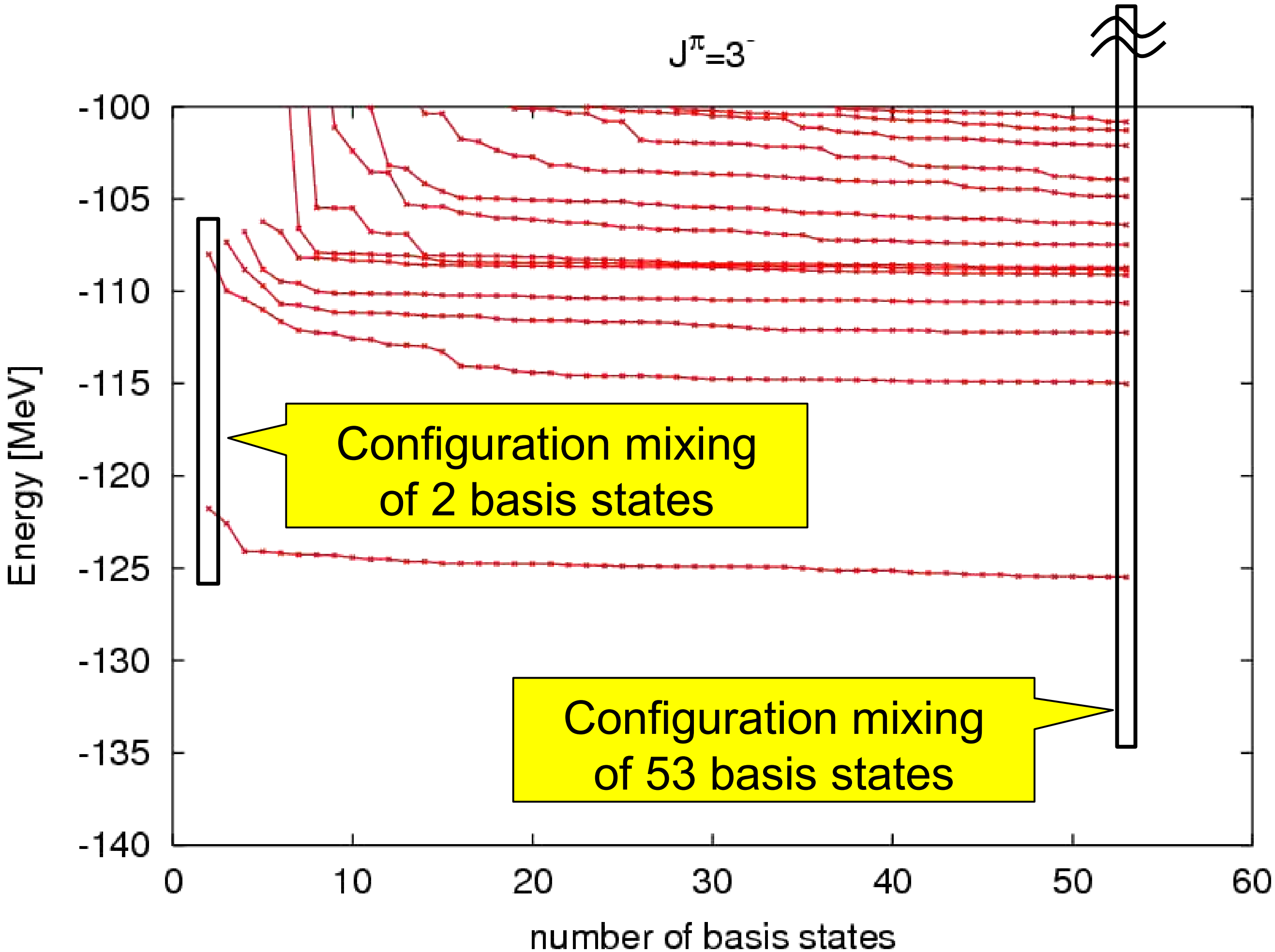
$$|\Phi^i\rangle \equiv |\mathcal{A}\{\phi^i_1 \phi^i_2 \cdots \phi^i_A\}\rangle$$

- Generalized eigenvalue problem

$$\{h^{J\pm} - E n^{J\pm}\} g = 0$$

$$\begin{Bmatrix} h^{J\pm}_{iKi'K'} \\ n^{J\pm}_{iKi'K'} \end{Bmatrix} = \langle \Phi^i | \begin{Bmatrix} \widehat{H} \\ 1 \end{Bmatrix} P^J_{KK'} P^{\pm} | \Phi^{i'} \rangle$$

Energy convergence of $J^{\pi}=3^{-}$ in ^{16}O (BKN interaction is used)

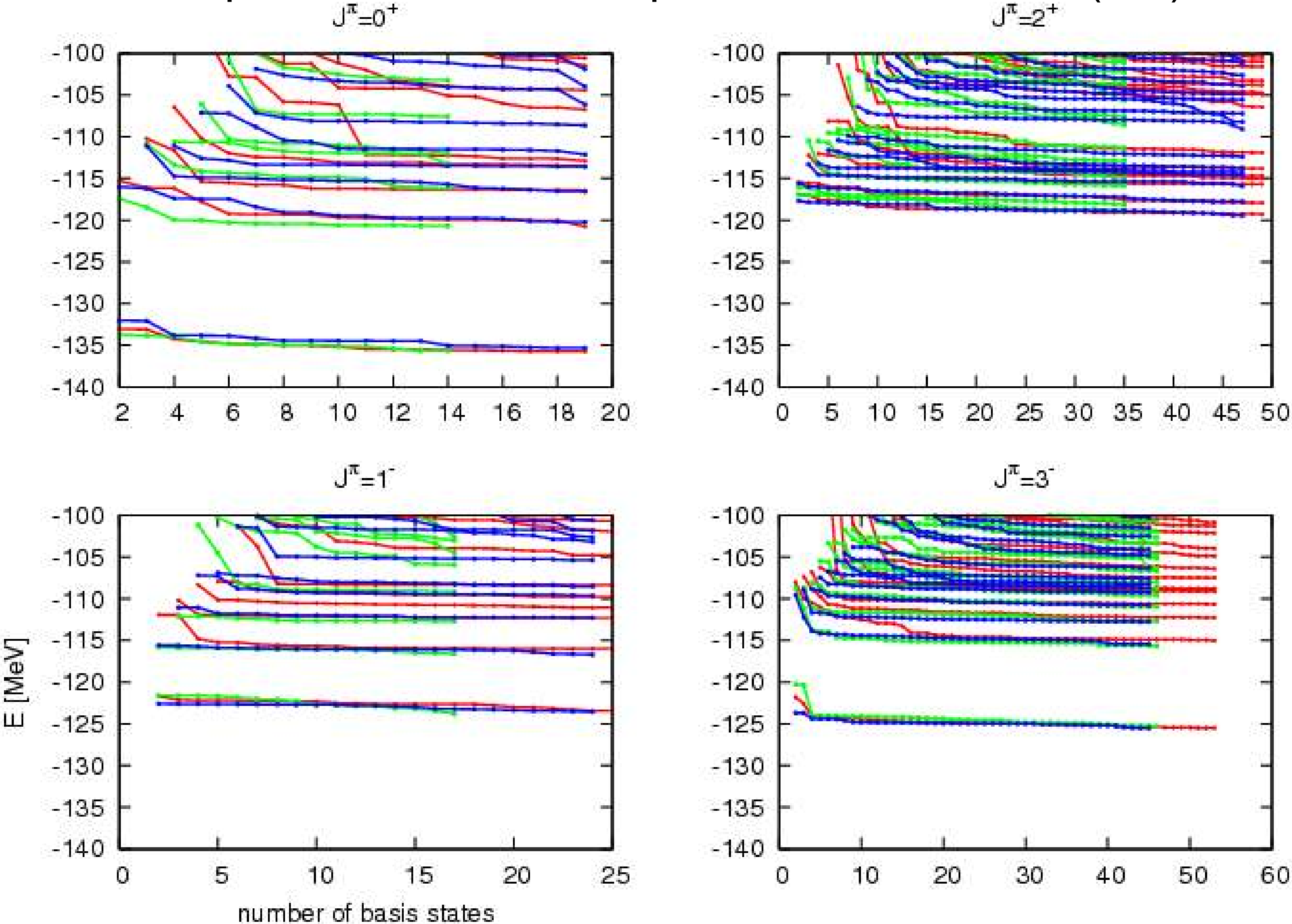


Results should be unique.

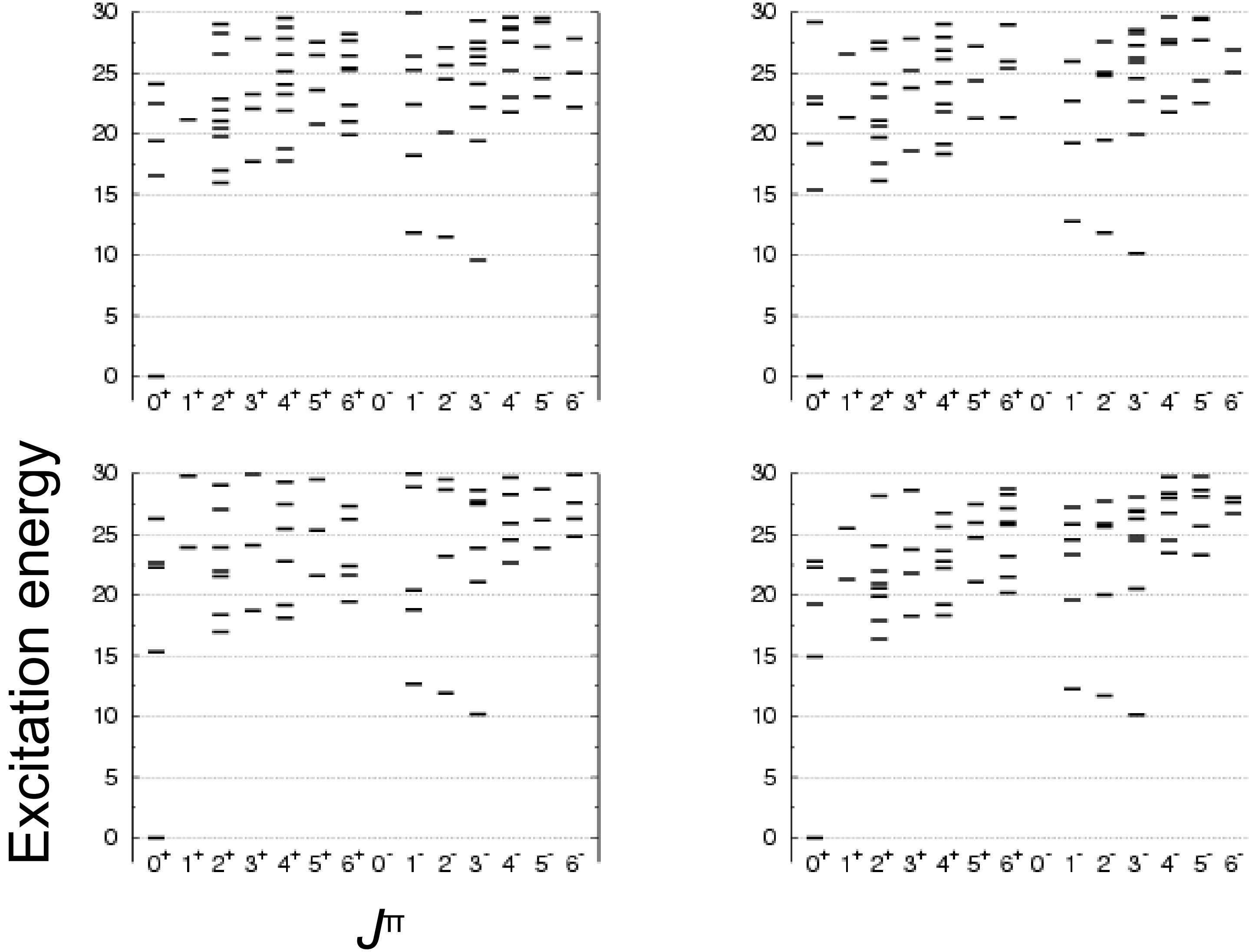
Random number set A	Random number set B
⇩	⇩
$\Phi^1, \Phi^2, \cdots, \Phi^{50}$	$\Psi^1, \Psi^2, \cdots, \Psi^{50}$
⇩	⇩
result A	result B

Result A and B should be identical.

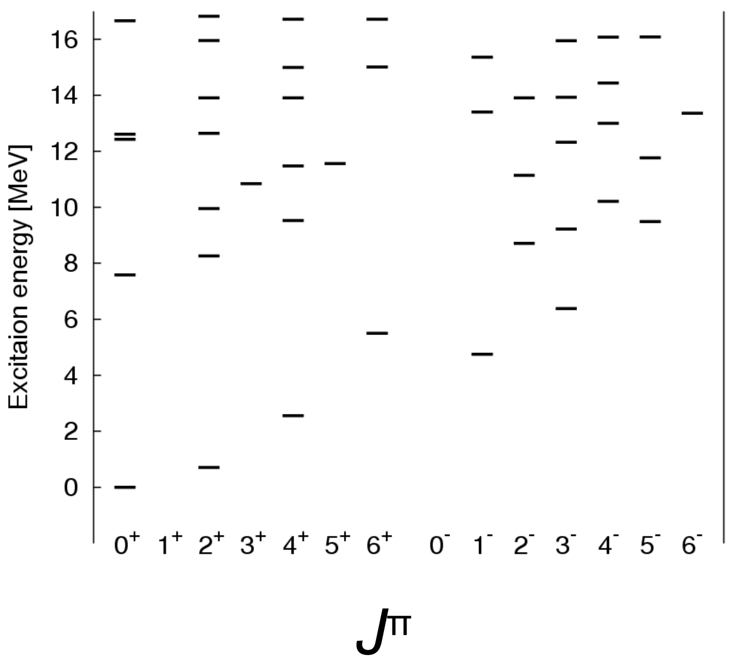
Comparison of three independent calculations (^{16}O)



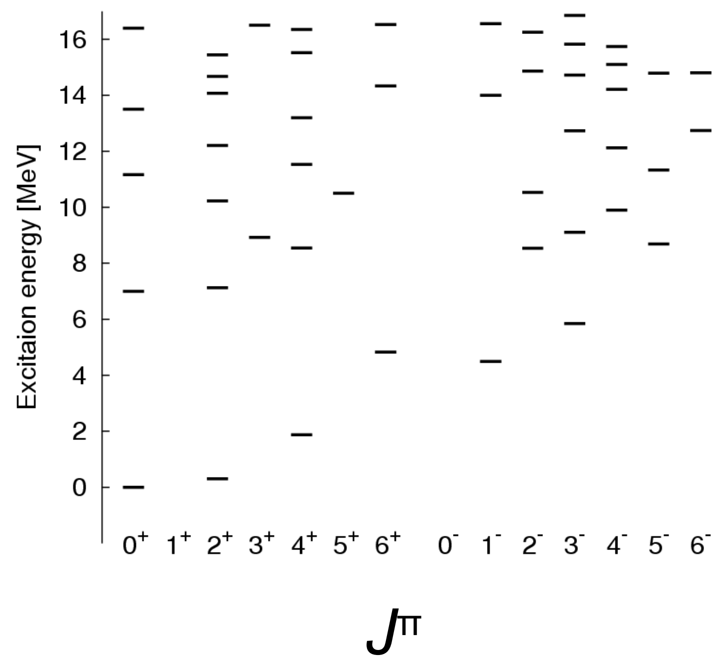
Comparison of four independent calculations
Excitation spectrum (^{16}O)



Comparison of two independent calculations Excitation spectrum (^{20}Ne)

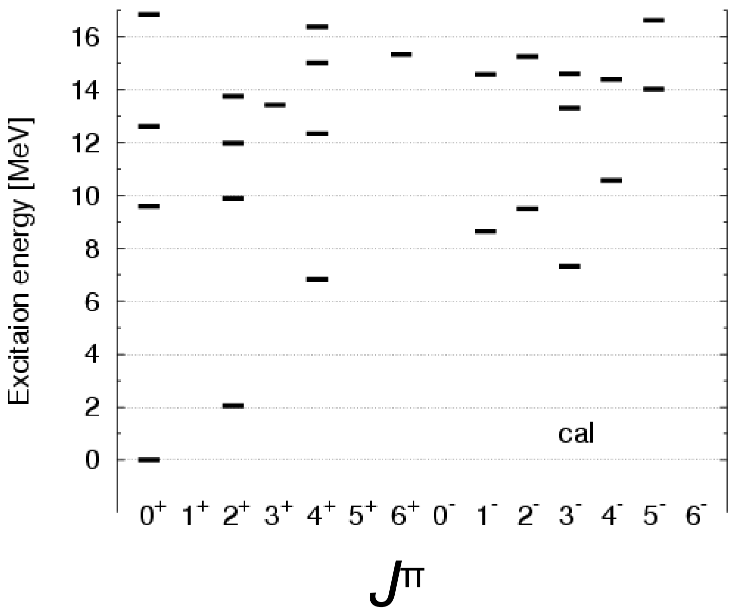


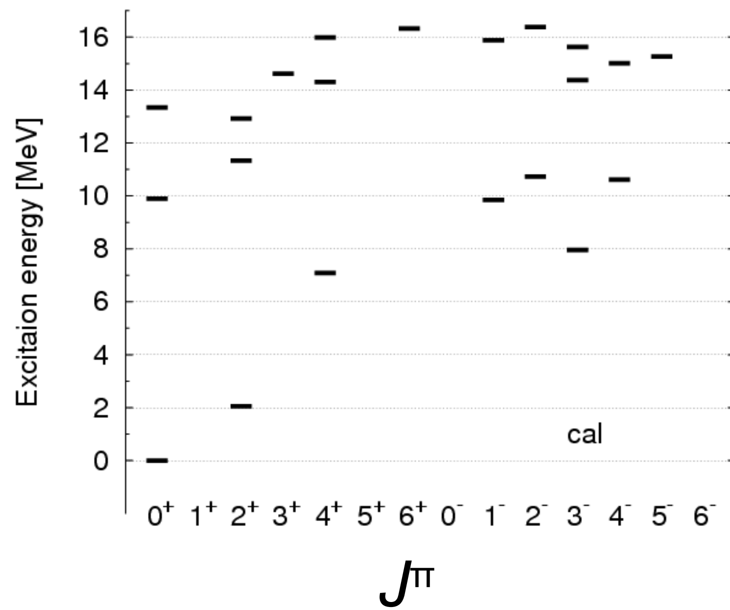
Random number set A



Random number set B

Comparison of two independent calculations Excitation spectrum (^{12}C)



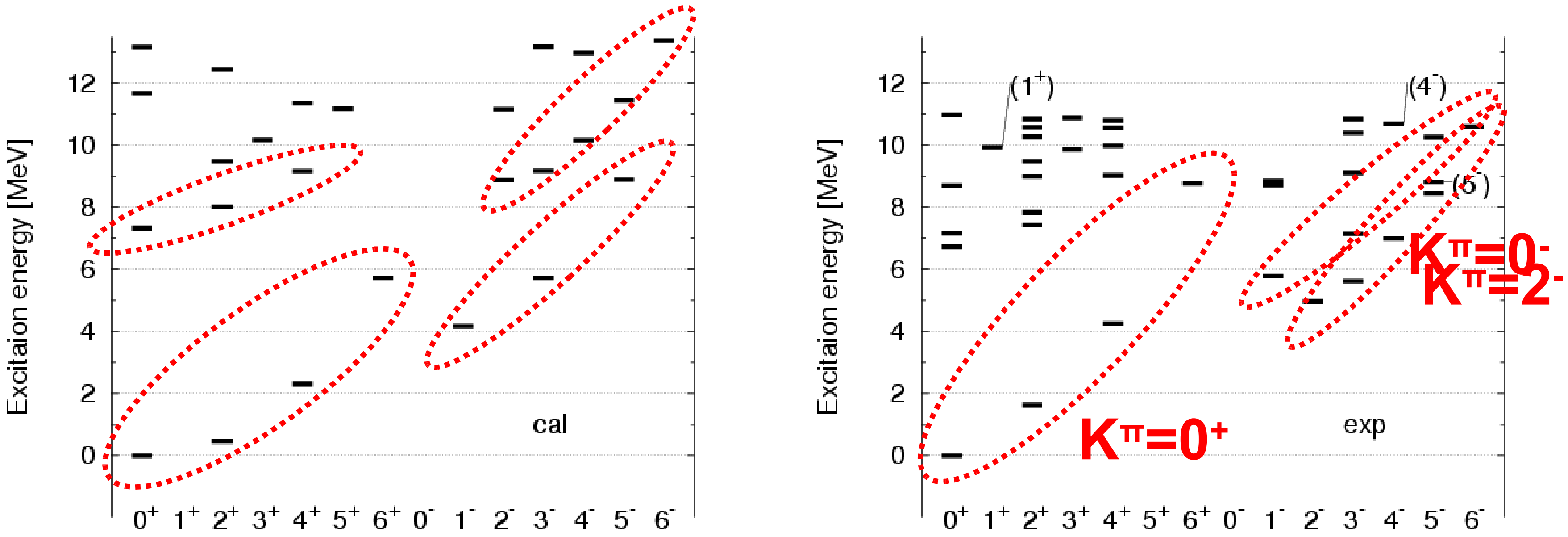


Random number set A **Random number set B**

- We examined accuracy of our method with BKN force.
  - Convergence and uniqueness of solutions
    - Results are promising.
  - Estimation of excitation energy is poor.

- Next
  - We will discuss the results of ^{20}Ne and ^{12}C in detail.

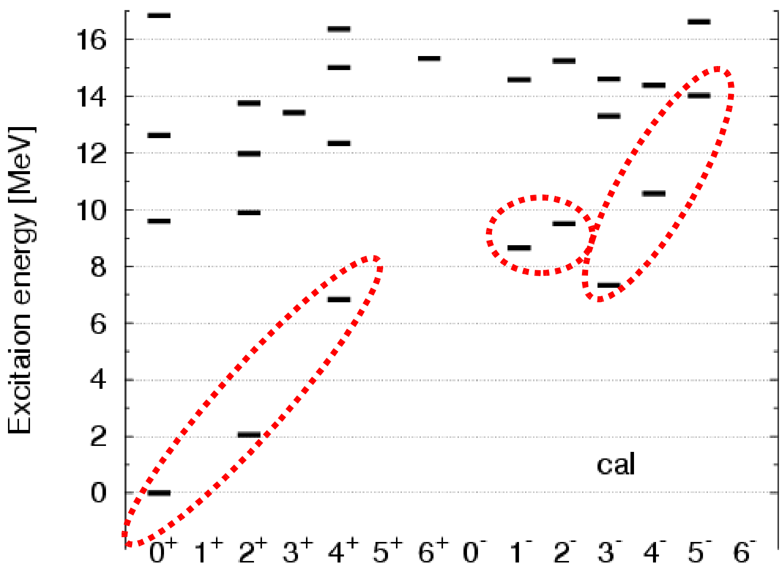
^{20}Ne



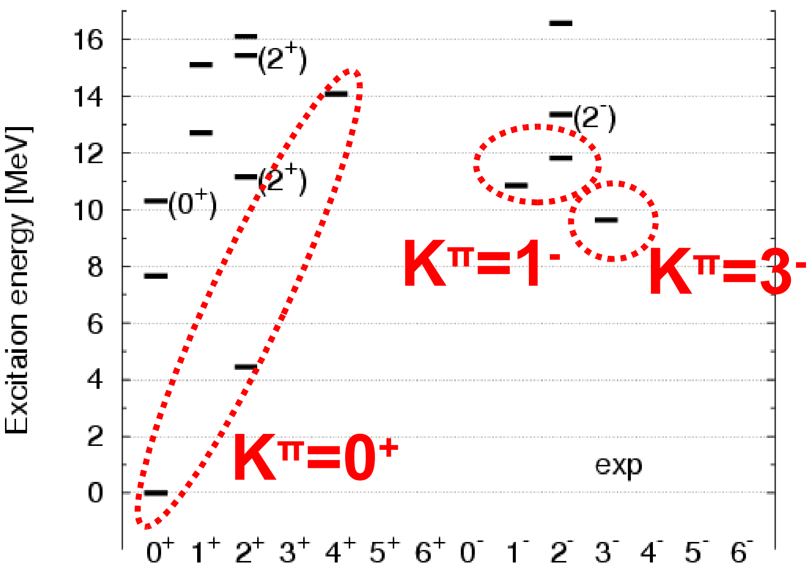
Excitaion energy [MeV]
0
2
4
6
8
10
12
0+ 1+ 2+ 3+ 4+ 5+ 6+ 0- 1- 2- 3- 4- 5- 6-
cal
Excitaion energy [MeV]
(1+)
(4-)
(5-)
Kπ=0-
Kπ=2-
Kπ=0+
exp

cal **exp**

^{12}C


Excitaion energy [MeV]
16
14
12
10
8
6
4
2
0
0+ 1+ 2+ 3+ 4+ 5+ 6+ 0- 1- 2- 3- 4- 5- 6-
cal

cal


Excitaion energy [MeV]
16
14
12
10
8
6
4
2
0
(2+)
(2-)
(2+)
(0+)
Kπ=1-
Kπ=3-
Kπ=0+
exp
0+ 1+ 2+ 3+ 4+ 5+ 6+ 0- 1- 2- 3- 4- 5- 6-

exp

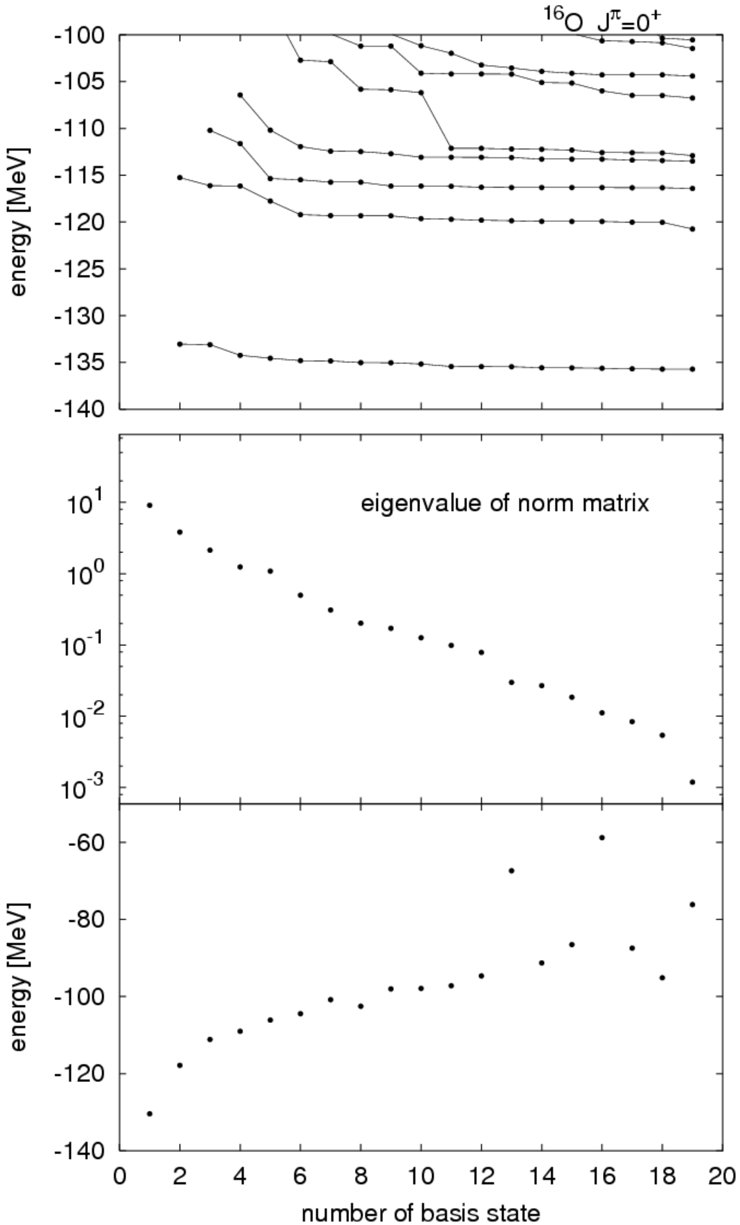
Summary

- Description of various low-lying excitations.
  - Without assuming nuclear shape.
  - Superposition of multiple Slater determinants.
- New stochastic method using imaginary-time method.
  - Initial Slater determinants are randomly-generated.
  - Local minima and soft-modes automatically appear during the imaginary-time evolution.
- We examined accuracy of our method with BKN force.
  - Convergence and uniqueness of solutions
  - Application to light nuclei (^{12}C, ^{20}Ne)
    - Results are promising.

Future Problem

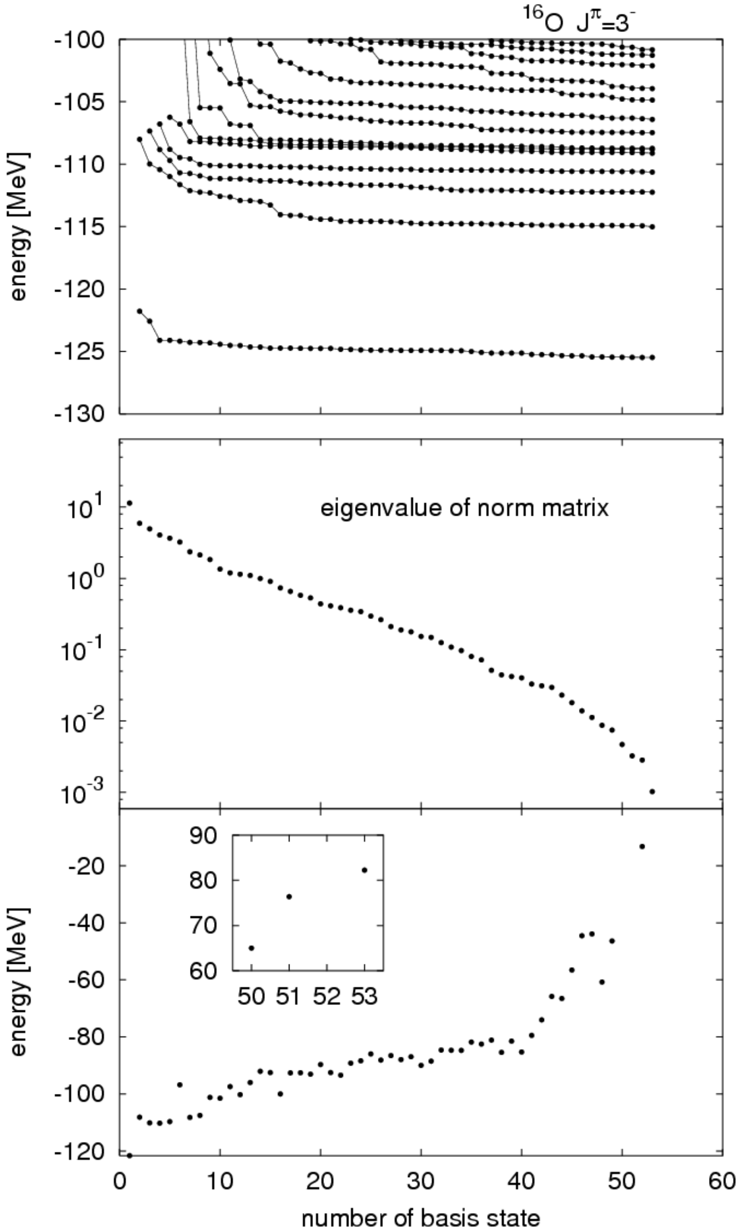
- Improvement of the method
  - We have to consider the way to select only important configurations that make the energy lower.

- Application with more realistic Skyrme force
  - Application to unstable nuclei



Energy convergence

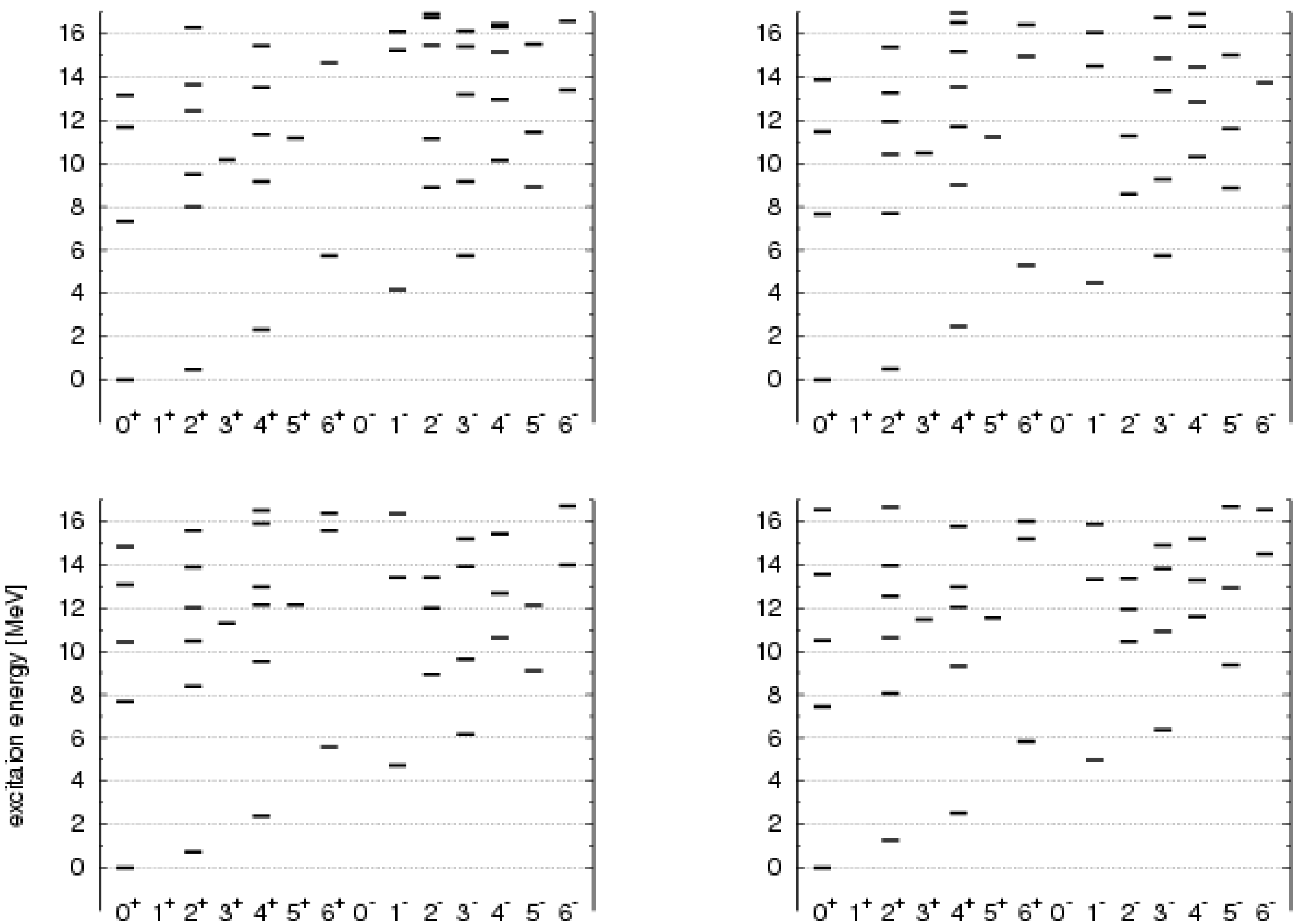
Eigenvelue of norm matrix



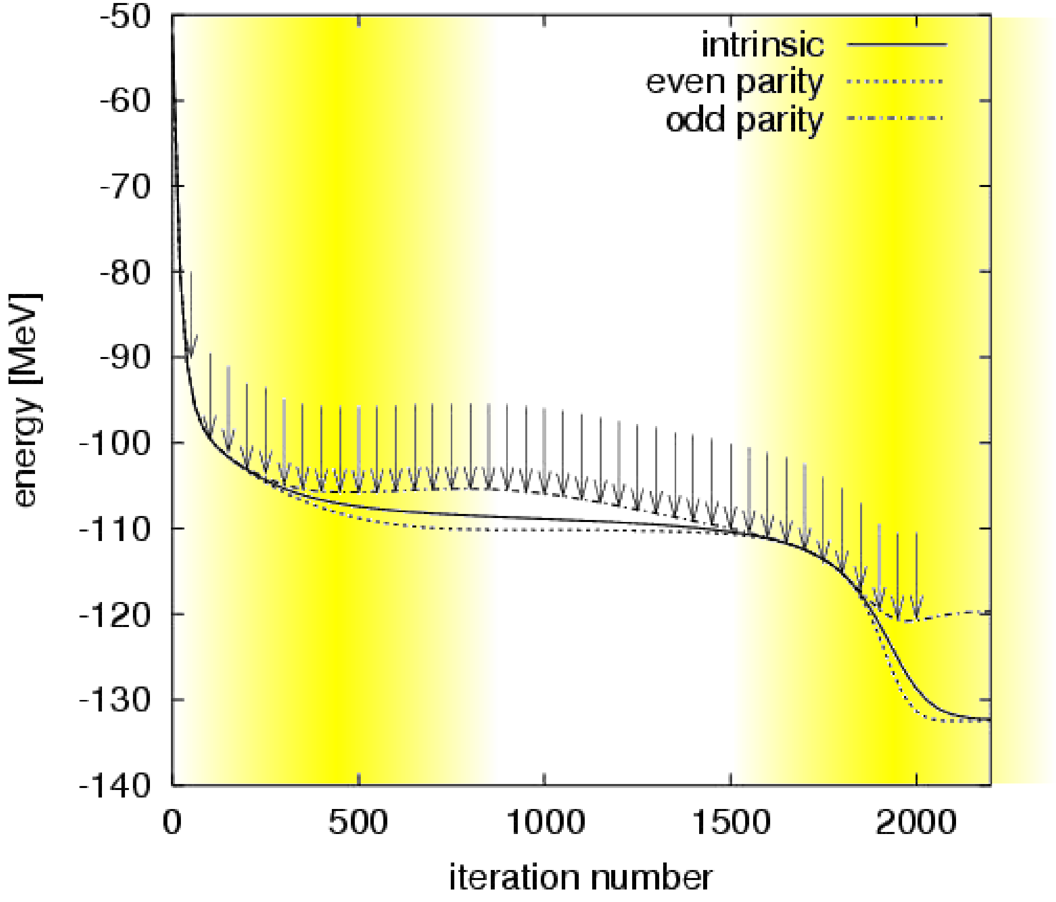
Energy convergence

Eigenvelue of norm matrix

^{20}Ne

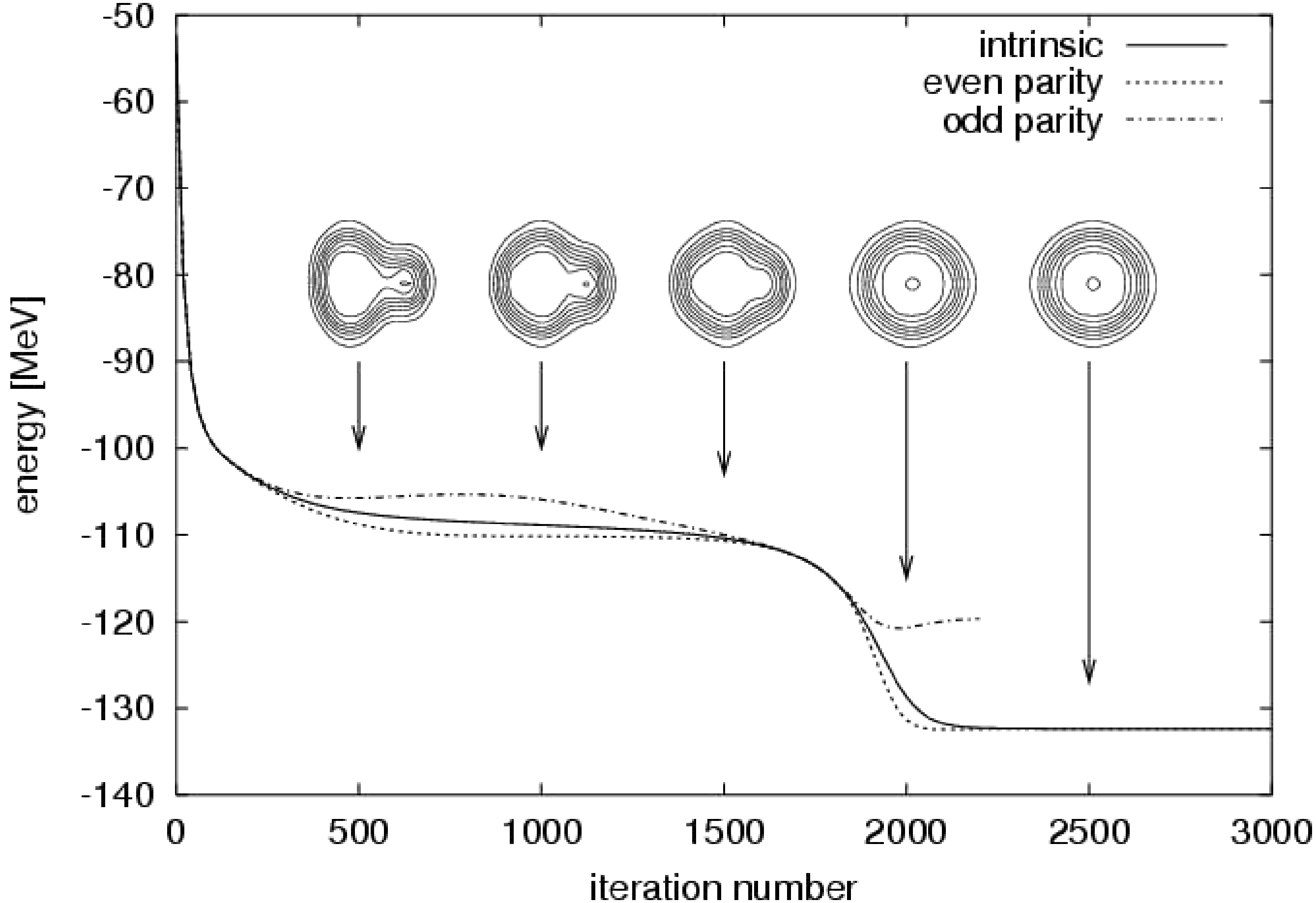


40 check points



An example of imaginary-time calculation

^{16}O



Comparison of four independent calculations Excitation spectrum (^{20}Ne)