Division of Astrophysics and Nuclear Physics: Nuclear Physics Group (Parallel session #2)

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Stochastic generation of low-energy configurations and configuration mixing calculation with Skyrme interactions

Graduate Student
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(expected to receive his PhD in March)

Fukuoka, Shinohara, Funaki, Nakatsukasa, Yabana, PRC 88, 014321 (2013)

Microscopic structure theories

- Ab-inito-type approaches
  - GFMC, NCSM, CCM, etc.
  - Computationally very demanding for heavier nuclei
- Shell model approaches
  - CI calculation in a truncated space
  - Difficulties in cross-shell excitations
- Microscopic cluster models
  - RGM, GCM, etc.
  - Interaction is tuned for each nucleus
- Energy density functional approaches
  - *New configuration-mixing (multi-ref.) calculation*

Toward low-energy complete spectroscopy

Shinohara, Ohta, Nakatsukasa, Yabana, PRC 84, 054315 (2006)

- Beyond the mean field
  - Correlations, excited states
- Beyond (Q)RPA
  - States very different from the g.s.
- Beyond GCM
  - Lift a priori generator coordinates

Toward the *theoretical complete spectroscopy* of low-lying states with *an effective Hamiltonian* and with a *very large model space*:

⇩

"Stochastic" approach to configuration mixing

Configuration mixing with parity and angular momentum projection

1. Generation and selection of Slater det's in the 3D Cartesian Coordinate space

$$\{\Phi^i\} \quad (i = 1, \cdots, N)$$

2. Projection on good J^π (3D rotation)

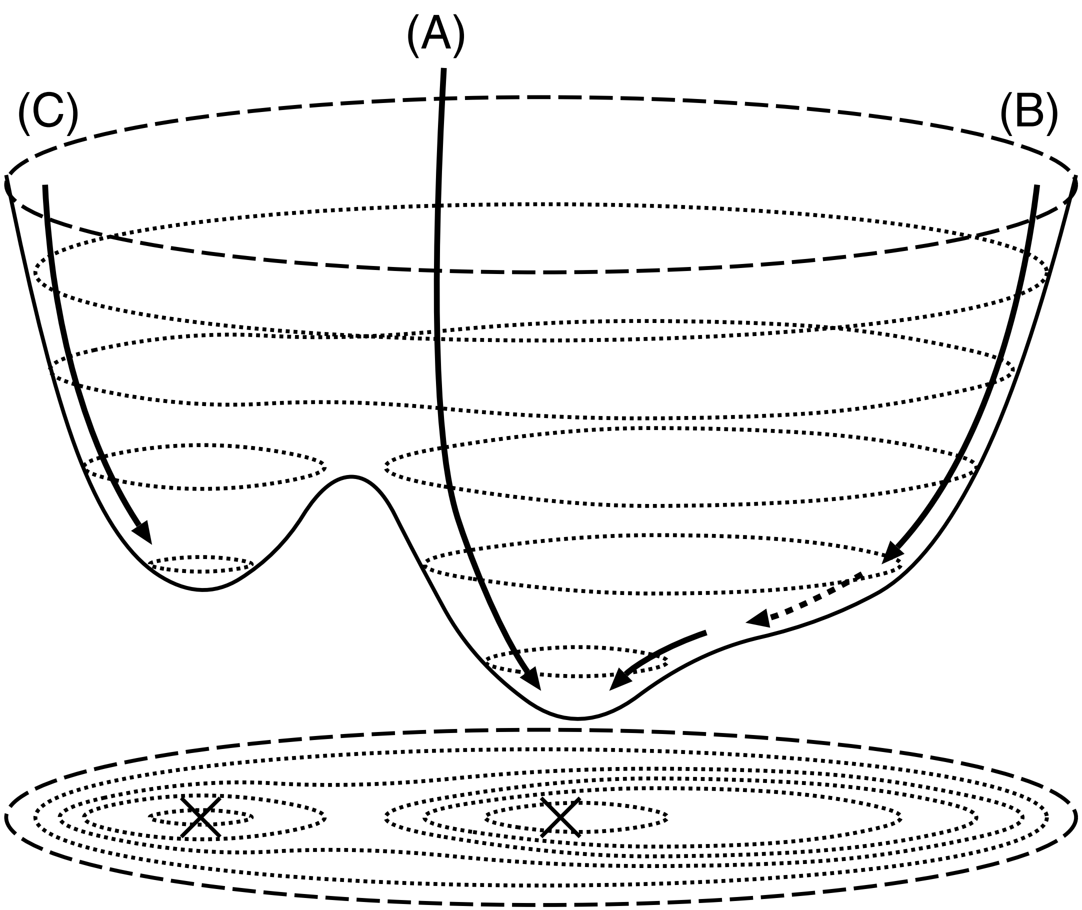
$$\left|\Phi^J_{MK}\right\rangle = P^\pm P^J_{MK}\left|\Phi\right\rangle$$

3. Solution of generalized eigenvalue eq.

$$\left(\mathbf{H}^{J\pm} - E\mathbf{N}^{J\pm}\right)\mathbf{g} = 0$$

$$\begin{matrix} H^{J\pm}_{nK,n'K'} \\ N^{J\pm}_{nK,n'K'} \end{matrix} = \left\langle \Phi^n \middle| \begin{Bmatrix} H \\ 1 \end{Bmatrix} P^\pm P^J_{KK'} \middle| \Phi^{n'} \right\rangle$$

Imaginary-time evolution



- Quickly removing high-energy (high-momentum) components
- Slowly moving on low-energy collective surface
- Finding local minima

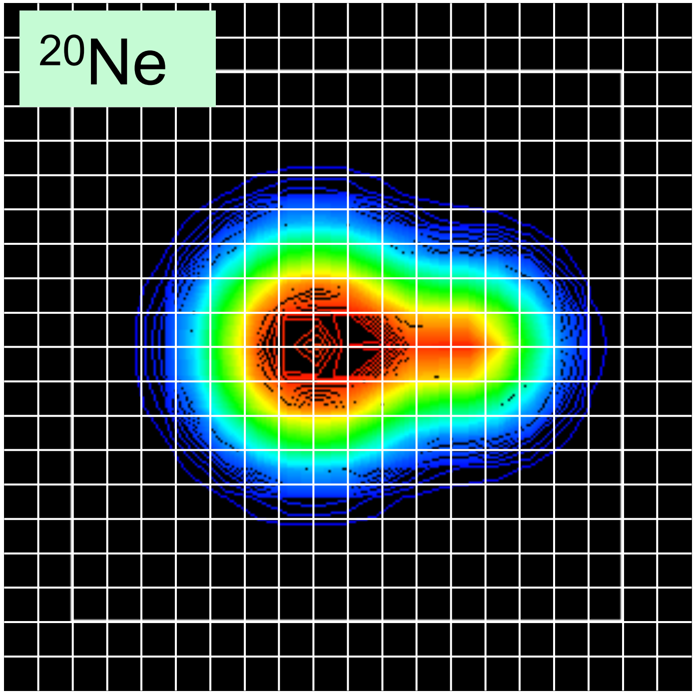
Efficient method to construct configurations associated with many kinds of low-energy collective motions

Generation of basis states: Imaginary-time method in 3D coordinate space

Long-range correlations in terms of the configuration mixing

Imaginary-time Method $\left|\phi_i^{(n+1)}\right\rangle = e^{-\Delta t\, h[\rho]}\left|\phi_i^{(n)}\right\rangle, \quad i = 1,\cdots A$

A well-known method in the Skyrme HF calculations

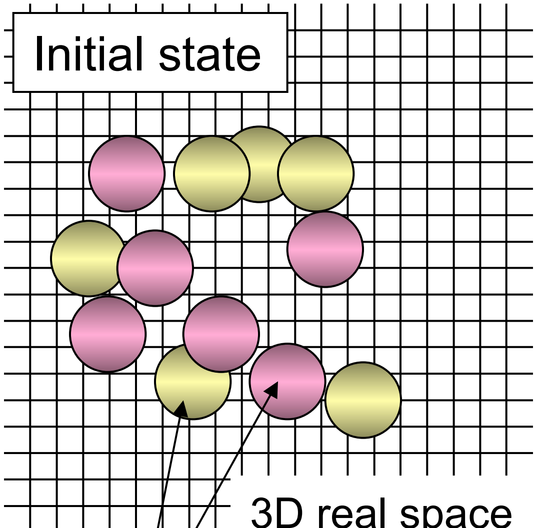


3D space is discretized in lattice

Single-particle orbital:

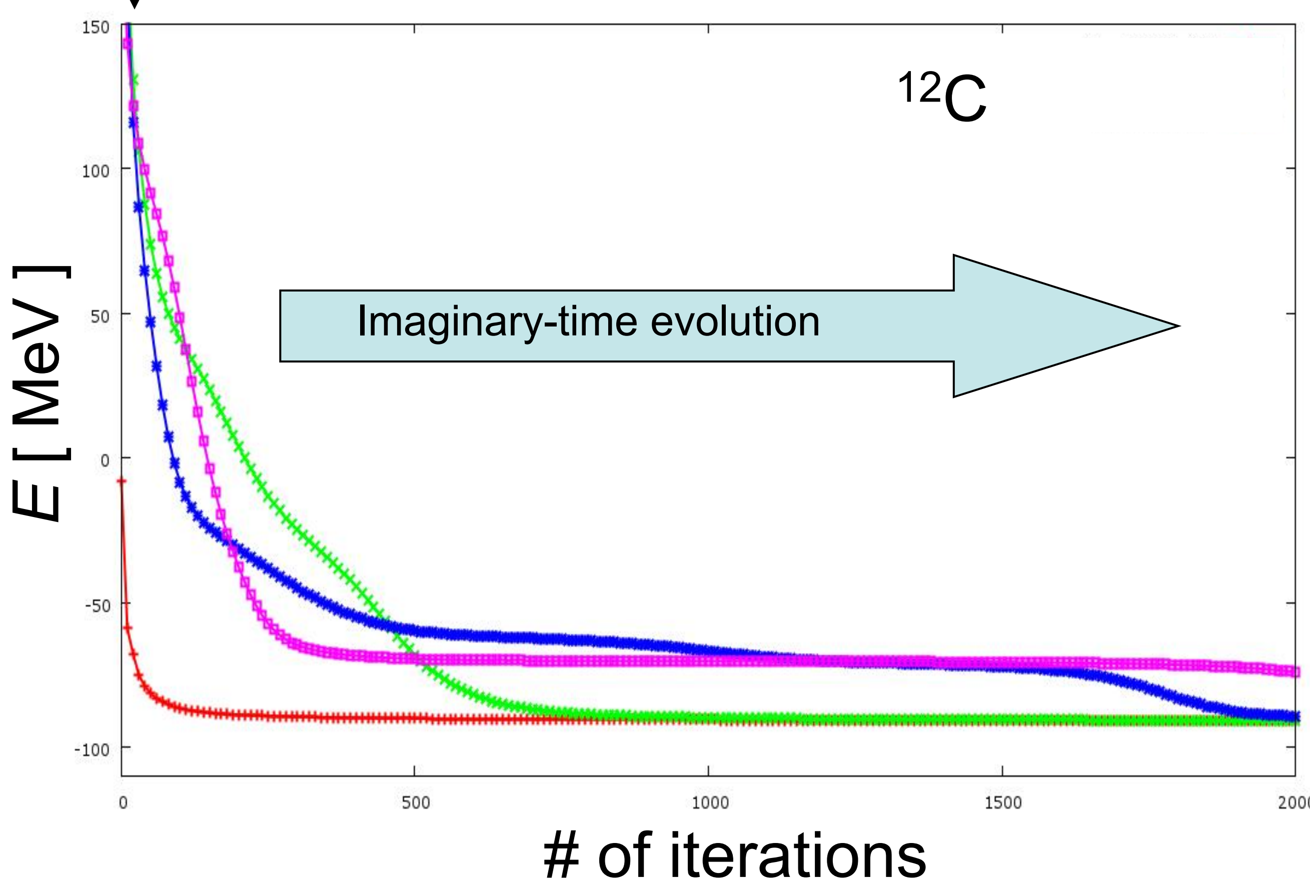
$$\phi_i(\mathbf{r}) = \{\phi_i(\mathbf{r}_k)\}_{k=1,\cdots Mr}, \quad i = 1,\cdots,N$$

Generation of many S-det's



Gaussian wave packets (n & p) whose positions are determined by random numbers.

$$\left|\phi_i^{(n+1)}\right\rangle = e^{-\Delta t\, h[\rho]}\left|\phi_i^{(n)}\right\rangle, \quad i = 1, \cdots A$$



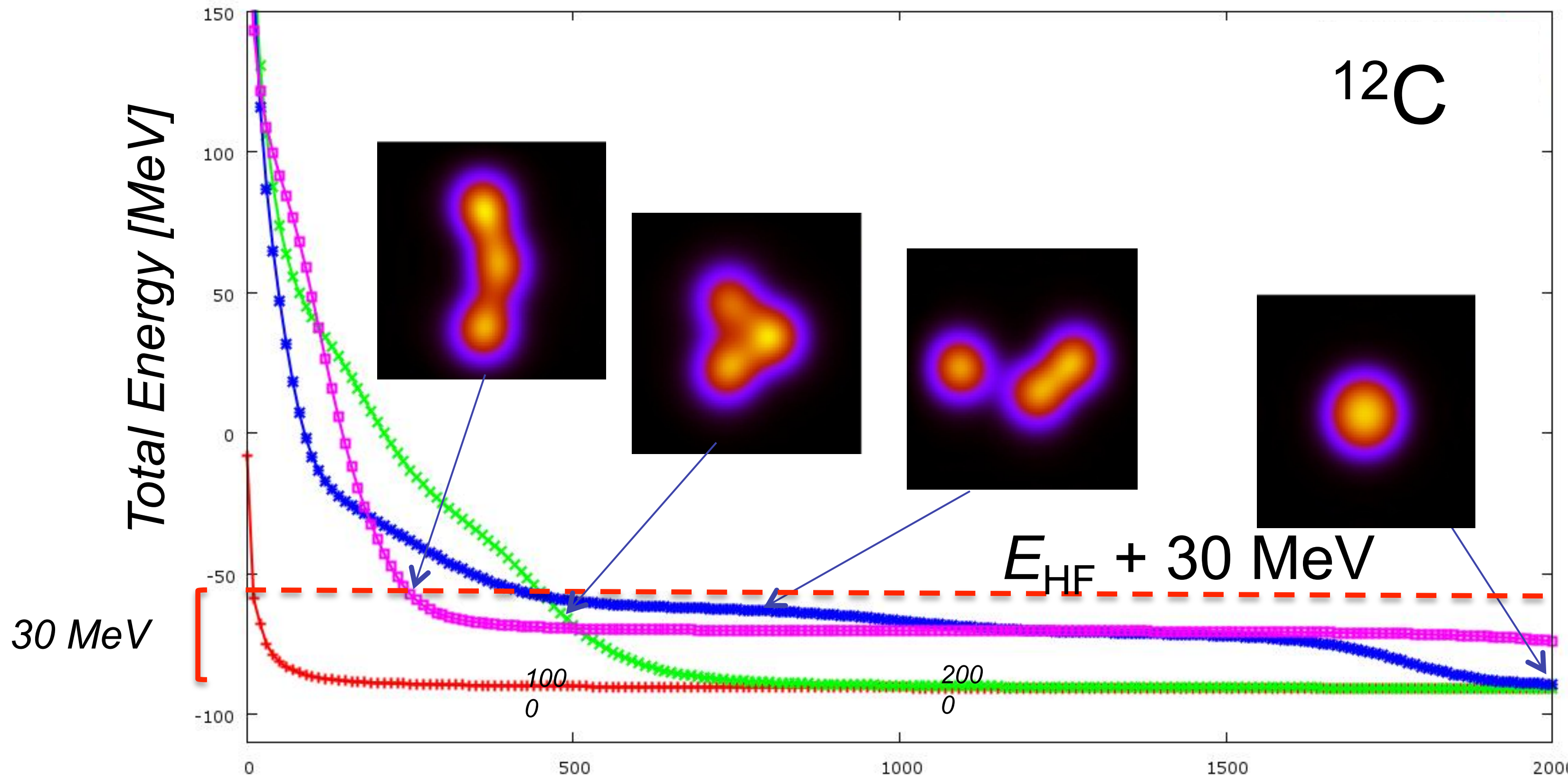
Screening of Slater determinants

Every one-hundred iterations,
we pick up a Slater determinant $\left|\Phi_i\right\rangle$

$\left|\Phi_i\right\rangle$ is adopted as the (M+1)-th basis configuration, if it satisfies

$$\left\langle\Phi_i\middle|H\middle|\Phi_i\right\rangle < E_{\mathrm{HF}} + 30\ \mathrm{MeV}$$

$$\left\langle\Phi_i\middle|\Phi_j\right\rangle < 0.7 \quad (j = 1, \cdots M)$$



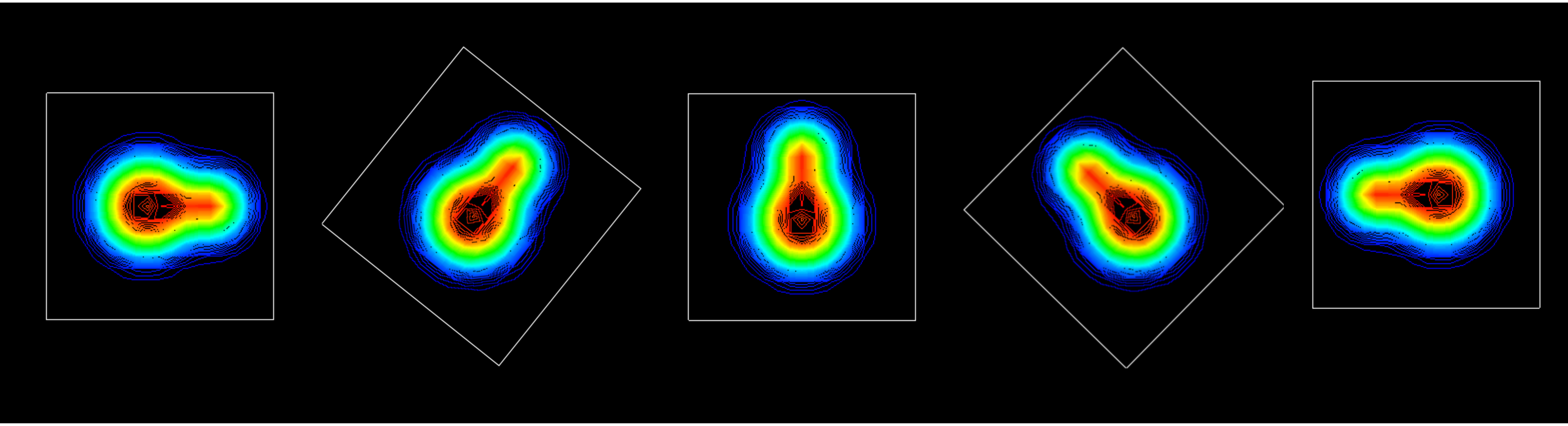
3D angular momentum projection

Parity and angular momentum projected state

$$\left|\Psi_M^{J\,(\pm)}\right\rangle = \frac{2J+1}{8\pi^2}\sum_K g_K \int d\Omega D_{MK}^{J\,*}(\Omega)\hat{R}(\Omega)\boxed{\left|\Phi^{(\pm)}\right\rangle}$$

$$\hat{\mathrm{R}}(\Omega) = \mathrm{e}^{-\mathrm{i}\alpha\hat{\mathrm{J}}_z}\mathrm{e}^{-\mathrm{i}\beta\hat{\mathrm{J}}_y}\mathrm{e}^{-\mathrm{i}\gamma\hat{\mathrm{J}}_z}$$

Parity-projected SD



Construct the angular momentum eigenstate by the explicit 3D rotation

Further Selection …

Eigenvalues of the norm matrix

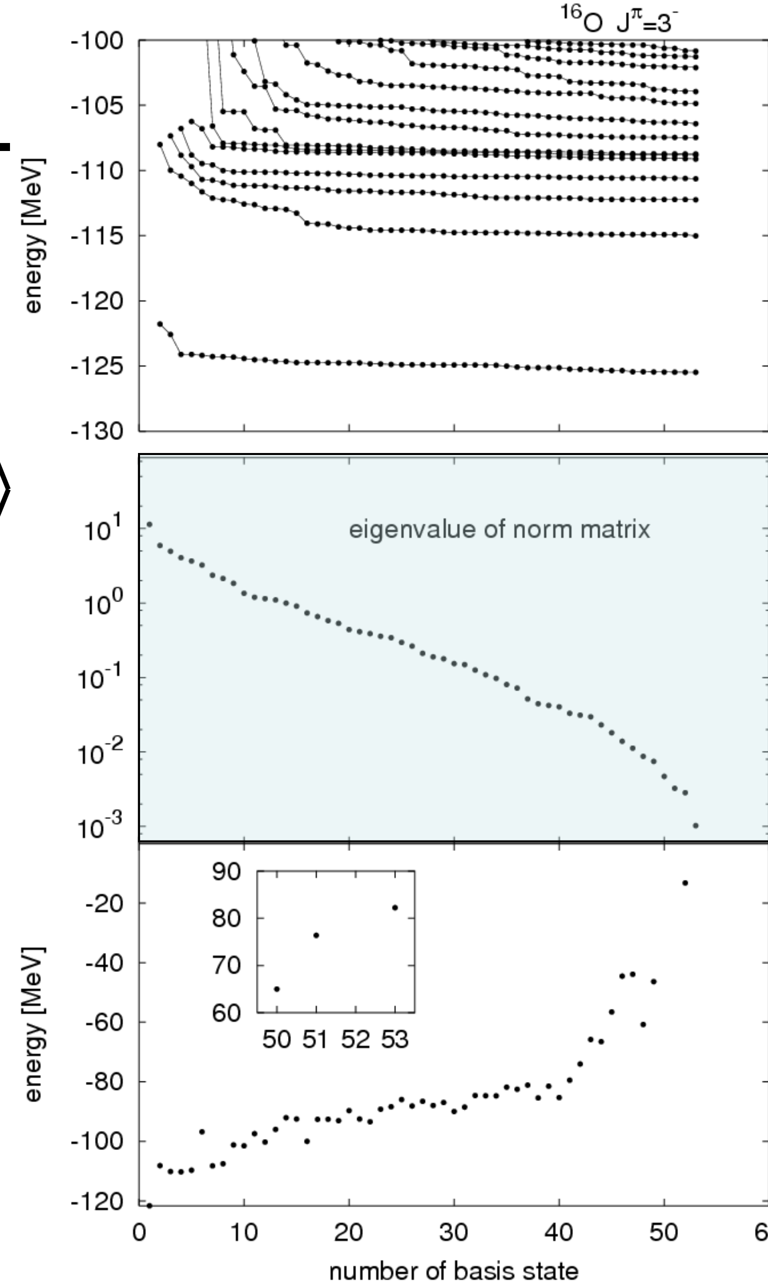
$$N^{J\pm}_{nK,mK'} = \left\langle \Phi^n \middle| P^J_{KK'} P^{\pm} \middle| \Phi^m \right\rangle$$

smaller than 10^{-3}

↓

Garbage box

BKN

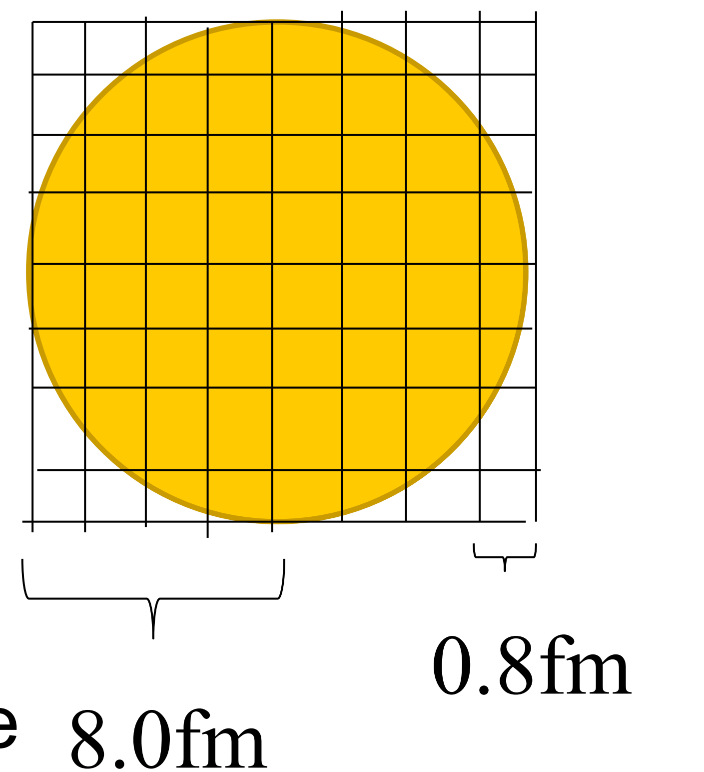


Numerical detail

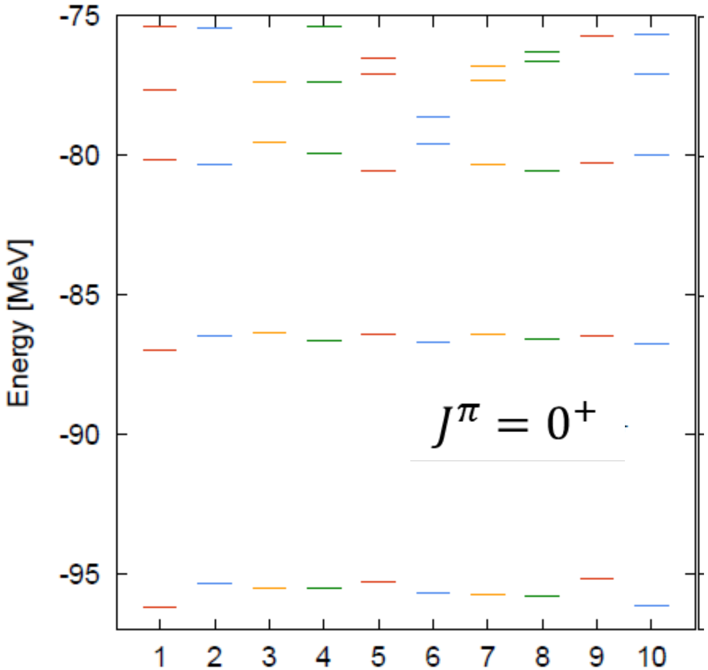
- Three-dimensional (3D) Cartesian mesh
  - Mesh size: 0.8 fm
  - All the mesh points inside the sphere of radius of 8 fm
- Euler angles
  - Discretization

$(\alpha,\beta,\gamma)=(18,30,18)$ points

- Numerical difficulties
  - Limiting number of SD
  - 50 Slater determinantns
  - About 10 h computation time with the use of 512 processors

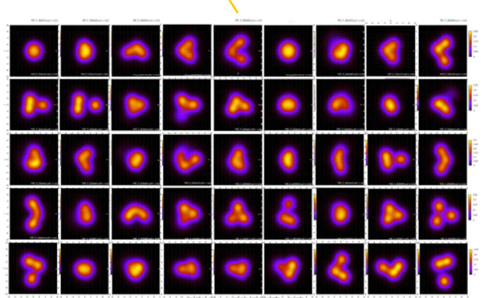


How *complete* is the calculation?

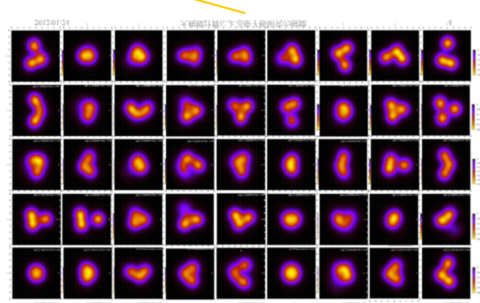


- Ten different sets of Slater determinants, generated with different random numbers.
- Low-energy spectra within several hundred keV
- Transition strength within about 10 %

^{12}C



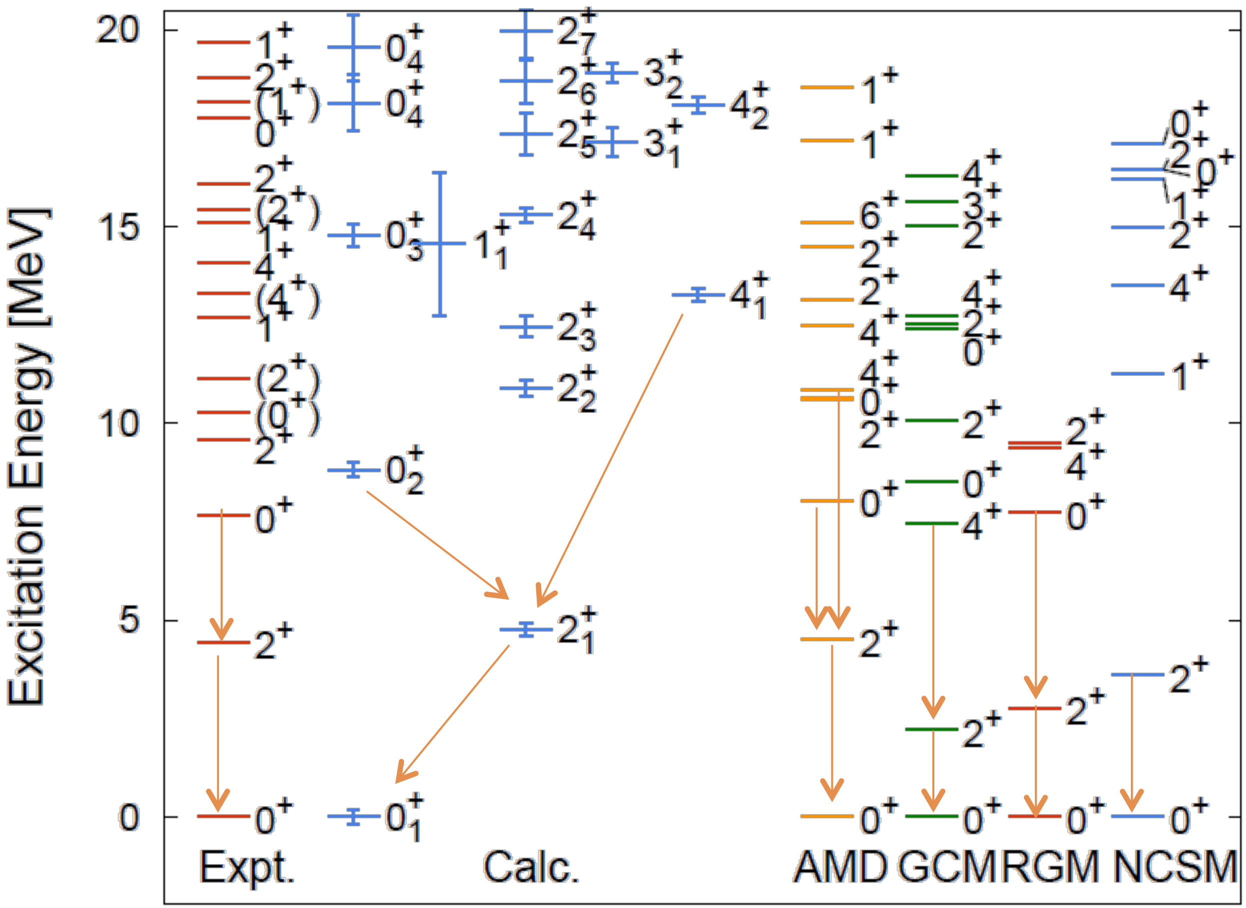
,



, …….(10 sets)

^{12}C (Sly4)

Exp: M. Chernykh *et al.*, PRL 98,032501 (2007)
AMD: Y. Kanada-En'yo, PTP117,655(2007)
GCM: E. Uegaki, *et al.*, PTP57,4 (1977)1262
RGM: M. Kamimura, NPA351,456-480(1981)
NCSM : P. Navrátil and W. E. Ormand, PRC 68, 034305 (2003)



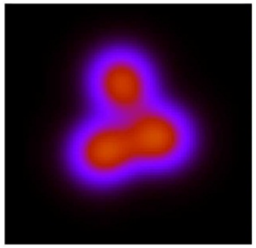
B(E2) in units of e^2fm^4

Calculation assuming three-alpha clusters

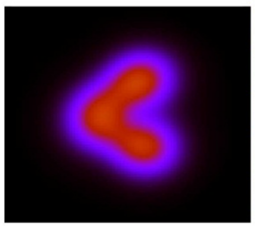
Tuning of the interaction

POSITIVE parity

Hoyle state : 0_2^+



41.2%



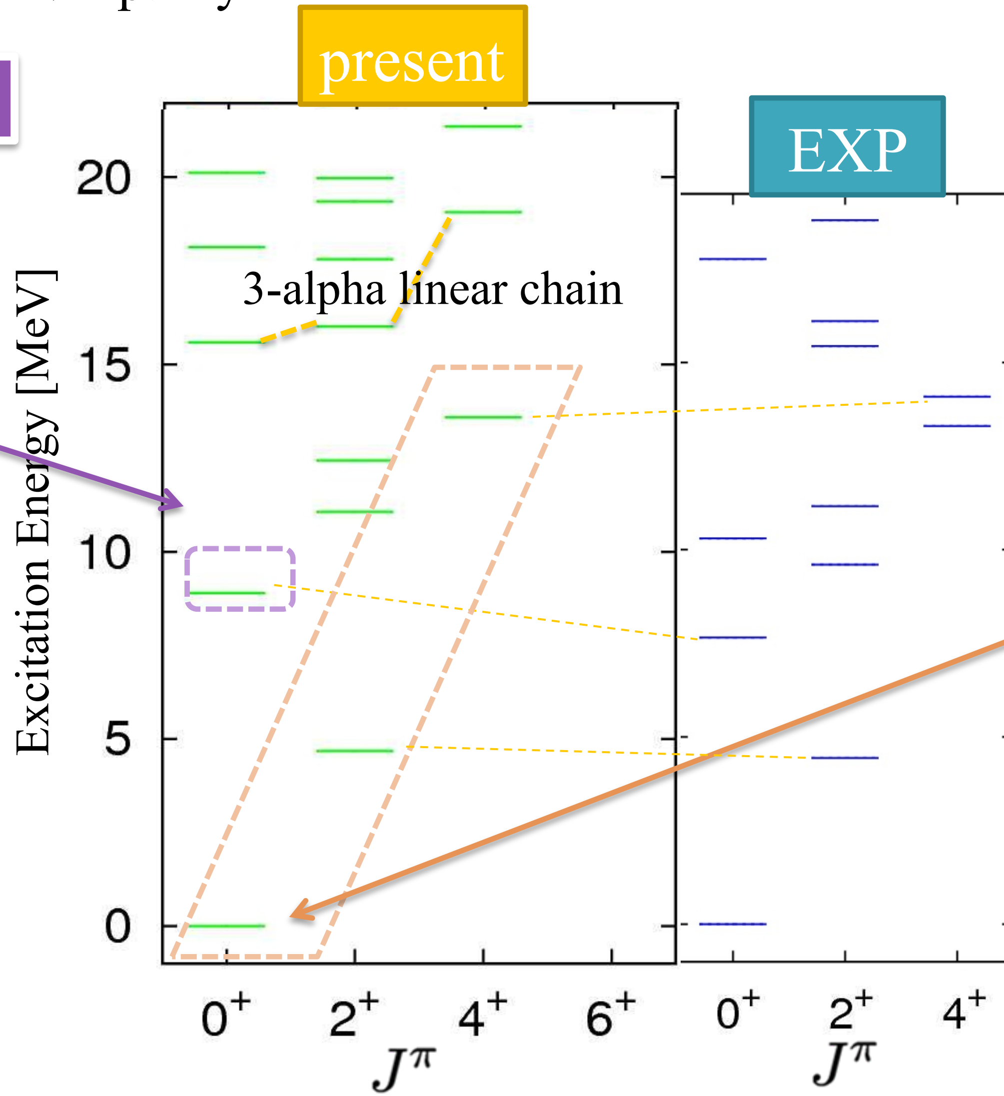
36.1%

31.7%

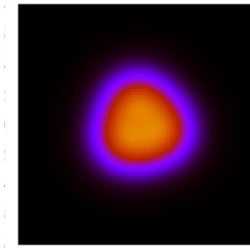
28.9%

⋮

superposition of many SDs



Ground state



0_1^+

89.8%

86.9%

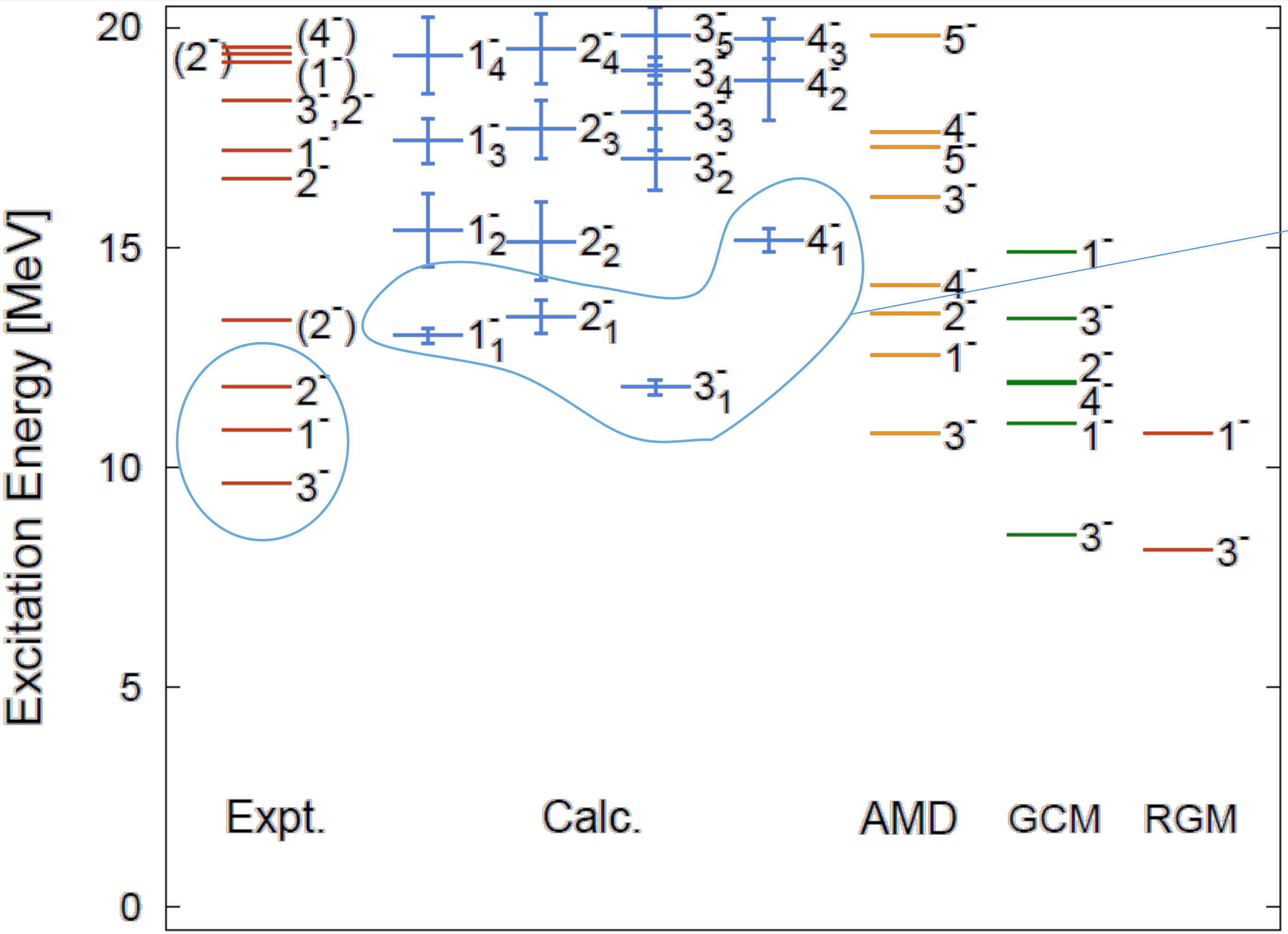
86.2%

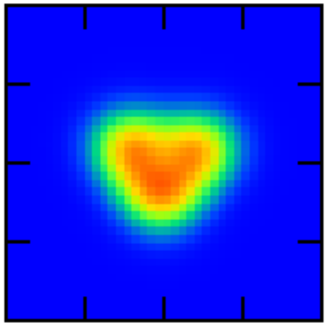
⋮

70% for HF state

- ✓ Correlation energy is 5 MeV
- ✓ Hoyle state is around 9 MeV
- ✓ Ground-state rotational band

^{12}C Negative-parity excited states





Overlap

$K^{\pi} = 1^{-}$

$1_1^- : 77\%$

$2_1^- : 75\%$

$K^{\pi} = 3^{-}$

$3_1^- : 81\%$

$4_1^- : 76\%$

Reliable results for the lowest state in each J^{π}

Similar to the AMD result

Hoyle state

Radius

J^π	present	AMD	FMD	3αRGM	BEC	3αGCM	
0_1^+	2.53 ± 0.03	2.53	2.39	2.40	2.40	2.40	
0_2^+	2.72 ± 0.003	3.27	3.38	3.47	3.83	3.40	Hoyle state
0_3^+	3.15 ± 0.02	3.98	4.62			3.52	Linear-chain state
2_1^+	2.61 ± 0.002	2.66	2.50	2.38	2.38	2.36	

Exp, FMD: M. Chernykh *et al.*, PRL 98,032501 (2007)
AMD: Y. Kanada-En'yo, PTP117,655(2007)
GCM: E. Uegaki, *et al.*, PTP57,4 (1977)1262
RGM: M. Kamimura, NPA351,456-480(1981)

Monopole transition

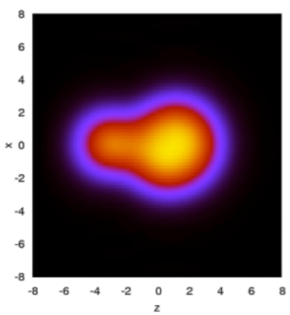
$$M(E0;0_1^+ \rightarrow 0_2^+) = 4.5 \pm 0.2 \text{ e fm}^2$$

5.4 ± 0.2 Experiment

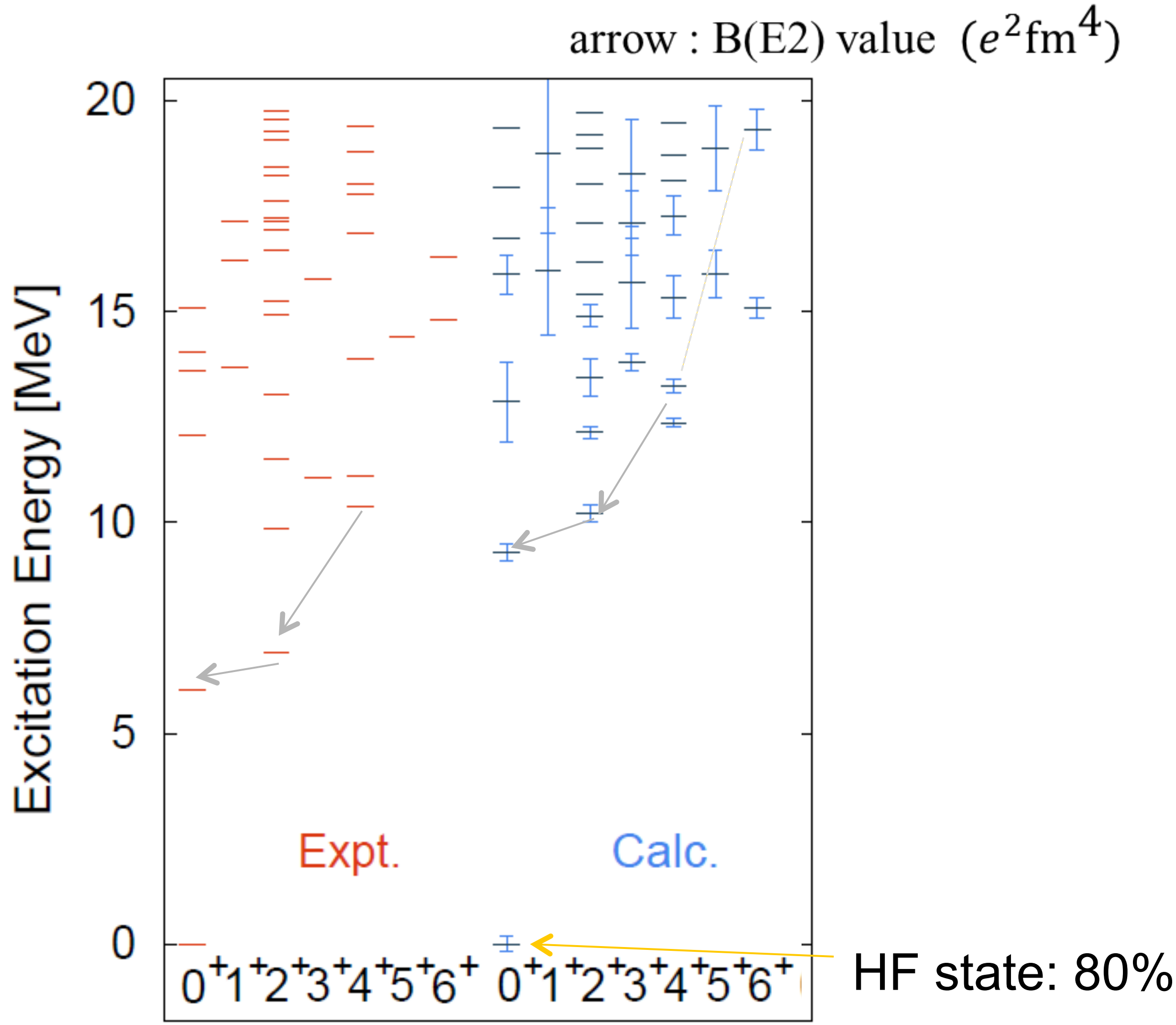
$6.5 - 6.7$ Other cal. based on the gaussian anzats

^{16}O POSITIVE parity

$^{12}C + \alpha(?)$ like

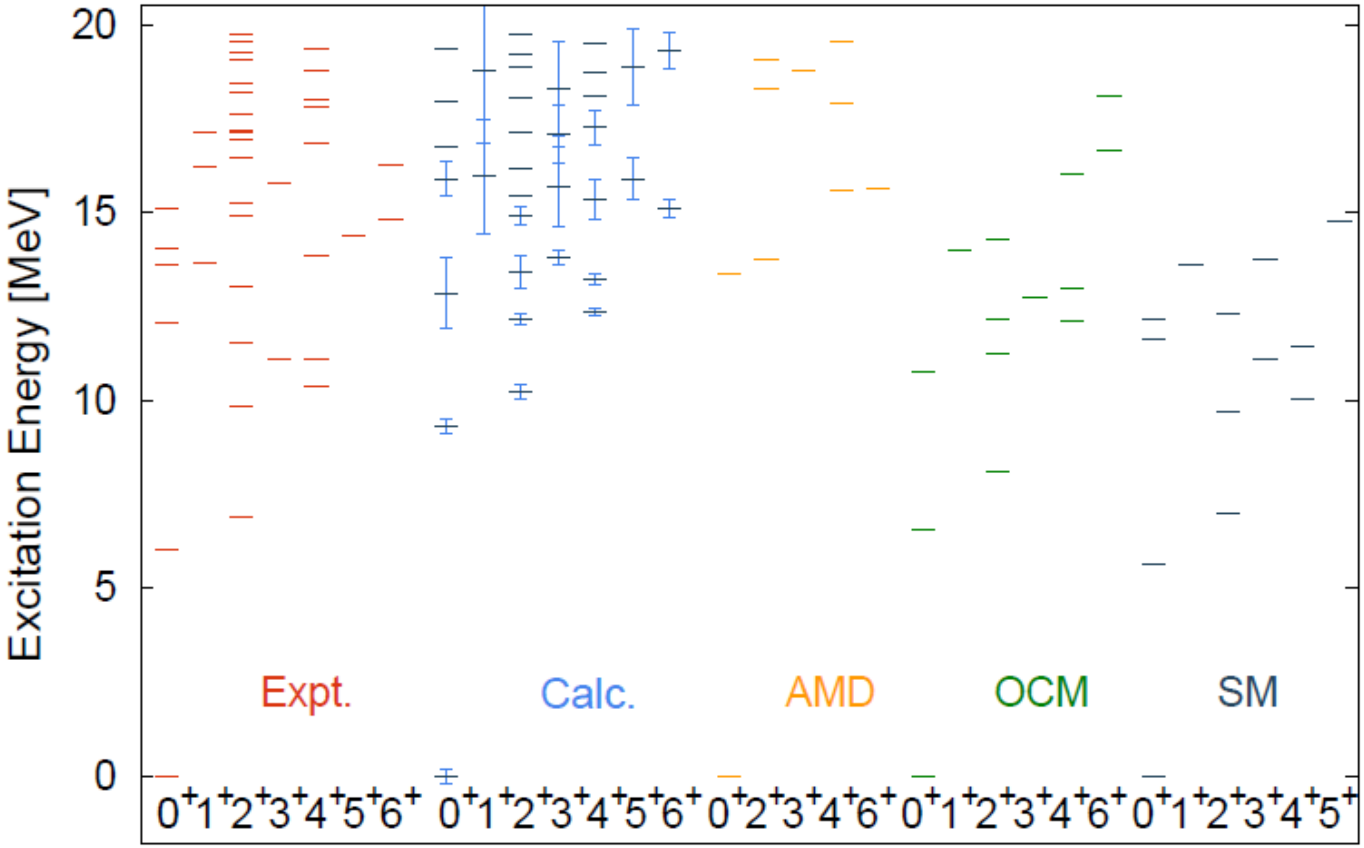


0_2^+ : 67.0%
2_1^+ : 66.4%
4_2^+ : 43.1%



✓ correlation energy is about 3 MeV

^{16}O Positive-parity states



Phenomenological fitting involved

Expt. : D. Tilley, et al., Nucl. Phys. A 636, 249 (1998)

AMD : N. Furutachi, et al., Prog. Thoer. Phys. 119, 403 (2008)

OCM: Y. Suzuki, Prog. Theor. Phys, 55, 1751 (1976)

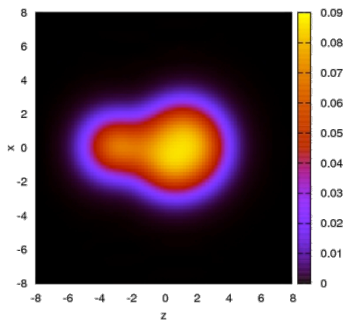
SM : W. C. Haxton and C. Johnson, Phys. Rev. Lett. 65, 1325 (1990)

Excitation energies are significantly lower than AMD.

^{16}O NEGATIVE parity

arrows : B(E2) (e^2fm^4)

^{12}C + α(?) like



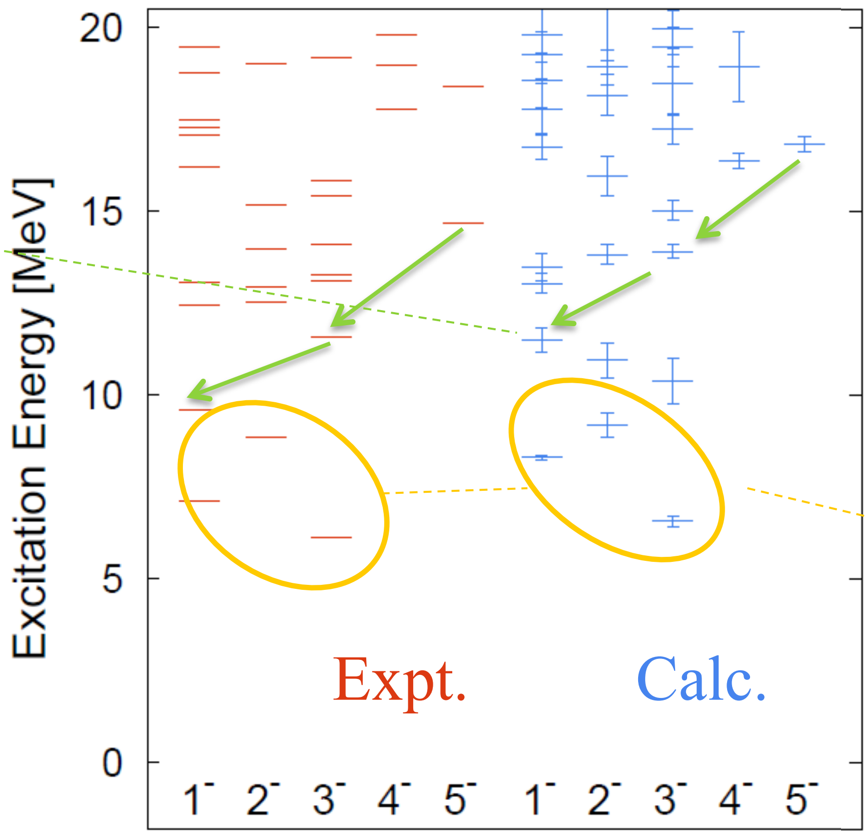
parity doublet partner

$K^\pi = 0^-$

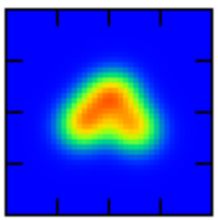
$1_2^- : 67\%$

$3_3^- : 45\%$

$5_1^- : 58\%$

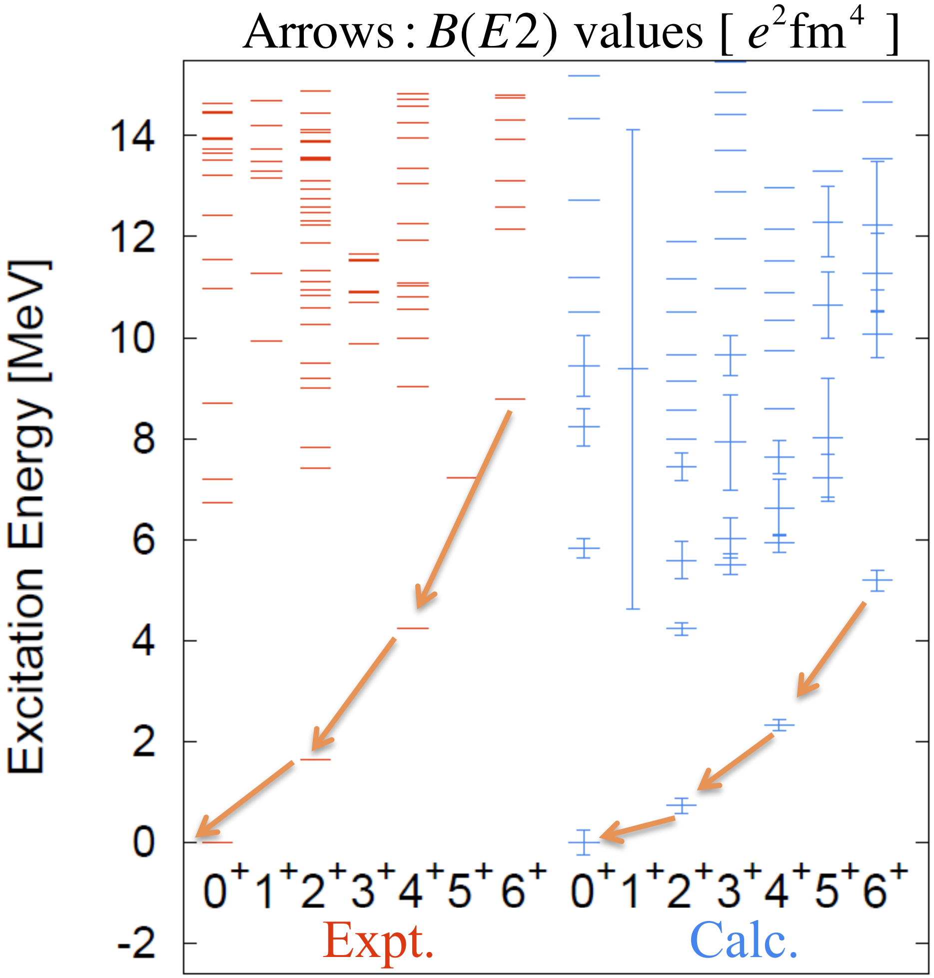


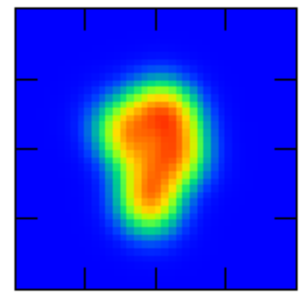
1p1h excitations



✓ particle-hole excitation is good agreement with experimental values

^{20}Ne: Positive-parity states

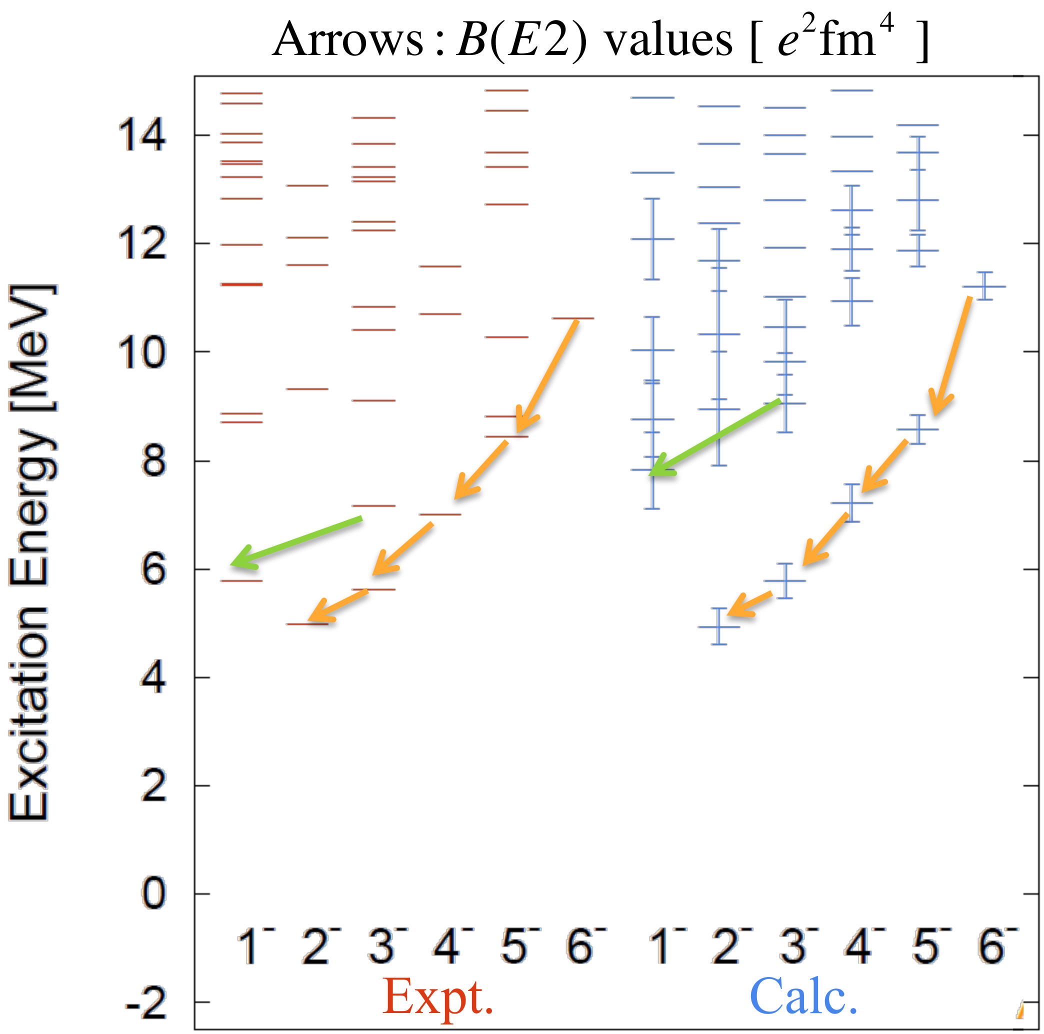


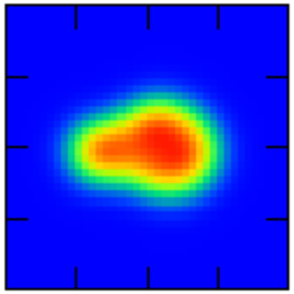


Hartree-Fock state: 80%

- Well reproduce B(E2) values
- Too large moment of inertia

^{20}Ne: Negative-parity states



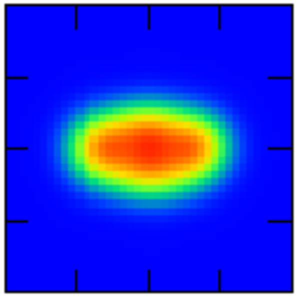


Overlap

$1_1^- : 60\%$

$3_2^- : 60\%$

$K^\pi = 2^-$



$2_1^- : 91\%$

$3_2^- : 87\%$

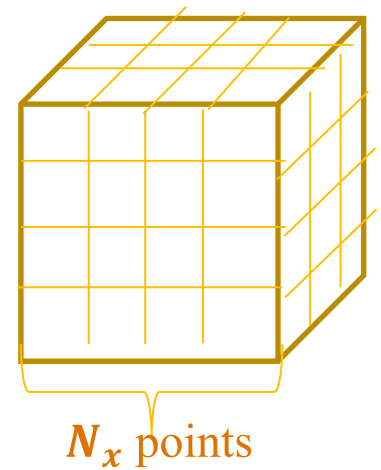
$4_4^- : 88\%$

$5_1^- : 78\%$

$6_1^- : 77\%$

$(0p)^{-1}(sd)^5$ structure

Computational cost of finite range interaction



■ Skyrme interaction

$$\left\langle \Phi \middle| \widehat{V_{t0}^{F}} \middle| \Phi \right\rangle = -\frac{t_0}{2} x_0 \sum_{i,j} \langle \phi_i \phi_j | \delta(\vec{r}_1 - \vec{r}_2) \hat{P}_r \hat{P}_\sigma \hat{P}_\tau | \phi_i \phi_j \rangle$$

$$= -\frac{t_0}{2} x_0 \sum_{\tau} \int d\vec{r}\, \rho(\vec{r}\,)^2 \qquad \rho(\vec{r}) = \sum_{i,\sigma} \phi_i^*(\vec{r},\sigma)\phi_i(\vec{r},\sigma)$$

Computational cost : $N_x^3 \times \underline{N_i}$

\# of orbits

■ Gogny interaction

$$\left\langle \Phi \middle| \widehat{V_{W_l}^{F}} \middle| \Phi \right\rangle = -\frac{W_l}{2} \sum_{\tau} \int d\vec{r} \int d\vec{r}\,'\rho(\vec{r}\sigma, \vec{r}\,'\sigma')\, \rho(\vec{r}\,'\sigma', \vec{r}\sigma) \exp\{-(\vec{r} - \vec{r}\,')^2/\mu_l^2\}$$

$$\rho(\vec{r}\sigma, \vec{r}\,'\sigma') \equiv \sum_{i,\sigma} \phi_i^*(\vec{r},\sigma)\phi_i(\vec{r}\,',\sigma')$$

Computational cost : $N_x^6 \times N_i$

- ✓ Same scaling of orbit as the case of Skyrme interaction
- ✓ scaling of space is power of two

Method 1: finite spherical lattice

W_l Fock term

$$V_{W_l}^F = -\frac{W_l}{2}\sum_\tau \int d\vec{r} \int d\vec{r}' \rho(\vec{r}\sigma,\vec{r}'\sigma')\,\rho(\vec{r}'\sigma',\vec{r}\sigma)\exp\{-(\vec{r}-\vec{r}')^2/\mu_l^2\}$$

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') \equiv \sum_{i,\sigma} \phi_i^*(\vec{r},\sigma)\underline{\phi_i(\vec{r}',\sigma')}$$

The range of Gogny interaction is about 4 fm.

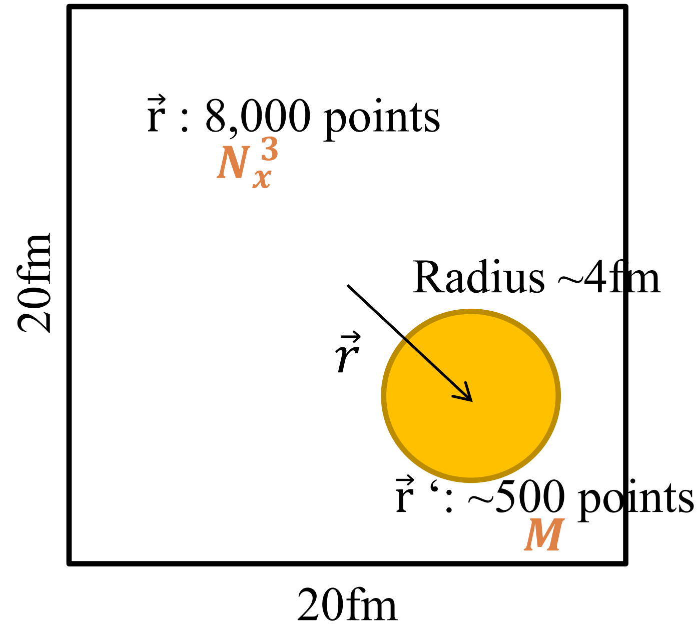
it is sufficient to integrate r' inside 4fm sphere.

Numerical cost : $N_x^3 \times M \times N_i$

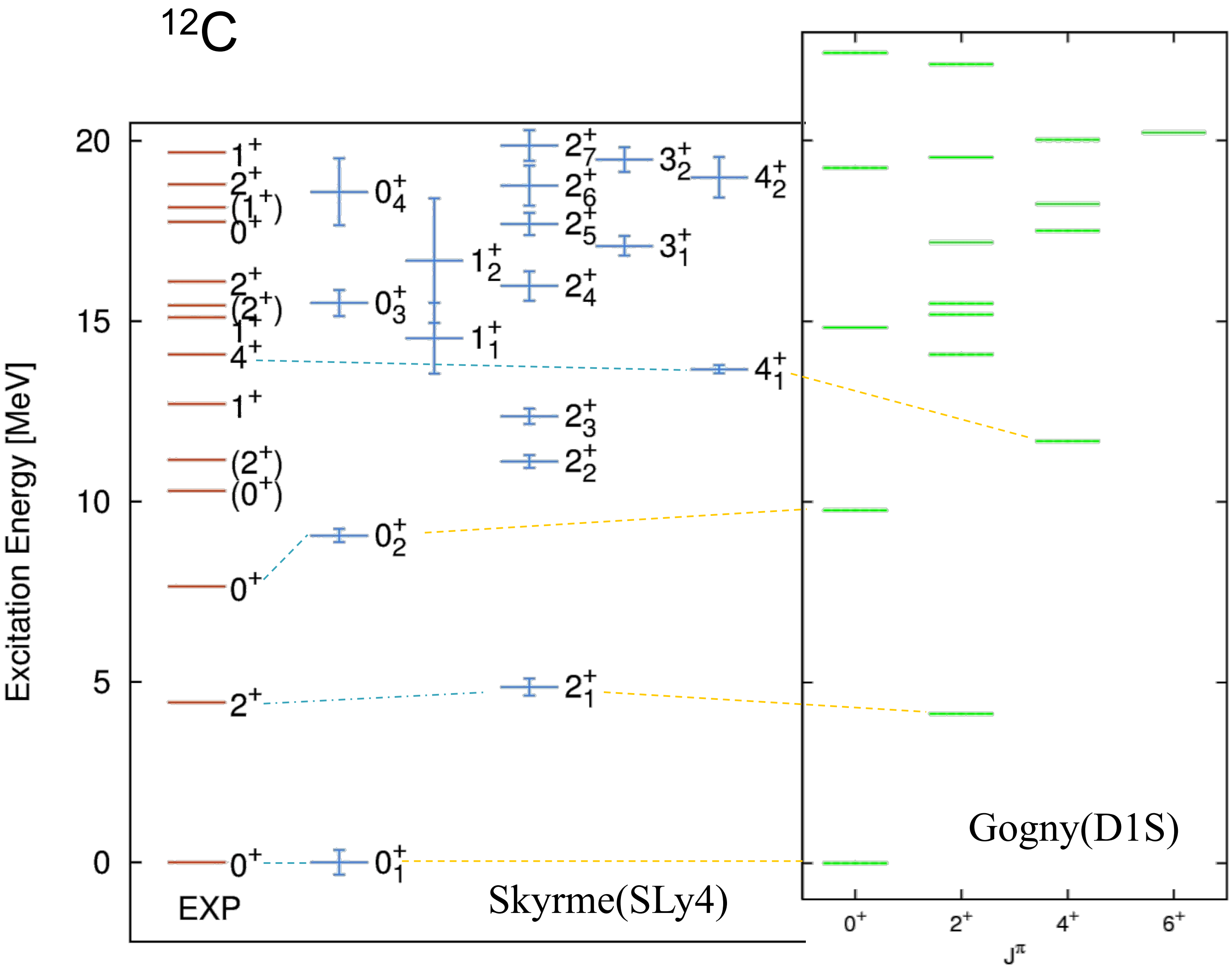
cf. Skyrme interaction

$N_x^3 \times N_i$

✓ Same scaling as the case of Skyrme interaction, except M



positive parity



CPU time

Integral points:
(α, β, γ)=(18, 20, 18)
512 core x 9h
31 SDs

7.5 times

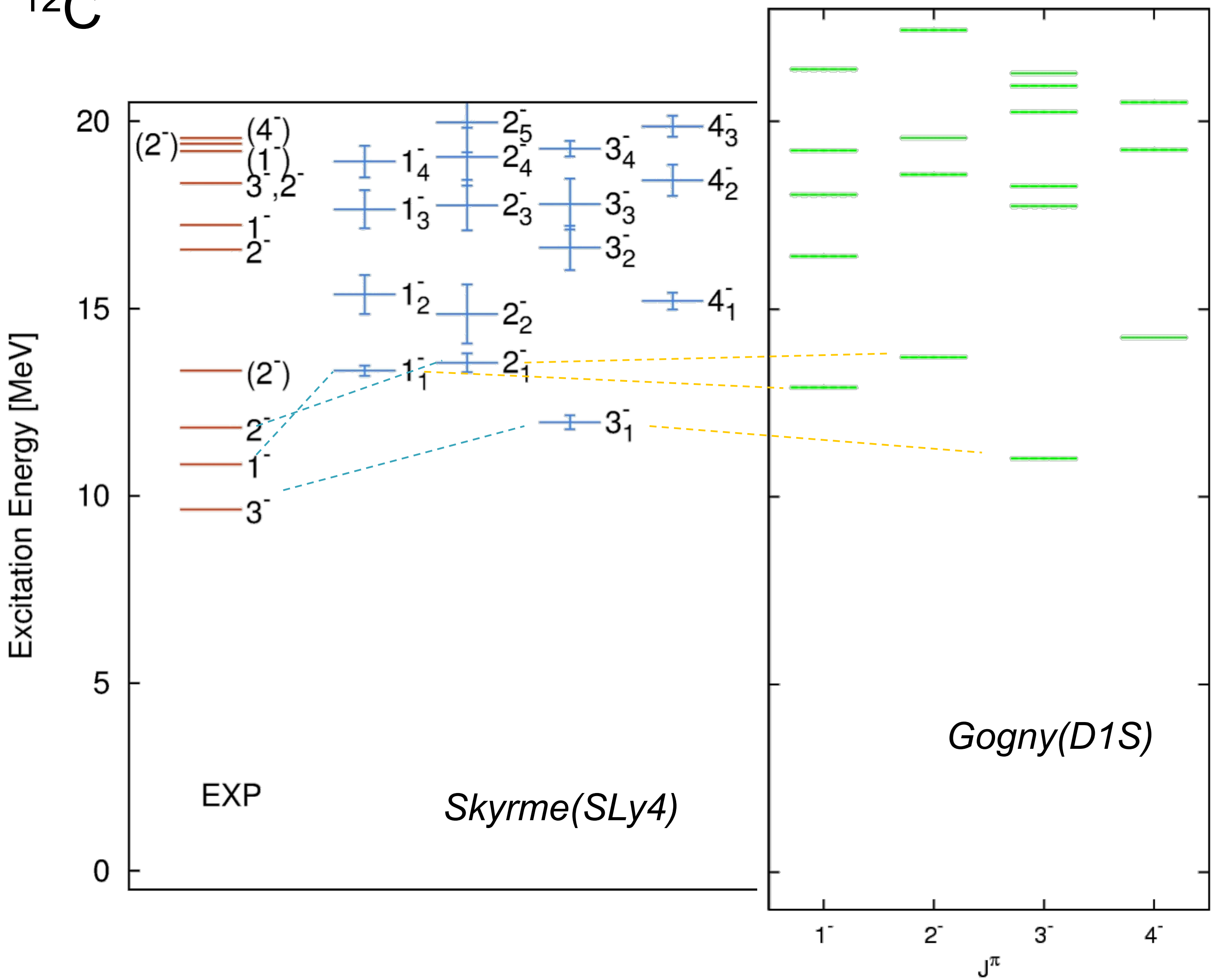
cf. Skyrme
(α, β, γ)=(18, 30, 18)
512 core x 1.8h
45 SDs

SR16000@YITP

- ✓ Computational cost is times
- ✓ Energy spectrum is almost same

negative parity

^{12}C



✓ *Energy spectrum is almost same*

Summary

Shinohara et al, PRC 74, 054315 (2006)
Fukuoka et al, PRC 88, 014321 (2013)

- Complete low-lying spectroscopy with the Skyrme Hamiltonian
- Capable of describing various excited states in a unified way

Problems

- 2^{nd} 0^+ state in ^{16}O
  - Energy too high by about 3 MeV
  - B(E2) Underestimated
  - Center of mass? Weak-coupling phenomena?
- Moment of inertia of ^{20}Ne
  - Too large
  - Pairing?
- Hoyle state in ^{12}C
  - Too small radius? Effect of the spin-orbit interaction?

Future issues

- Coordinate-space calculation with finite-range interaction
- Reaction studies