Stochastic generation of low-energy configurations and configuration mixing calculation

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INT workshop,   April 15, 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, TN, 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.

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

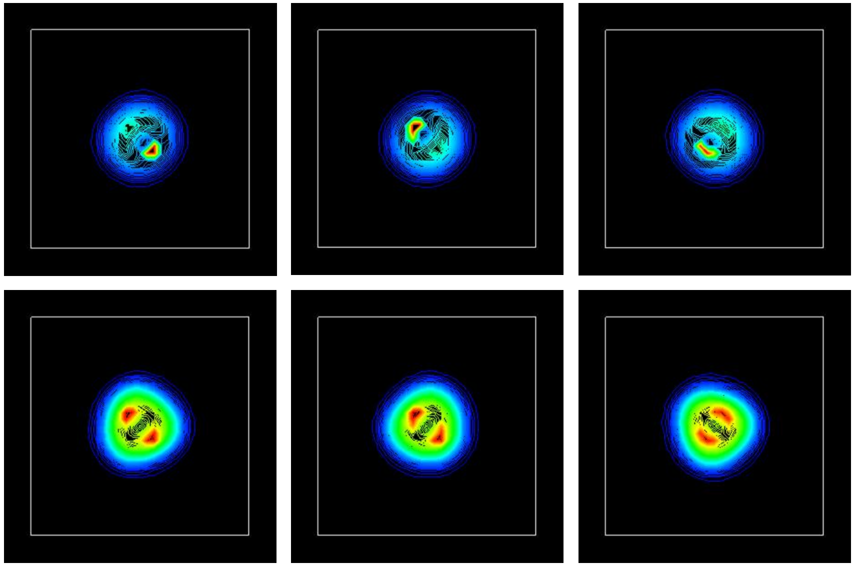
$$\begin{matrix} H^{J\pm}_{nK,n'K'} \\ N^{J\pm}_{nK,n'K'} \end{matrix} = \left\langle \Phi^n \left| \begin{Bmatrix} H \\ 1 \end{Bmatrix} P^\pm P^J_{KK'} \right| \Phi^{n'} \right\rangle$$

Variational approach

^{16}O
BKN interaction
Two Parity-projected Slater determinants

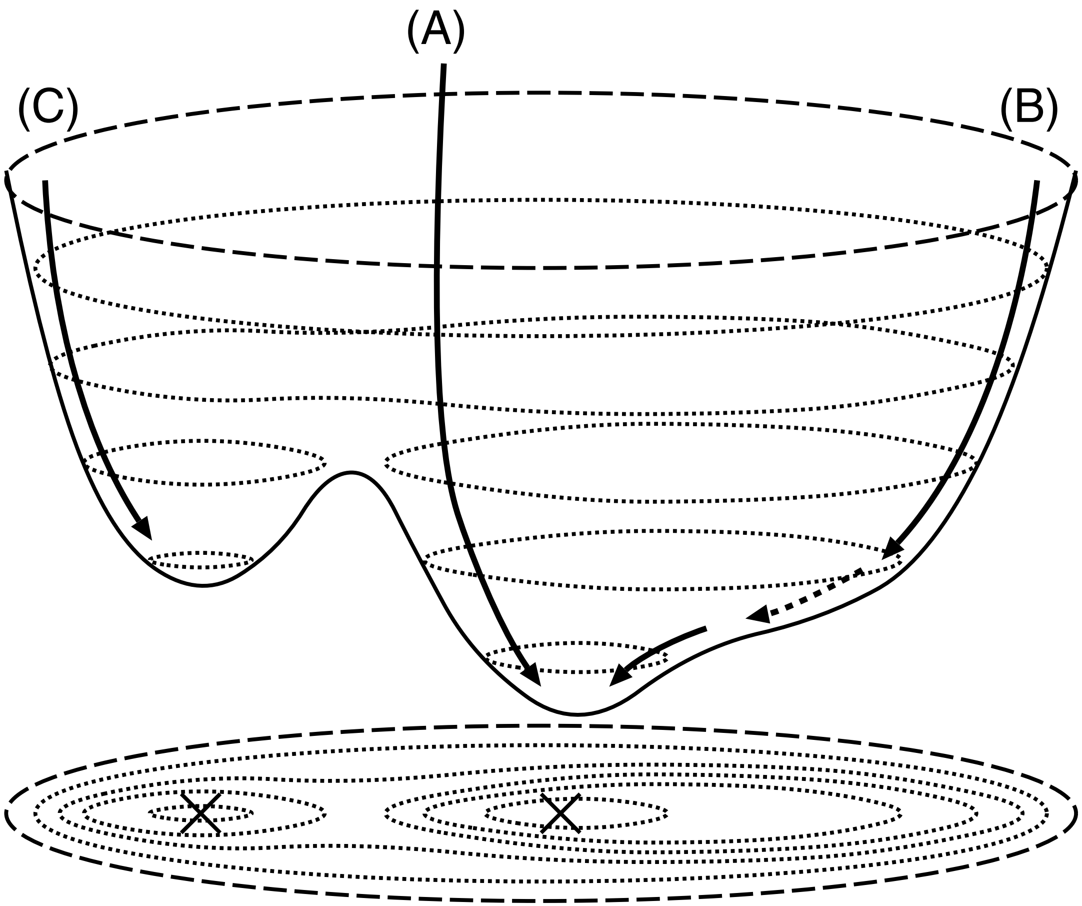
$$\Psi^{1(+)} = 0.72\,\Phi^{1(+)} - 0.24\,\Phi^{2(+)}$$
$$\Psi^{2(+)} = 1.12\,\Phi^{1(+)} - 1.40\,\Phi^{2(+)}$$

	E
Variational	−142.54
PPHF	−133.35



“Singular” Slater determinants

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

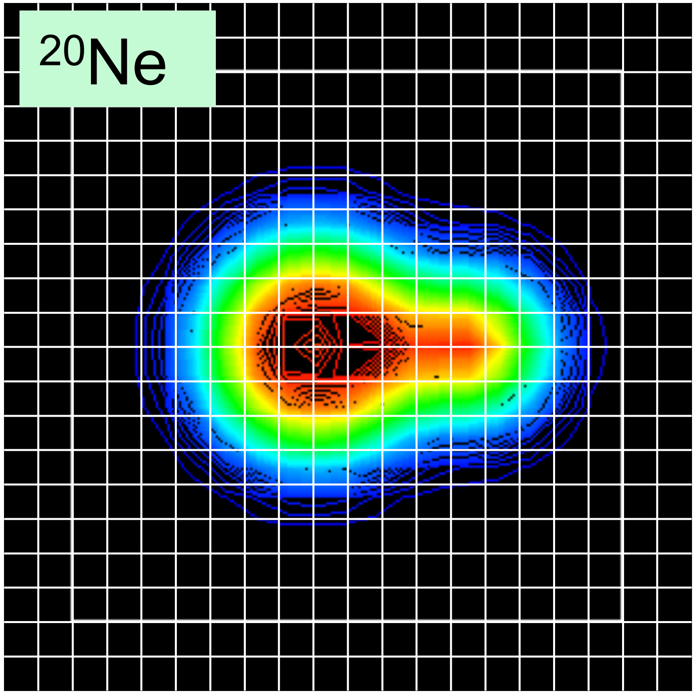
Generation of basis states: Imaginary-time method in 3D coordinate space

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

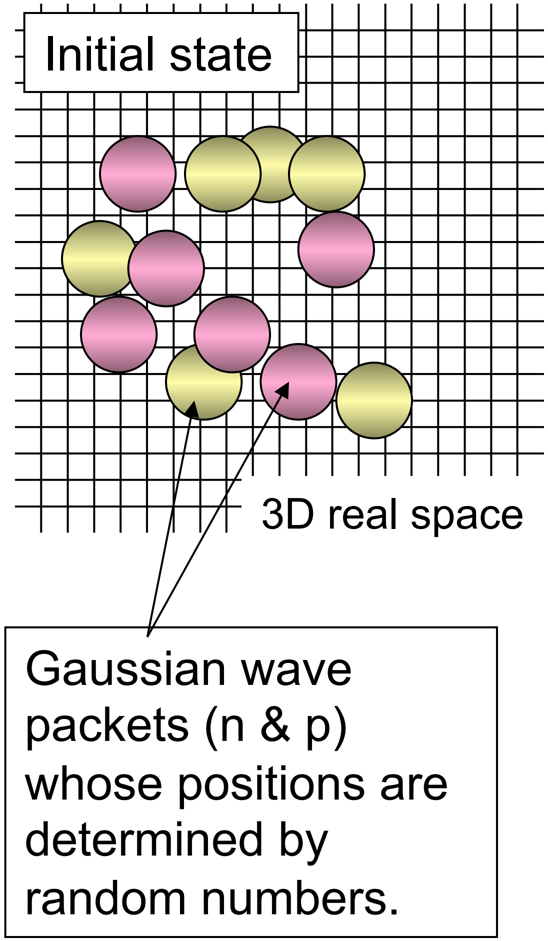


3D space is discretized in lattice

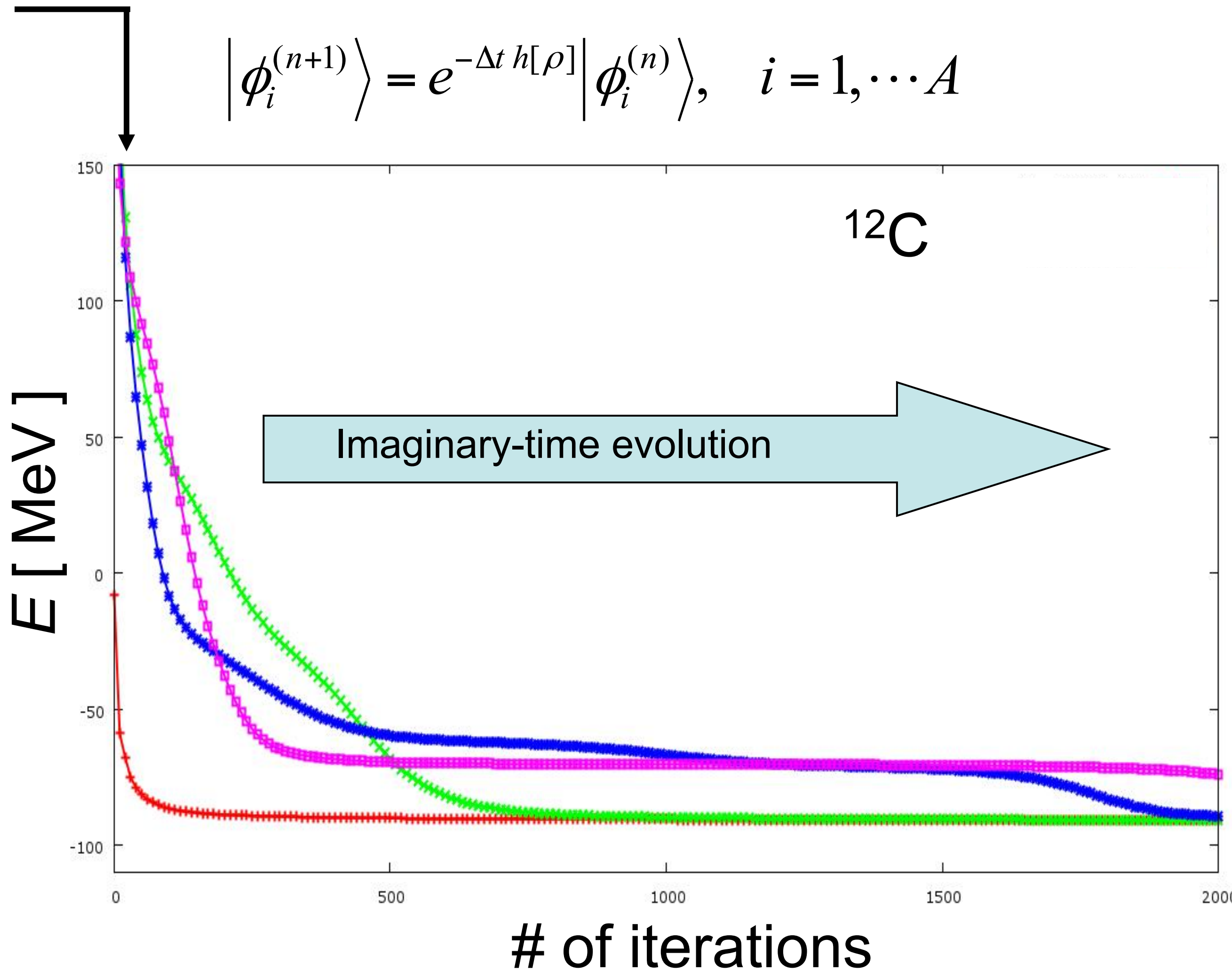
Single-particle orbital:

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

Generation of many S-det’s



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



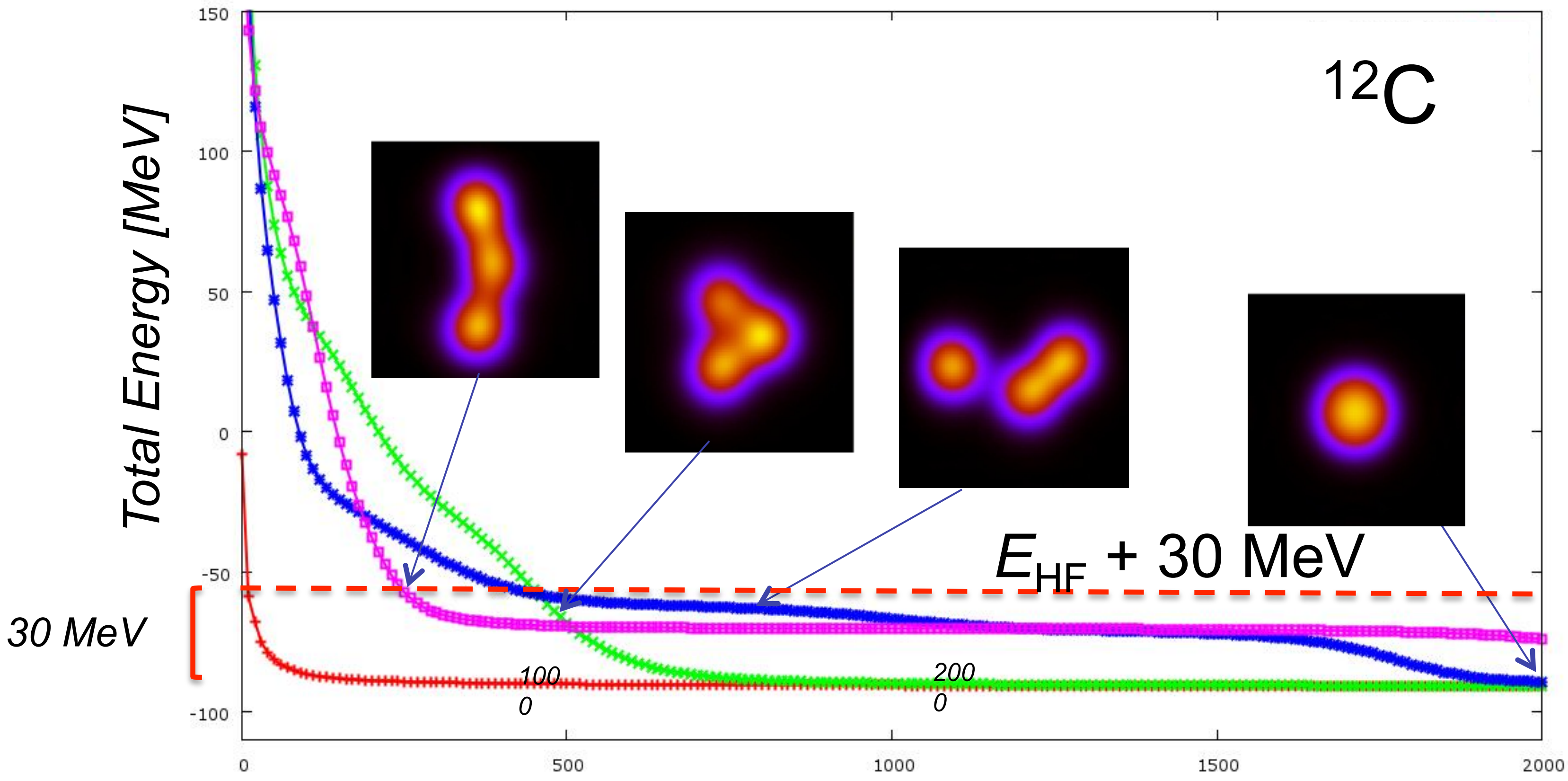
Screening of Slater determinants

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

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

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



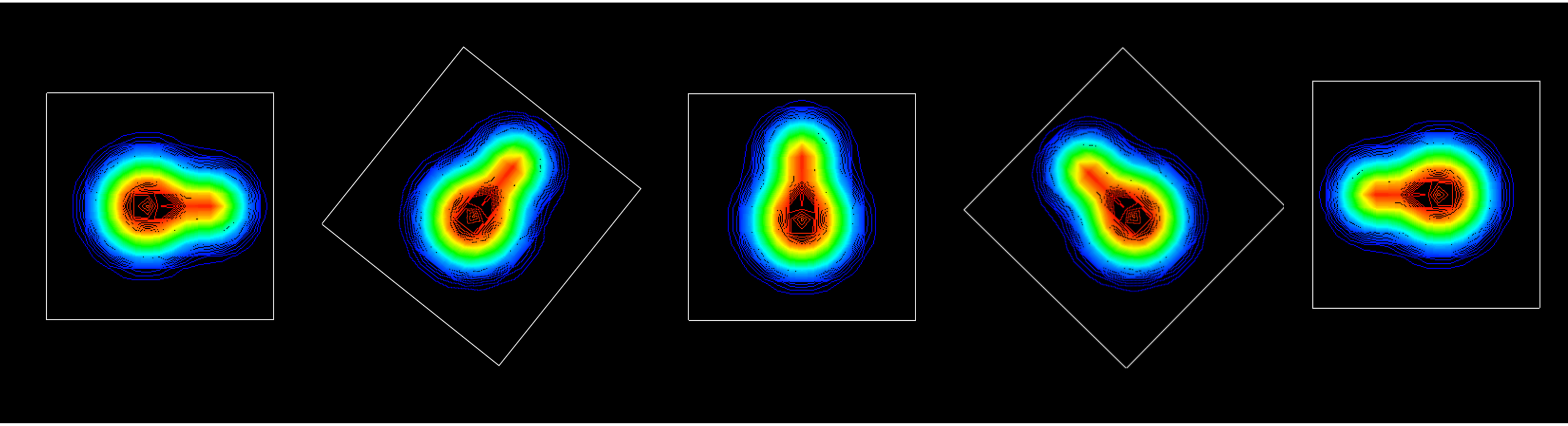
3D angular momentum projection

Parity and angular momentum projected state

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

Parity-projected SD

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



Construct the angular momentum eigenstate
by the explicit 3D rotation

Further Selection …

Eigenvalues of the norm matrix

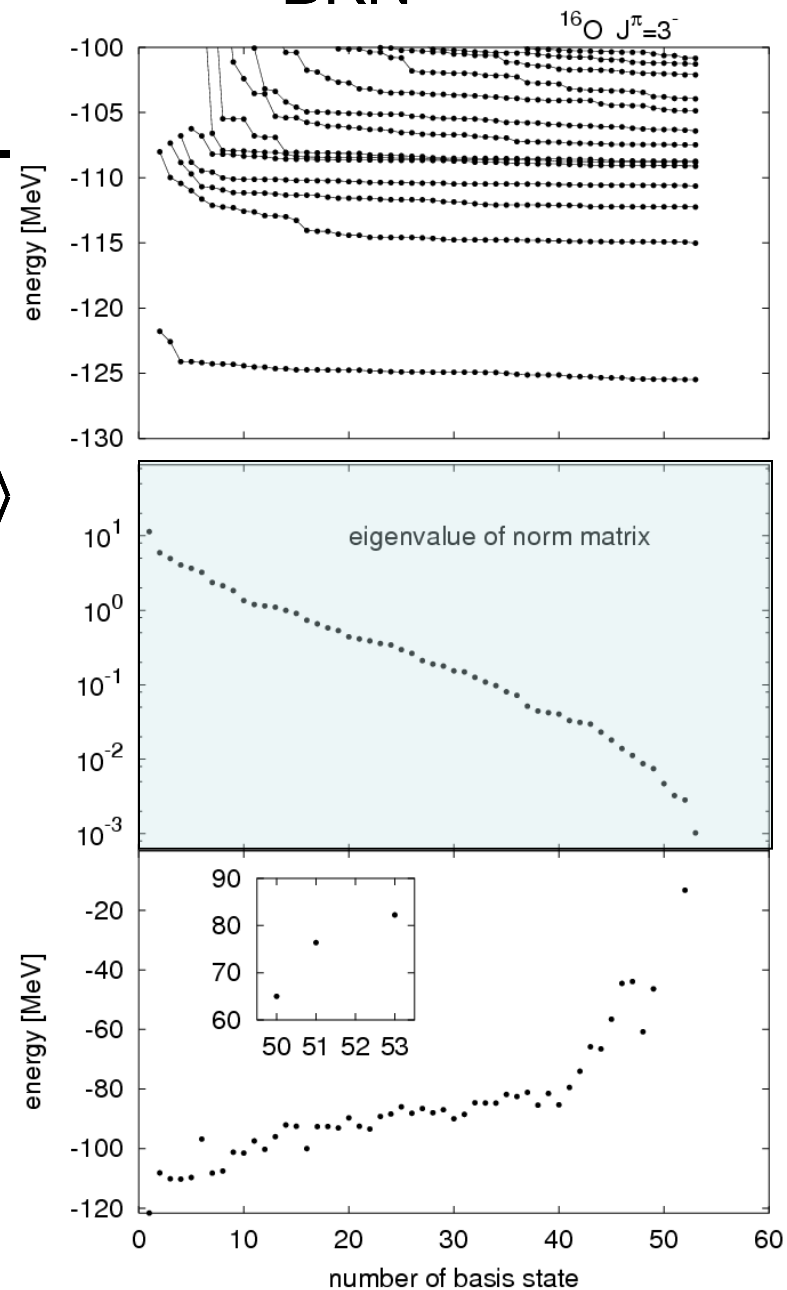
$$N^{J\pm}_{nK,mK'} = \left\langle \Phi^n \middle| P^J_{KK'} P^{\pm} \middle| \Phi^m \right\rangle$$

smaller than 10^{-3}

↓

Garbage box

BKN

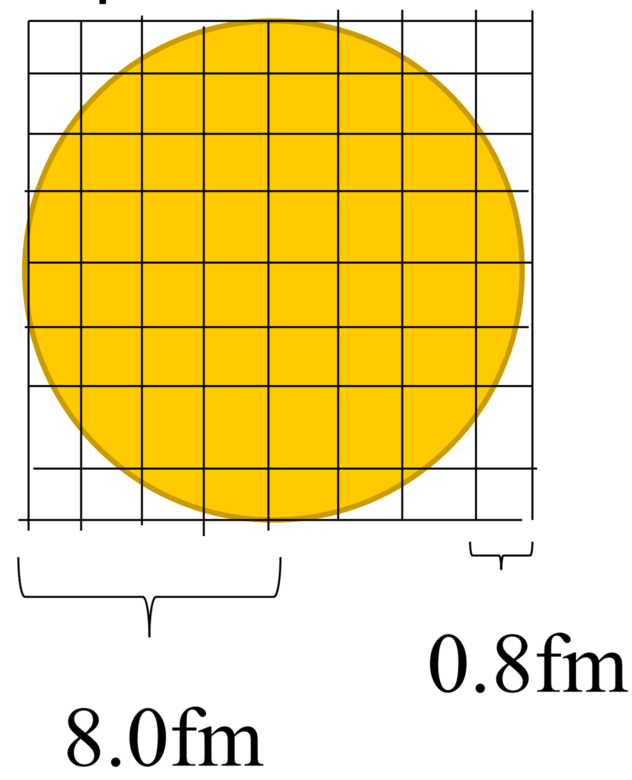


Numerical detail

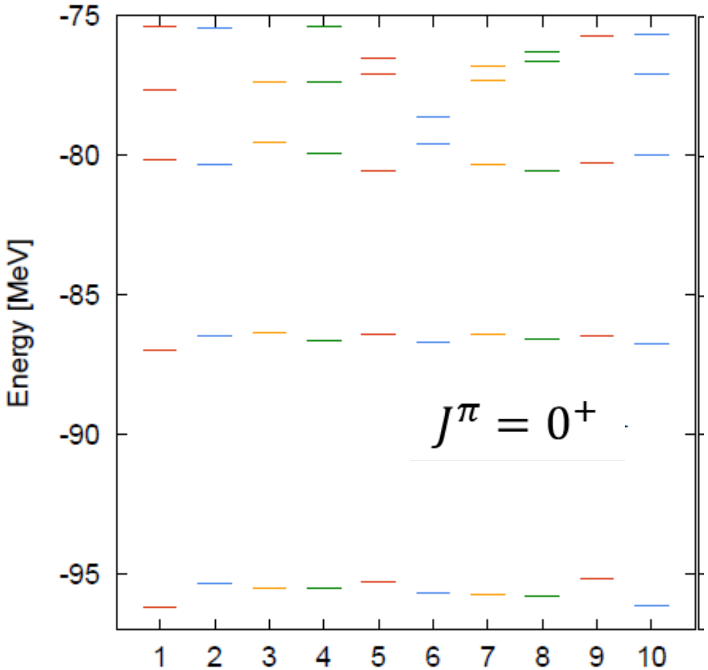
- Three-dimensional (3D) Cartesian mesh
  - Mesh size: 0.8 fm
  - All the mesh points inside the sphere of radius of 8 fm
- Euler angles
  - Discretization

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

- Numerical difficulties
  - Limiting number of SD
  - 50 Slater determinantns

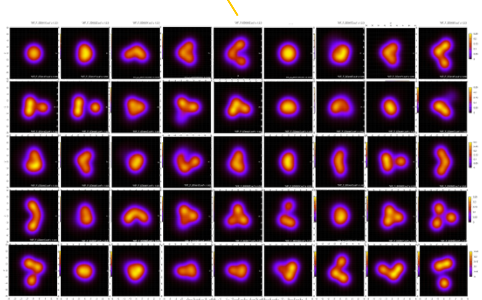


How *complete* is the calculation?

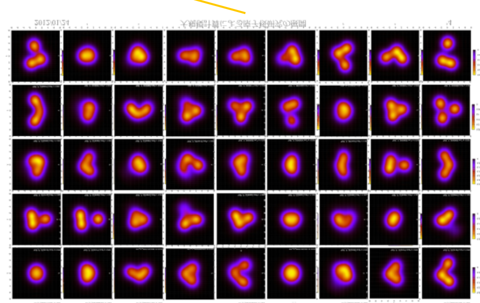


- Ten different sets of Slater determinants, generated with different random numbers.
- Low-energy spectra within several hundred keV
- Transition strength within about 10 %

^{12}C



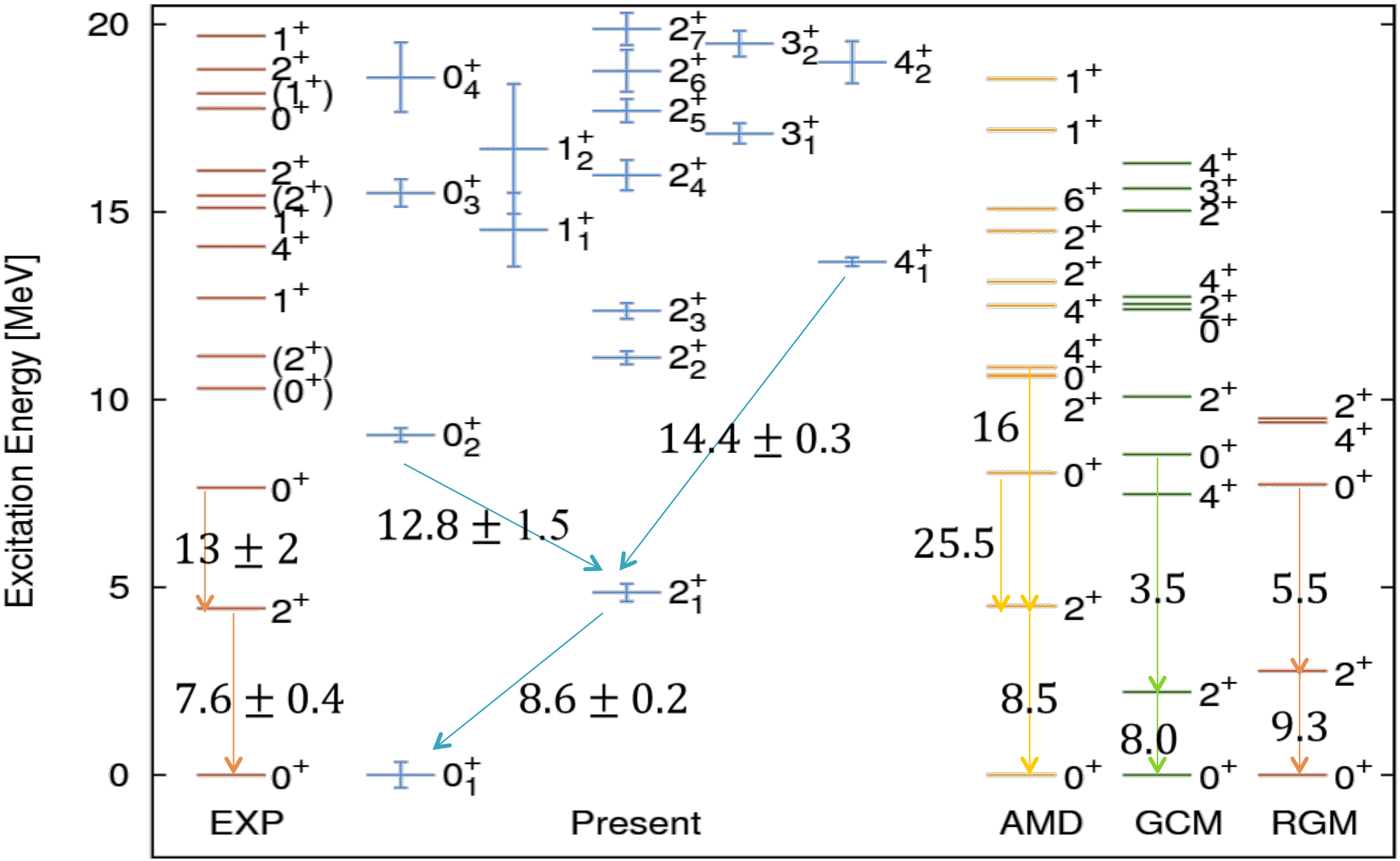
,



, …….(10 sets)

^{12}C (Sly4)

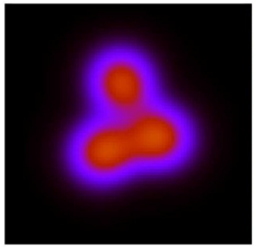
Exp: M. Chernykh *et al.*, PRL 98,032501 (2007)
AMD: Y. Kanada-En'yo, PTP117,655(2007)
GCM: E. Uegaki, *et al.*, PTP57,4 (1977)1262
RGM: M. Kamimura, NPA351,456-480(1981)



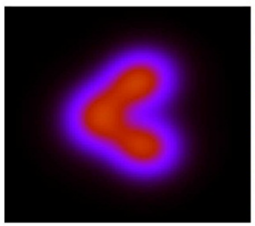
B(E2) in units of e^2fm^4

POSITIVE parity

Hoyle state : 0_2^+



41.2%



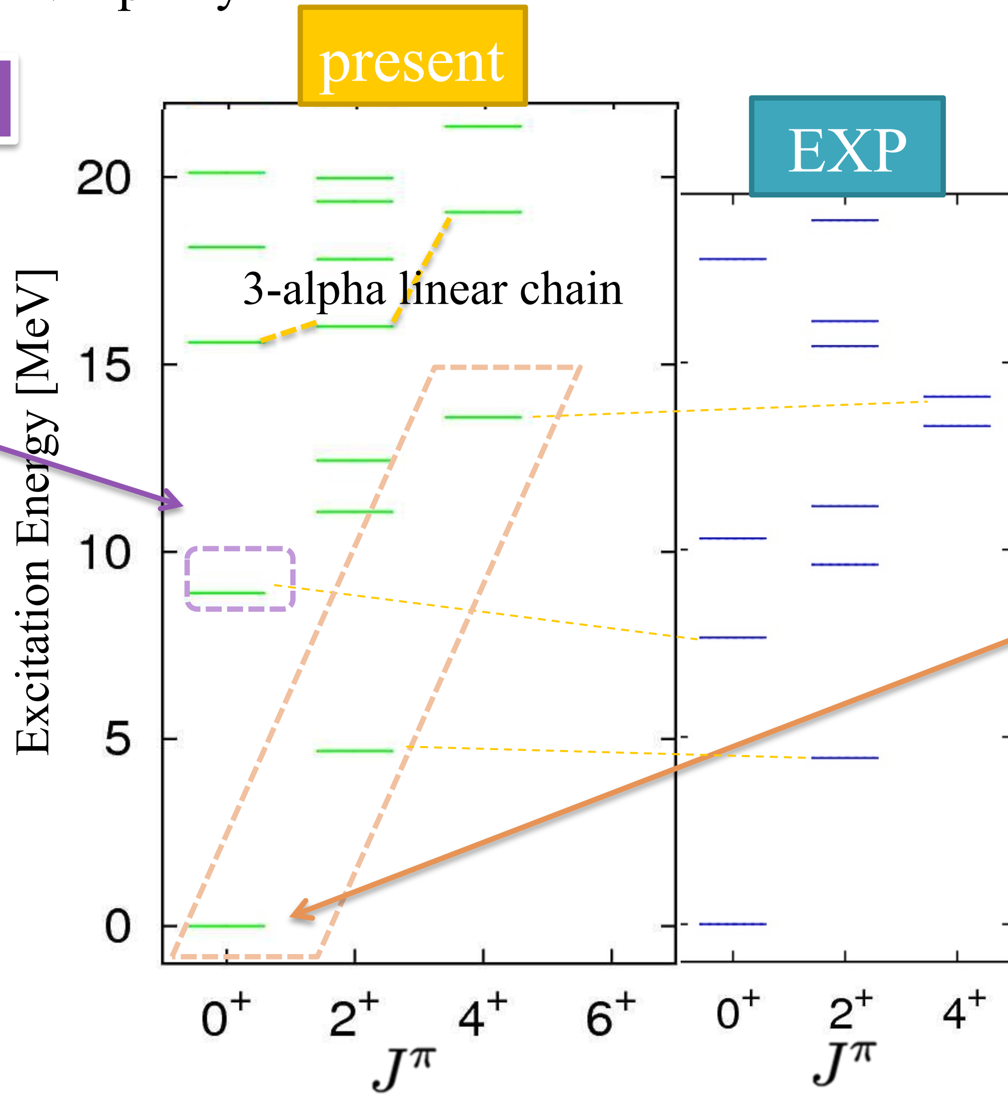
36.1%

31.7%

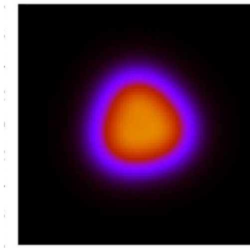
28.9%

⋮

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

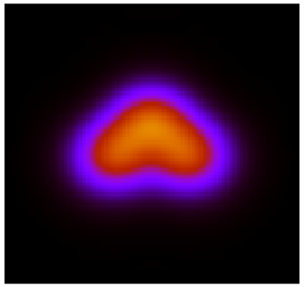
Radius, B(E2), B(E3), M(E0)

J^π	EXP	present
0_1^+	2.31(2)	2.52±0.01
0_2^+		2.73±0.02
0_3^+		3.20±0.05
2_1^+		2.60±0.01
	fm	fm

Linear-chain state

	Transitions	Exp	Cal
	$B(E2; 2_1^+ \to 0_1^+)$	7.6±0.4	8.6 ±0.2
	$B(E2; 4_1^+ \to 2_1^+)$		13.4±0.5
	$B(E2; 0_2^+ \to 2_1^+)$	13±2	13.6±1.2
	$B(E2; 2_2^+ \to 0_2^+)$		0.17±0.23
	$B(E2; 2_3^+ \to 0_2^+)$		5.9±0.7
	$B(E2; 2_4^+ \to 0_2^+)$		10±1
	$B(E2; 2_4^+ \to 0_3^+)$		91±13
e^2fm^4	$B(E2; 4_2^+ \to 2_4^+)$		131±22
e^2fm^6	$B(E3; 3_1^- \to 0_1^+)$	107 ± 14	77 ± 4
efm^2	$M(E0; 0_1^+ \to 0_2^+)$	5.4±0.2	4.5±0.2

^{12}C NEGATIVE parity



Overlap

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

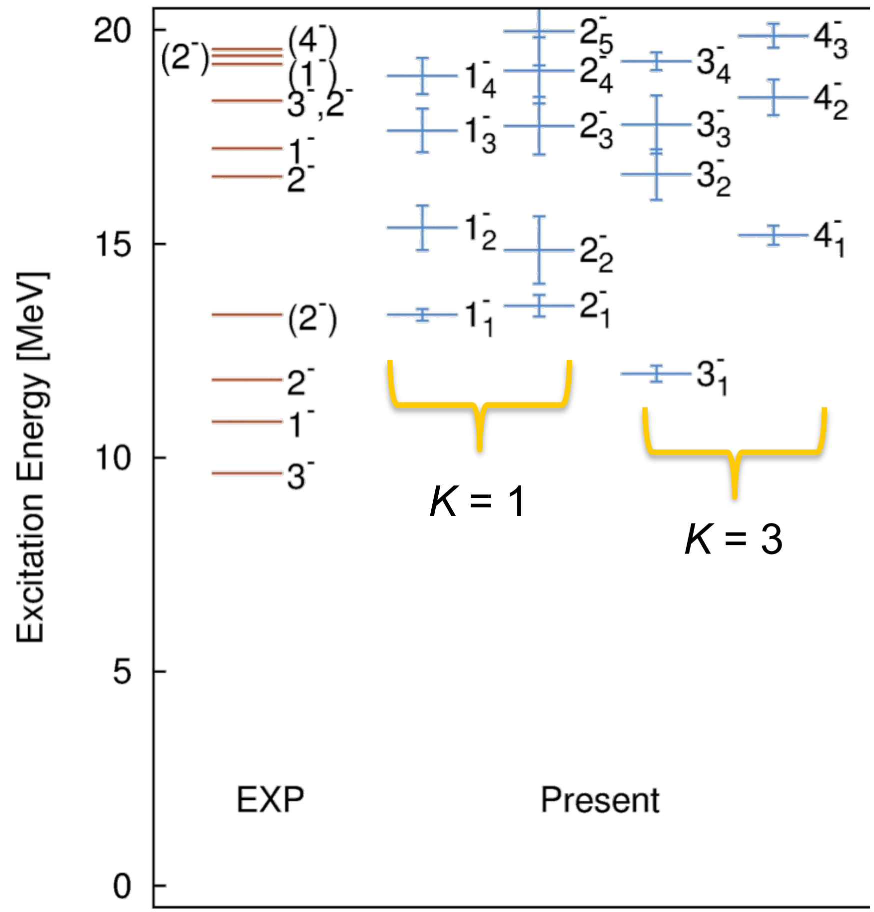
$1_1^- : 85.0\%$

$2_1^- : 73.0\%$

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

$3_1^- : 83.4\%$

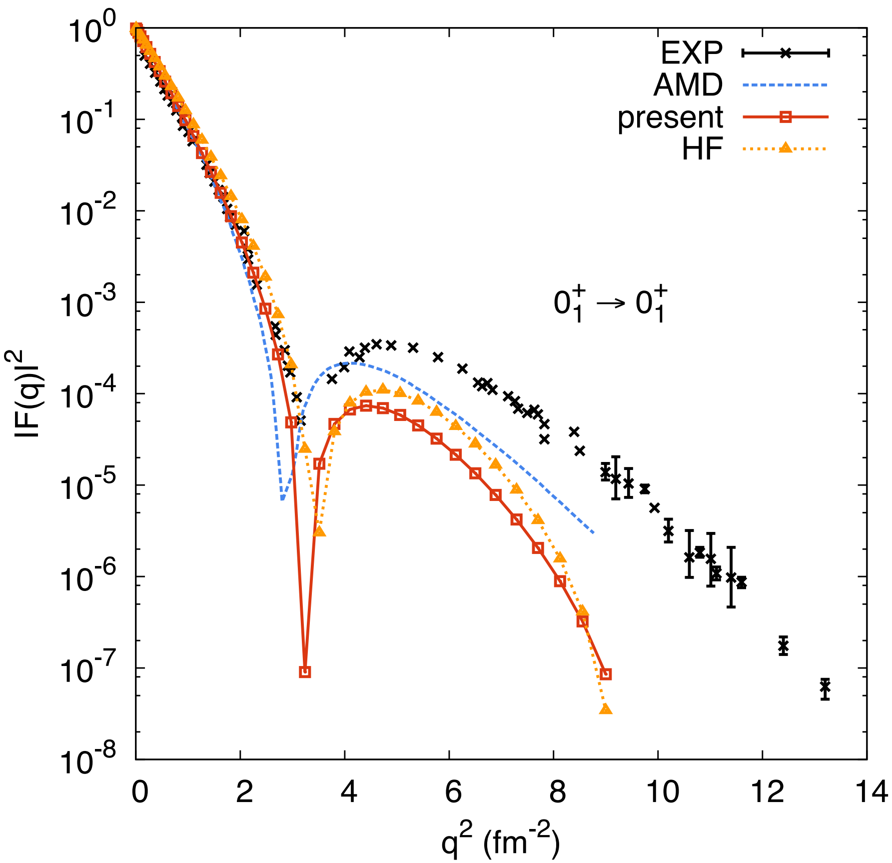
$4_1^- : 71.8\%$



The lowest negative-parity state in each J
A few MeV higher than experiment.

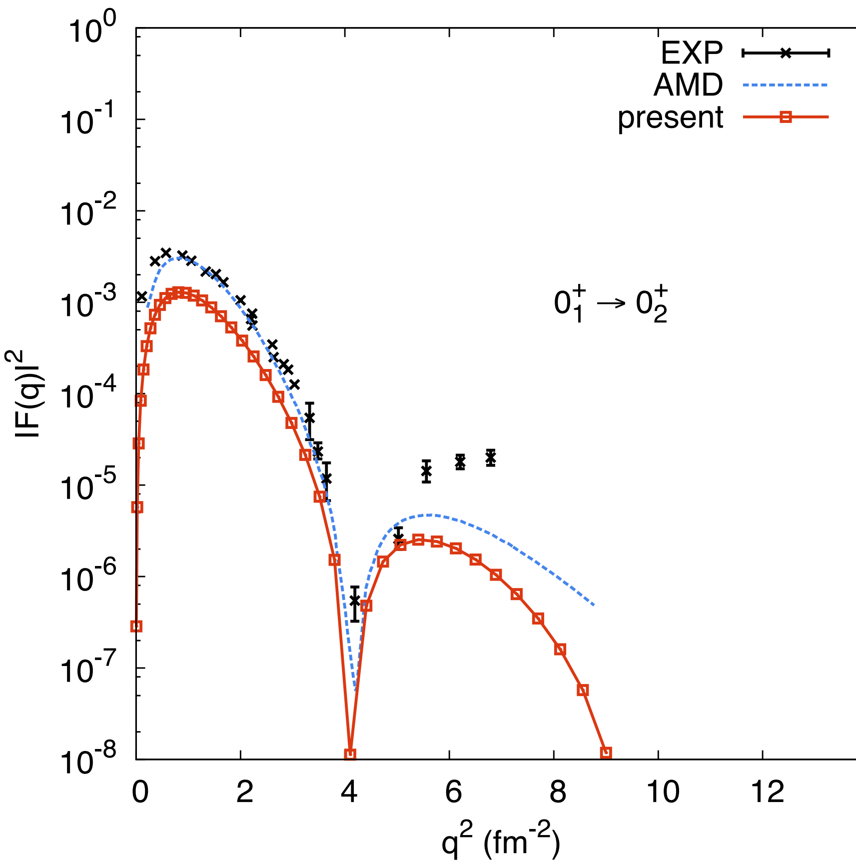
Charge form factors

- Elastic (ground)



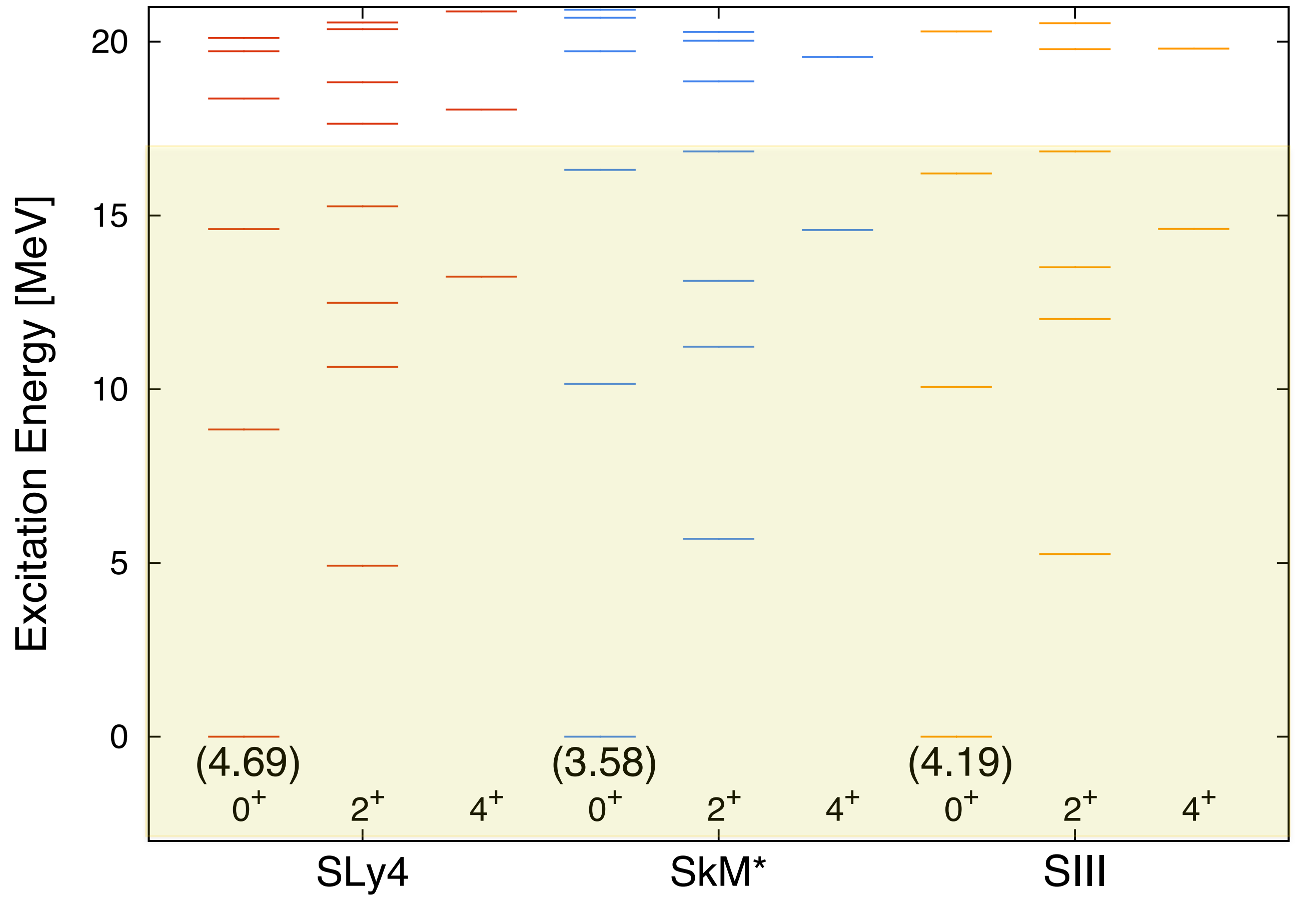
Too large diffuseness

Inelastic ($0_1^+ \to 0_2^+$)



Functional dependence

- Robust result
  - G.s. correlation energy varies by about 1 MeV



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

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

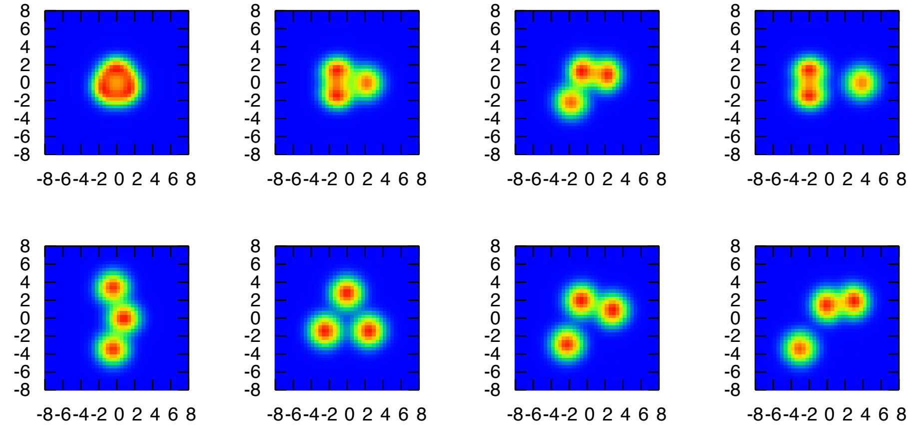
5.4 ± 0.2 Experiment

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

Shrinkage of the Hoyle state

3-alpha configurations used in the GCM calculation by Uegataki et al.

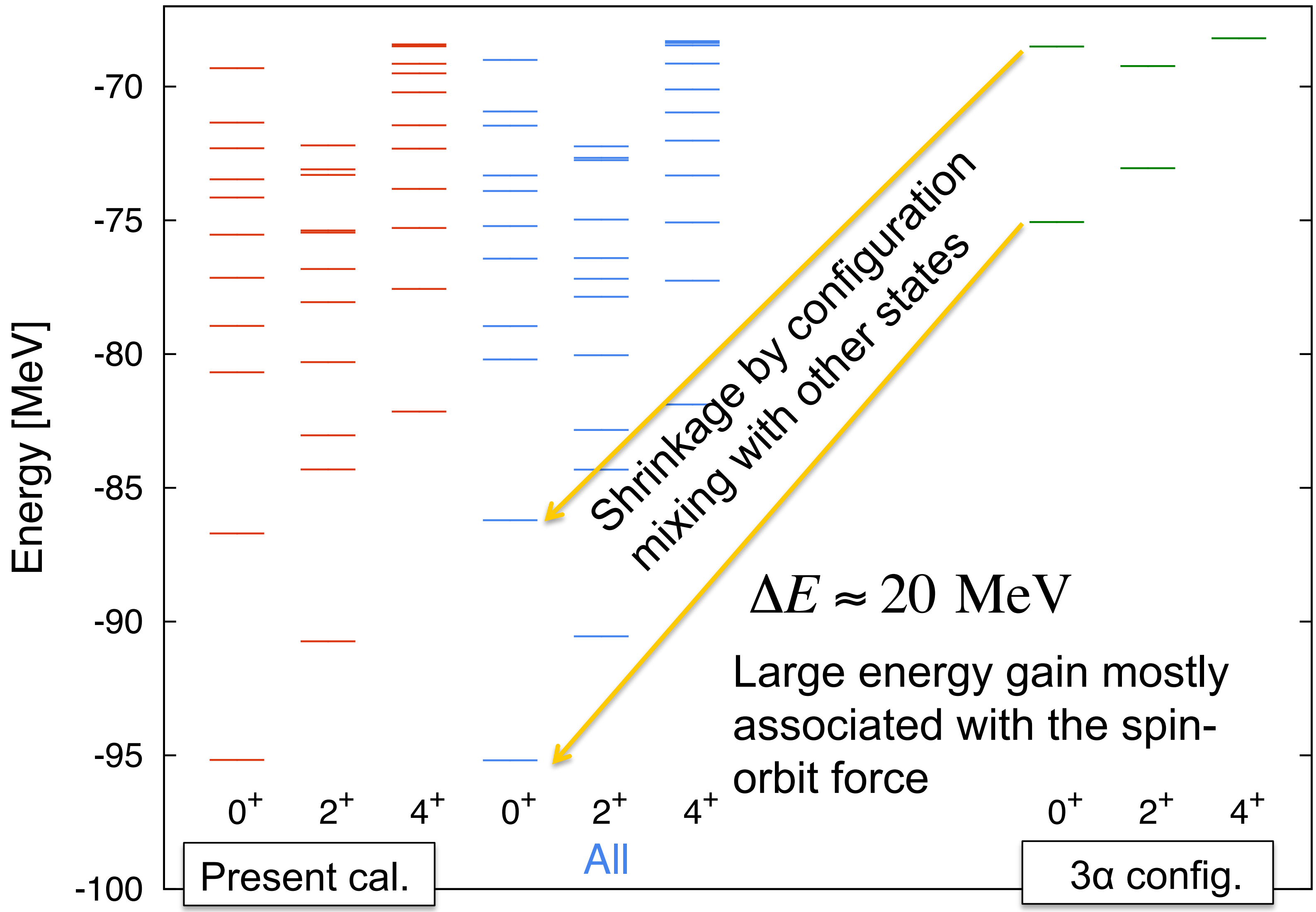
E. Uegaki, *et al.*, PTP57,4 (1977)1262



	EXP	IT	IT + 3α	3α	3α(Uegaki)
radius(0_1^+)	2.31±0.02	2.53	2.54	2.80	2.40
radius(0_2^+)		2.76	2.73	3.31	3.40
$M(E0; 0_2^+ \to 0_1^+)$	5.4± 0.2	4.57	4.13	8.72	6.6

- 3-alpha configurations keep the radius of Hoyle state large.
- Other configurations generated by the imaginary-time propagation makes it much smaller.

SLy4

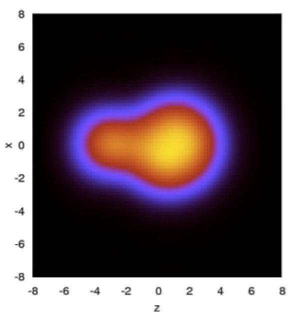


E_{HF}=−90.6 MeV

Adopting the three-alpha configurations utilized in GCM: E. Uegaki, *et al.*, PTP57,4 (1977)1262

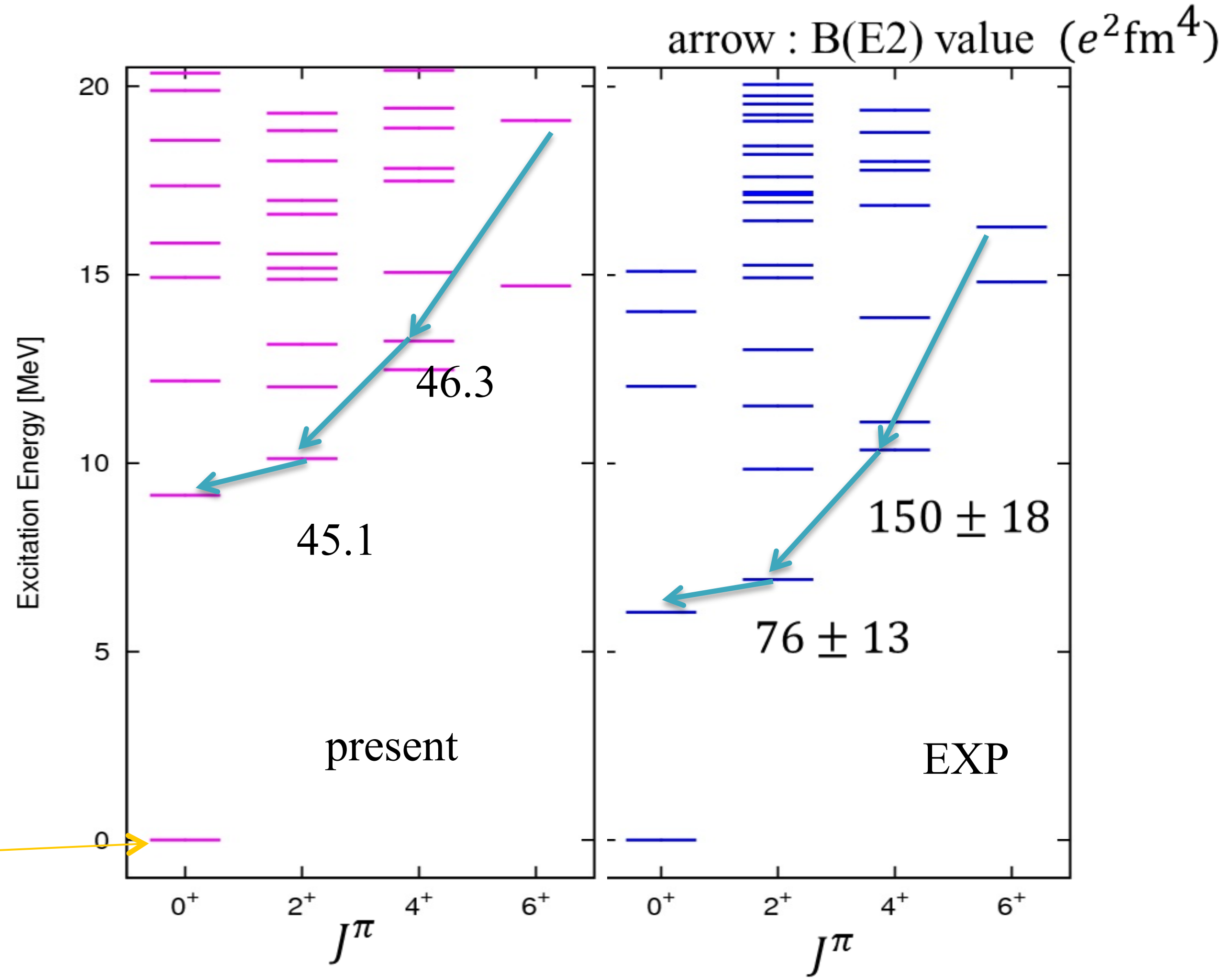
^{16}O POSITIVE parity

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



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

HF state: 80%

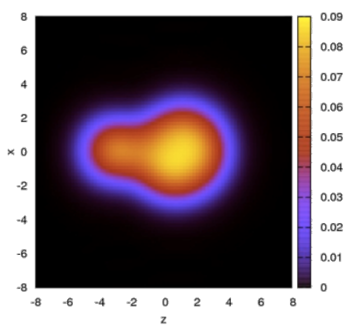


✓ correlation energy is 3.3MeV

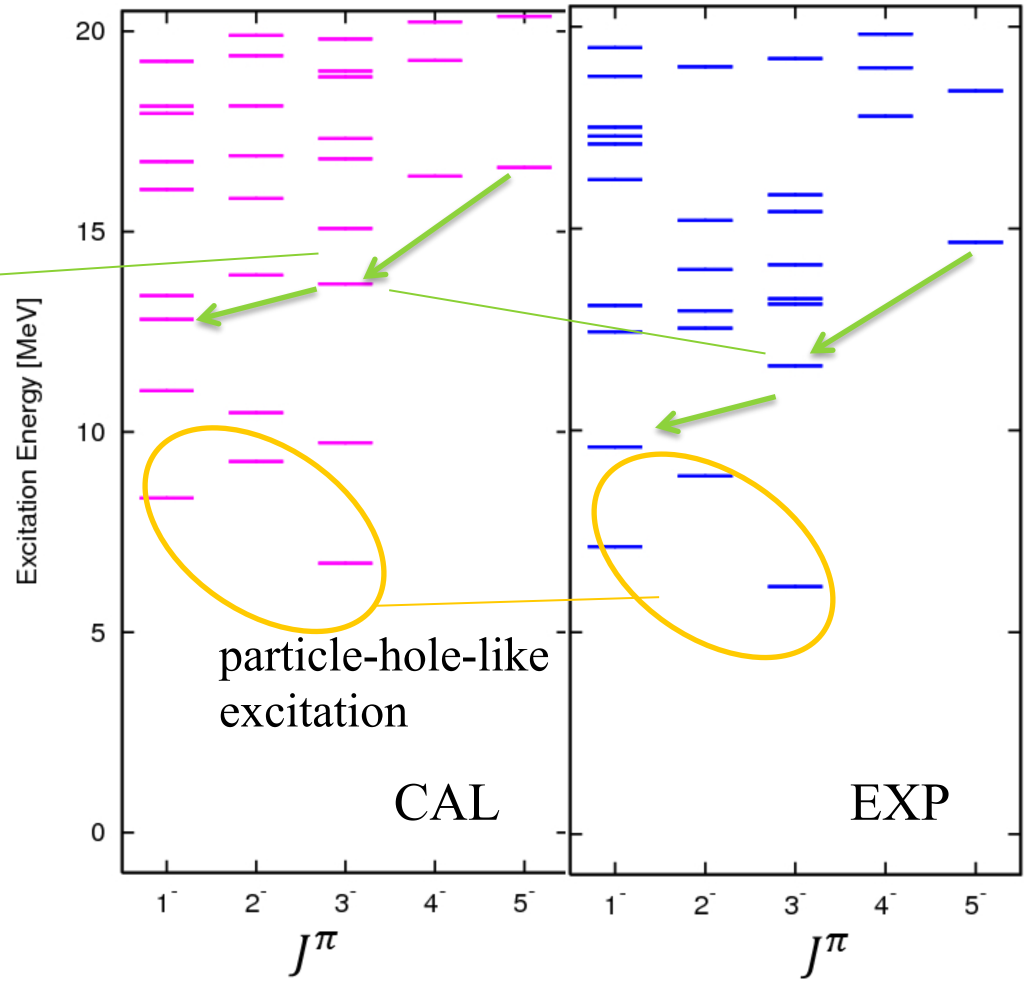
^{16}O NEGATIVE parity

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

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



parity doublet partner

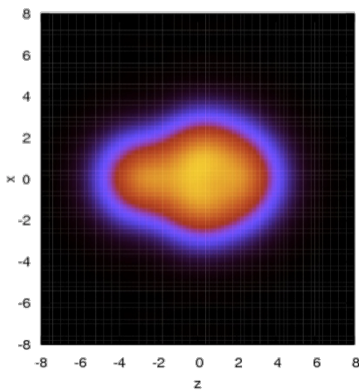


✓ particle-hole excitation is good agreement with experimental values

^{20}Ne (Sly4)

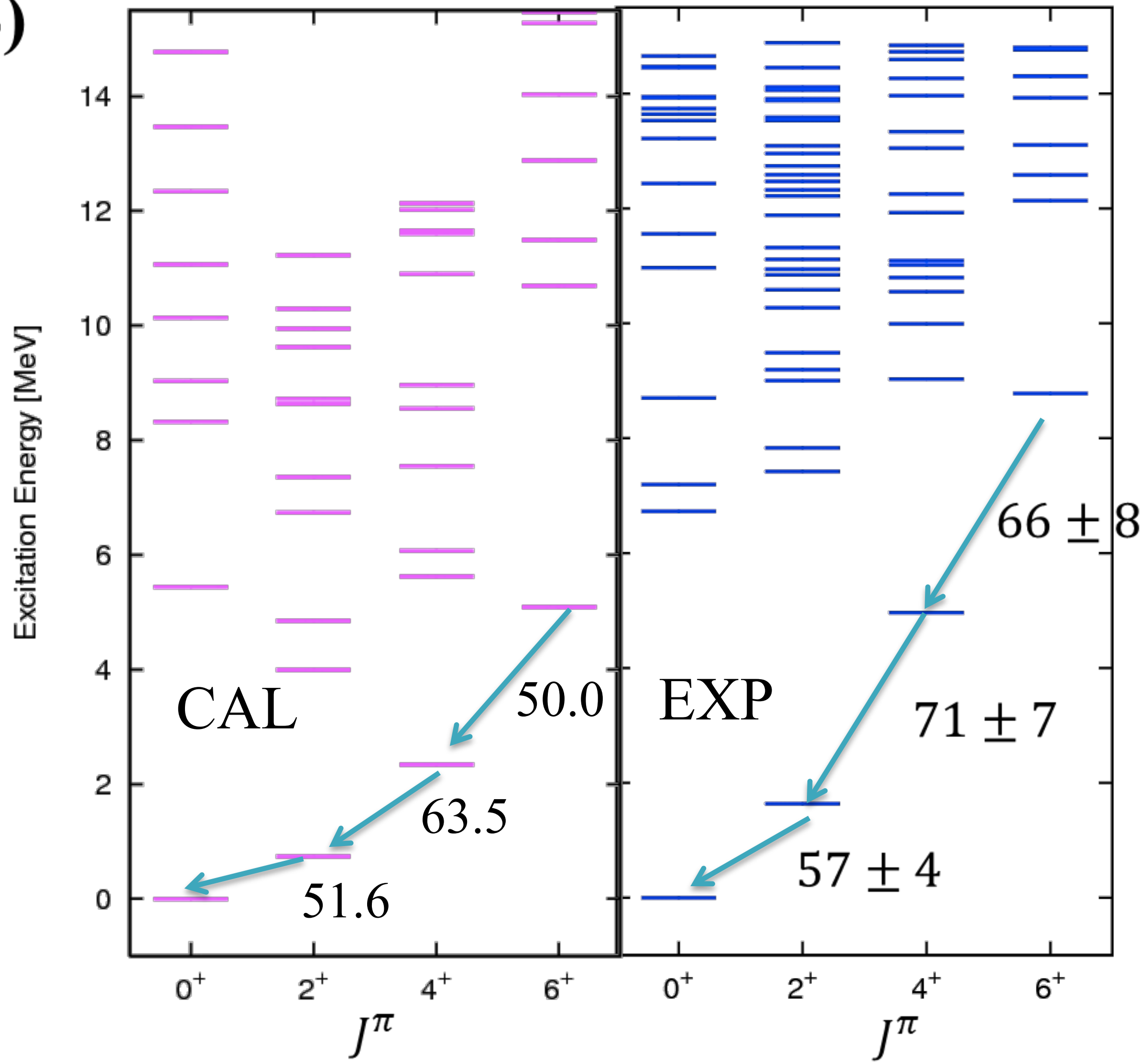
POSITIVE parity

$^{16}O + \alpha$ (?)



0_1^+ : 81.4%
2_1^+ : 83.1%
4_1^+ : 66.8%

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

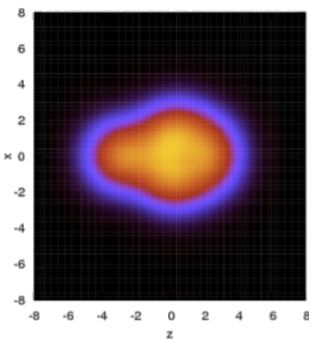


- ✓ Correlation energy of about 6 MeV
- ✓ B(E2) in good agreement
- ✓ Too large moment of inertia

^{20}Ne (Sly4) NEGATIVE parity

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

$K^\pi = 0^-$



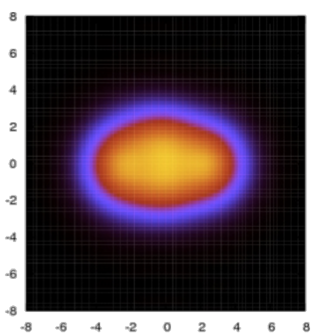
Overlap

1^-_2 : 78.7%

3^-_4 : 75.8%

5^-_4 : 66.0%

$K^\pi = 2^-$



Overlap

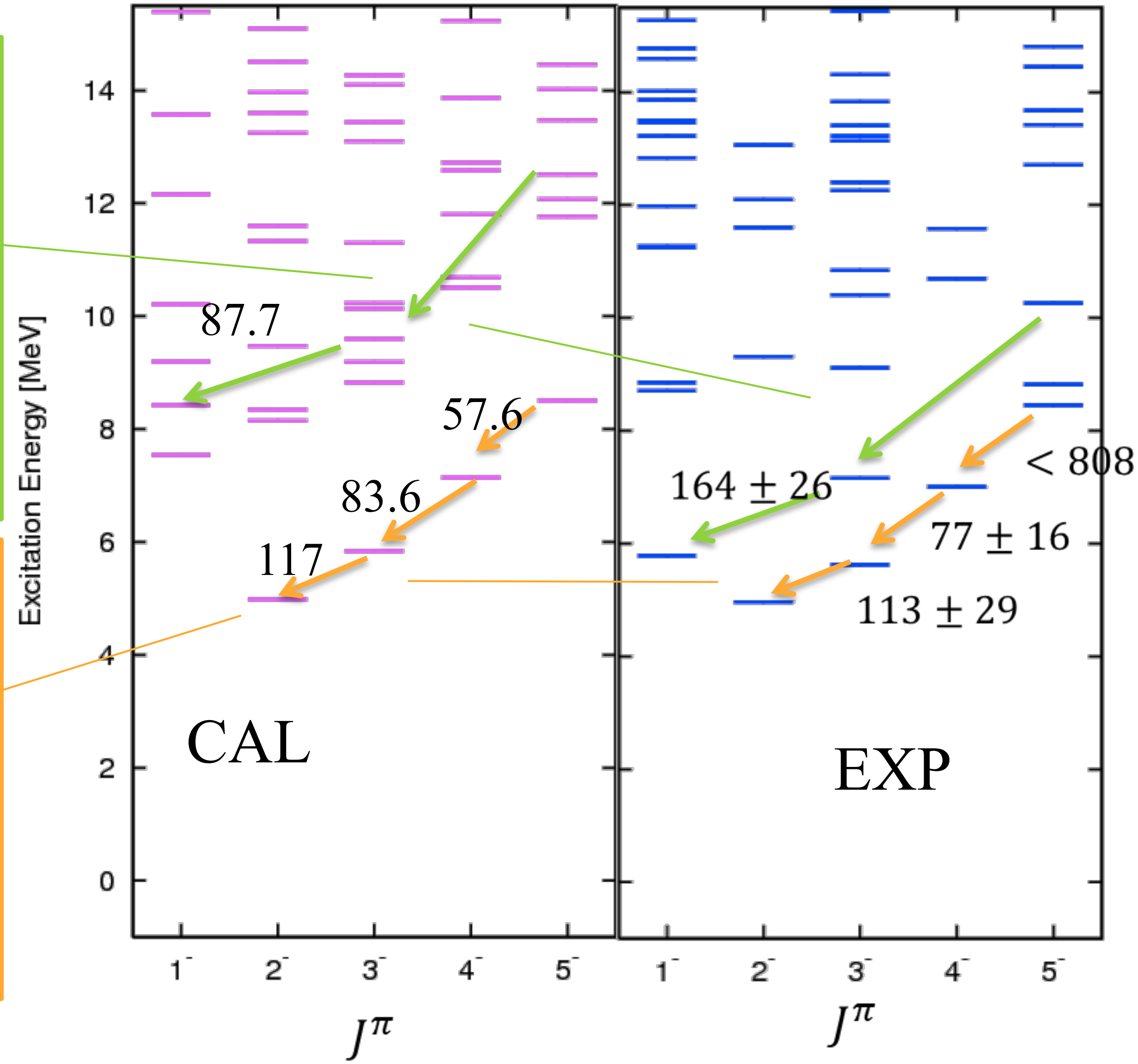
2^-_1 : 90.5%

3^-_1 : 85.8%

4^-_4 : 83.1%

5^-_1 : 74.6%

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



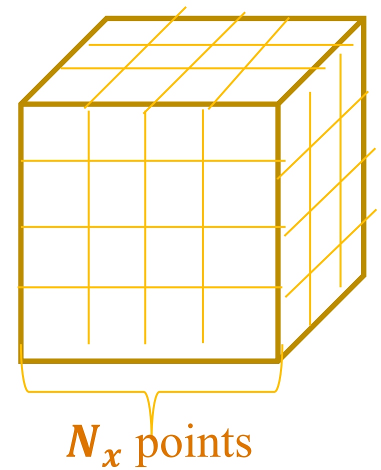
- ✓ Candidate for parity-doublet partner
- ✓ K^π=2$^-$ band: $(p)^{-1}(sd)^5$

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 : $N_x^3 \times N_i$

# 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

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

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

The range of Gogny interaction is about 4 fm.

⇓

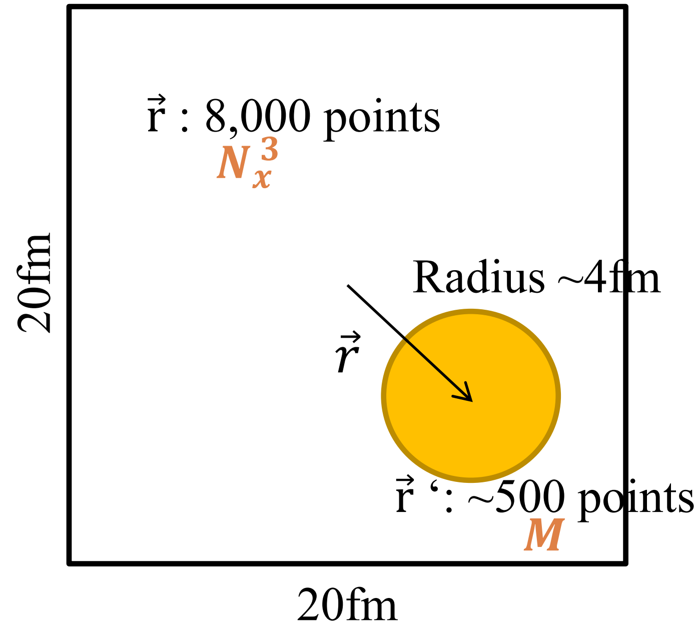
it is sufficient to integrate r' inside 4fm sphere.

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

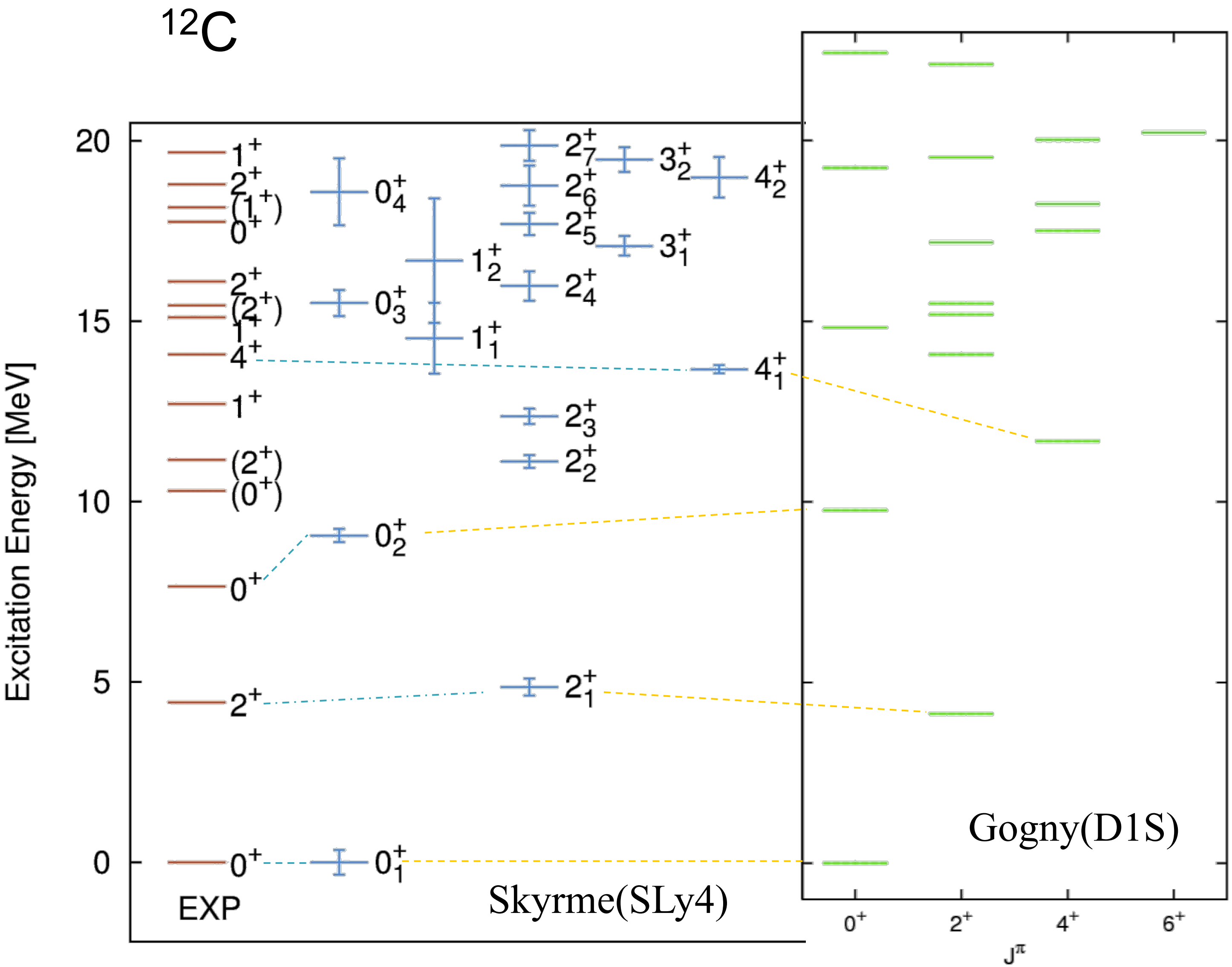
cf. Skyrme interaction

$N_x^3 \times N_i$

✓ 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

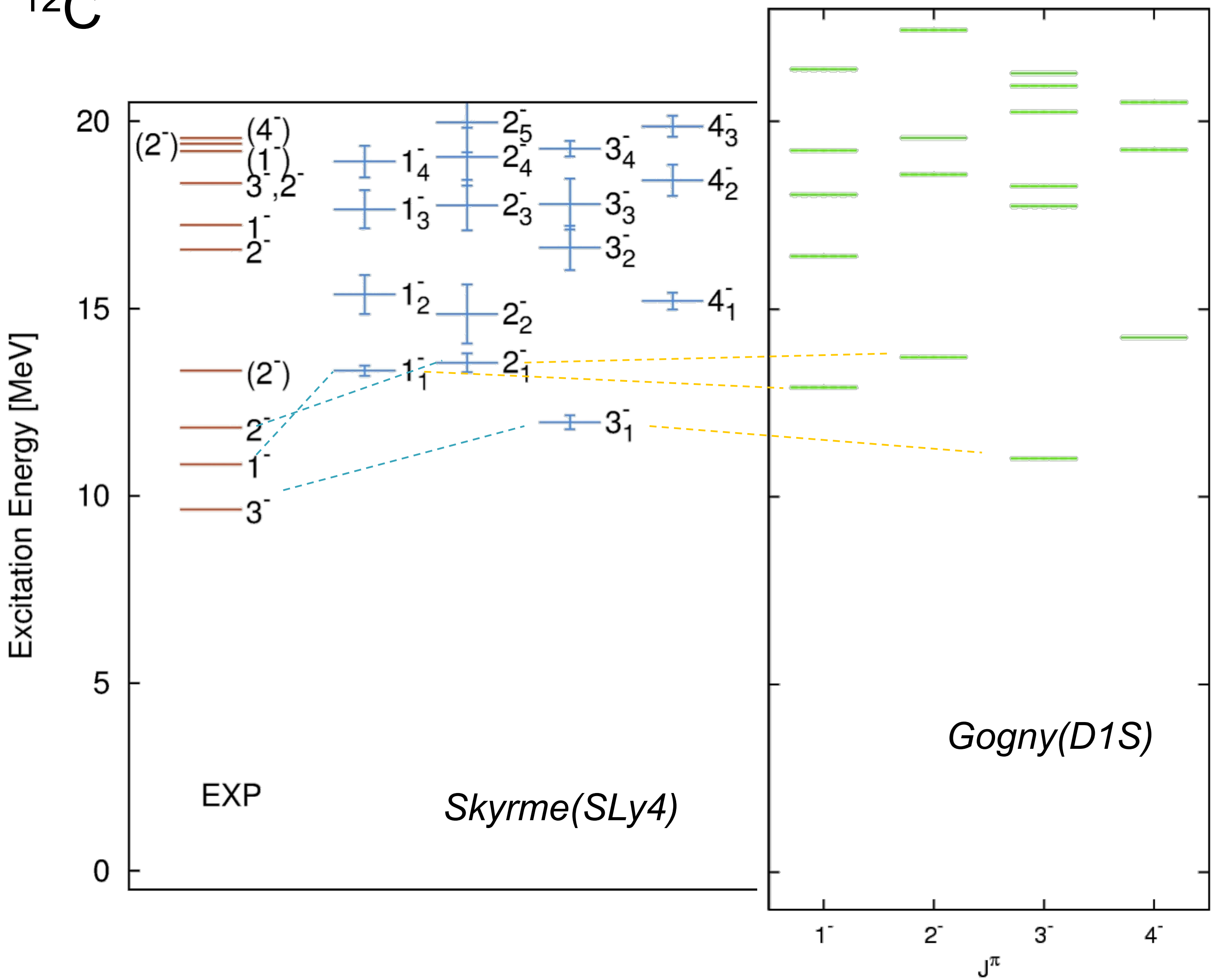
cf. Skyrme
(α, β, γ)=(18, 30, 18)
512 core x 1.8h
45 SDs

SR16000@YITP

- ✓ Computational cost is 7.5 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, in preparation

- Complete low-lying spectroscopy with the Skyrme Hamiltonian
- Capable of describing a variety of excited states in a unified way, such as vibrational excitations, cluster excitations, single-particle excitations.

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
  - All properties reasonably agree with experiments, except for its radius.
  - Three-alpha configurations produce a large radius
  - Configuration mixing with other states makes the Hoyle state shrunk