# No-Core Monte Carlo Shell Model calculation for $^{10}Be$ and $^{12}Be$ low-lying spectra


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# Outline

- **Introduction**
- **Theoretical framework**
  1) **Unitary Correlation Operator Method**
  2) **Monte Carlo Shell-Model**
- **Results and discussion**

  **Low lying spectra for $^{10}$Be and $^{12}$Be**
- **Summary and outlook**

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# Introduction

- **One of the major goals in nuclear physics is to understand the structure of nuclei starting from realistic nuclear interactions.**
- **In the last decades, many progresses have been made in obtaining an accurate representation of realistic nucleon-nucleon (*NN*) potentials.**

**Argonne interaction, CD-Bonn interaction, Nijim I & II, $N^3LO$ …**

✓ Wiringa, *et al.*, PRC 1984; 1995; Machleidt, PRC 2001; Stoks, *et al.*, PRC 1994; Entem and Machleidt, PRC 2003.

- **By using these realistic *NN* interactions, nuclear *ab initio* calculations have been performed in light nuclei, e.g.**

**Green's Function Monte Carlo (GFMC) A~12**

✓ Pieper and Wiringa, ARNP 2001; Pieper, *et al.*,PRC 2002; Pieper, NPA 2005

**No-Core Shell Model (NCSM) A~14**

✓ Navrátil, *et al.*, PRC 2000; JPG 2009; Caurier, *et al.*, PRC 2002

**Tensor Optimized Shell Model (TOSM) Li isotopes**

✓ Myo-san's talk yesterday

# Introduction

- **The direct application of these realistic *NN* potentials to many-body calculations, e.g. shell model calculation, is difficult.**

- strong short-range repulsive core;
- tensor correlation;
- …

- huge Hamiltonian matrix dimension for medium and heavy nuclei,
  e.g. $10^{9\sim10}$ M-scheme dimension for medium-mass nuclei

- **The Unitary Correlation Operator Method (UCOM) is one of the methods to solve this problem by introducing a unitary transformation.**

✓ Feldmeier, *et al.*, NPA 1998;
✓ Neff and Feldmeier, NPA 2003;
✓ Roth, *et al.*, PPNP 2010

- **Monte Carlo shell model has been proposed to solve this problem by diagonalizing the Hamiltonian in a small subspace (~ 100 dimension), which are generated by a stochastic way.**

✓ Otsuka, *et al.*, PPNP 2001

# In this work

**Realistic *NN*-interaction *V***

**UCOM transformation**

**$V_{UCOM}$ + MCSM**

**For the first time, we apply the MCSM to investigate $^{10}$Be and $^{12}$Be in an *ab initio* way.**

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# UCOM

- **Introduction of unitary operator**

| Correlated | Unitary correlation operator | Uncorrelated |
| --- | --- | --- |
| $\vert\Psi\rangle$ & $\vert\psi\rangle$ <br> $\hat{B}$ | $\vert\Psi\rangle = C\vert\Phi\rangle$ <br> $\hat{B} = C^{-1}BC$ | $\vert\Phi\rangle$ & $\vert\phi\rangle$ <br> $B$ |

$$C = \exp\{-iG\} \quad G = \sum_{i<j}^{A} g(i,j) + \ three - body\ term\ + \ higher\ terms$$

- **Nuclear structures are greatly affected by two kinds of correlation:**
  1) **Short-range correlation;**
  2) **Tensor correlation.**

$$C = C_\Omega C_r = \exp\,[-i\sum_{i<j} g_{\Omega,ij}]\,\exp\,[-i\sum_{i<j} g_{r,ij}]$$

**Fitting Energy minimum point to determine 4 parameters in $g_\Omega$ and $g_r$**

# UCOM potential

- **Main idea of UCOM**

$$\langle\Psi|H|\Psi'\rangle = \langle\Phi|C^{\dagger}HC|\Phi'\rangle = \langle\Phi|C^{-1}HC|\Phi'\rangle = \langle\Phi|\hat{H}|\Phi'\rangle$$

- **Correlated Hamiltonian and the UCOM potential**

$$\begin{aligned}\hat{H} &= C^{\dagger}HC = C^{\dagger}(T+V_{real.})C \\ &= \hat{T}^{[1]}+\hat{T}^{[2]}+\hat{V}^{[2]} = T_{int}+V_{UCOM}\end{aligned}$$

$$T^{[1]} = T_{int.}$$

**where any correlated operator is rewritten as:**

$$\begin{aligned}\hat{B} = C^{-1}BC &= \exp\{+iG\}B\exp\{-iG\} \\ &= B+[G,B]+\frac{1}{2!}[G,[G,B]]+\cdots\end{aligned}$$

# Monte Carlo Shell Model

**Imaginary-time evolution operator**

$$e^{-\beta H}$$

↓

$$e^{-\beta H}|\Phi\rangle = \sum_i e^{-\beta E_i} c_i |k_i\rangle$$

↓ $\beta \to \infty$

$$e^{-\beta E_1} c_1 |k_1\rangle$$

**β is a real number, *H* is general time independent Hamiltonian**

$$|\Phi\rangle = \sum_i c_i |k_i\rangle$$

**$E_i$ : i-th eigenvalue of *H*,**
**$|k_i\rangle$ : its eigenfunction,**
**$c_i$: amplitude.**

# Monte Carlo Shell Model

- **For example, a simple Hamiltonian:** $H = \frac{1}{2} V O^2$

O: one-body operator
V<0: coupling constant

$$e^{-\beta H} = e^{-\frac{1}{2}\beta V O^2}$$

Hubbard-Stratonovich (HS) transformation

$$e^{-\frac{1}{2}\beta V O^2} = \int_{-\infty}^{\infty} d\sigma_\alpha \sqrt{\frac{\beta|V|}{2}}\, e^{-\frac{\beta}{2}|V|\sigma_\alpha^2} \cdot e^{-\beta|V|\sigma_\alpha O}$$

σ: auxiliary fields

$$e^{-\frac{1}{2}\beta V O^2} \approx \sum_{MC:\sigma_\alpha} \sqrt{\frac{\beta|V|}{2\pi}} \cdot e^{-\beta|V|\sigma_\alpha O}$$

$$G(\sigma_\alpha) = e^{-\frac{\beta}{2}|V|\sigma_\alpha^2}$$

Probability weight
σ: random numbers

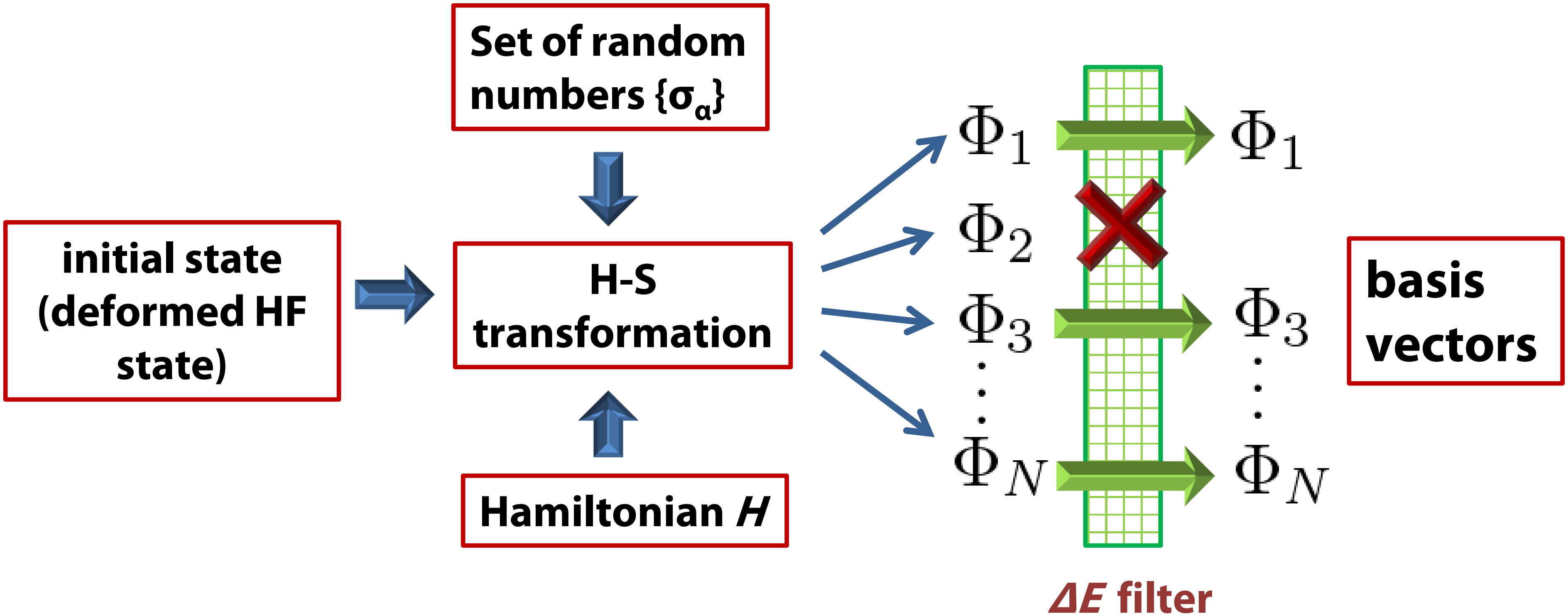
Monte Carlo sampling

$$e^{-\beta H}|\Phi\rangle \Rightarrow \sum_{MC:\sigma_\alpha} e^{-\beta h(\sigma_\alpha)}|\Phi\rangle$$

$$h(\sigma_\alpha) = V\sigma_\alpha O$$

One-body Hamiltonian

# Basis Generation process



# Symmetry restoration

➢ **Treatment of spurious center-of-mass motion**

**Lawson's prescription:**

✓ Gloeckner and Lawson, PLB 1974

$$H' = H_{SM} + \beta_{c.m.} H_{c.m.}$$

$$H_{c.m.} = \frac{\mathbf{P}^2}{2AM} + \frac{1}{2} M A \omega^2 \mathbf{R}^2 - \frac{3}{2}\hbar\omega$$

➢ **Full projection of angular momentum**

$$|\Phi(\sigma_i)\rangle \rightarrow P_{J,M} |\Phi(\sigma_i)\rangle$$

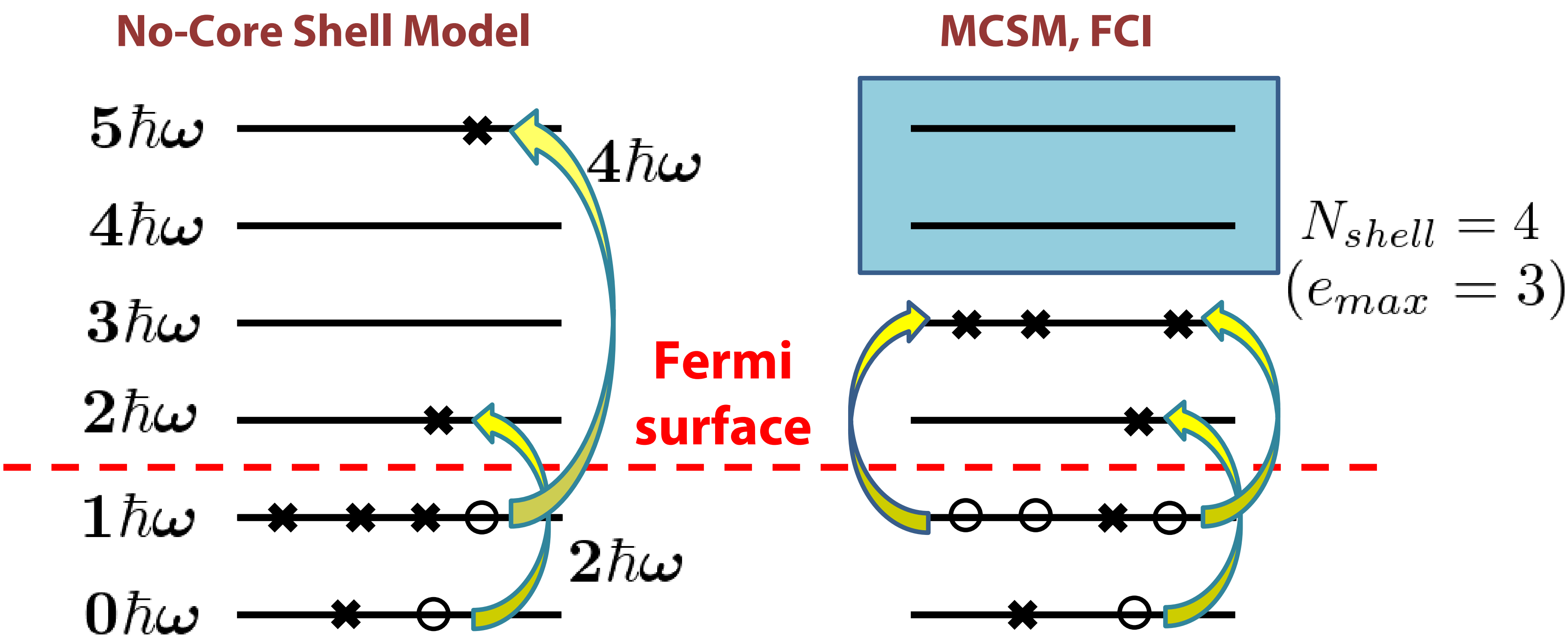
✓ Ring and Schuck, 1980

$$P_{J,M} = \frac{2J+1}{8\pi^2} \int D^{J*}_{MK}(\Omega) R(\Omega) d\Omega$$

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

$$\langle \Phi(\sigma_i) | H P_{J,M} | \Phi(\sigma_j) \rangle$$

# Truncation Scheme for *ab-initio* shell-model calculation




**Excitation energy up to** $N_{max}\hbar\omega$

$$2\hbar\omega + 4\hbar\omega = 6\hbar\omega \leq N_{max}\hbar\omega$$

**Single particle energies up to** $e_{max}\hbar\omega$

$$e_{max} = 2n + l$$

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# Numerical detail

- **$e_{max}=2n+l$, which is the quantum number of Harmonic oscillator major shell;**

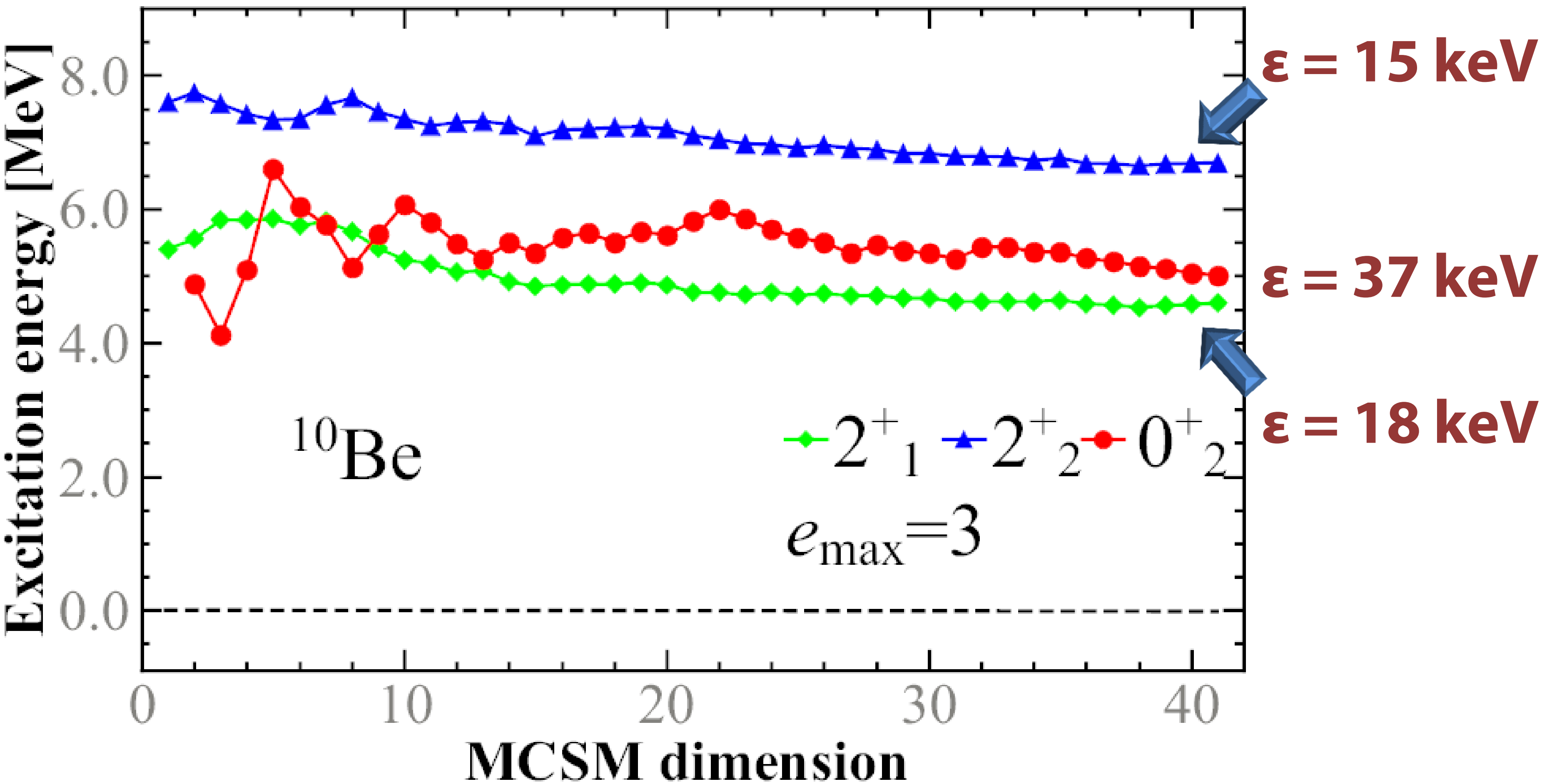
- **The input potential is $V_{UCOM}(N^3LO)$ and $V_{UCOM}(AV18)$;**

- **Coulomb interaction is NOT included in present calculation.**

# Beryllium low-lying spectra

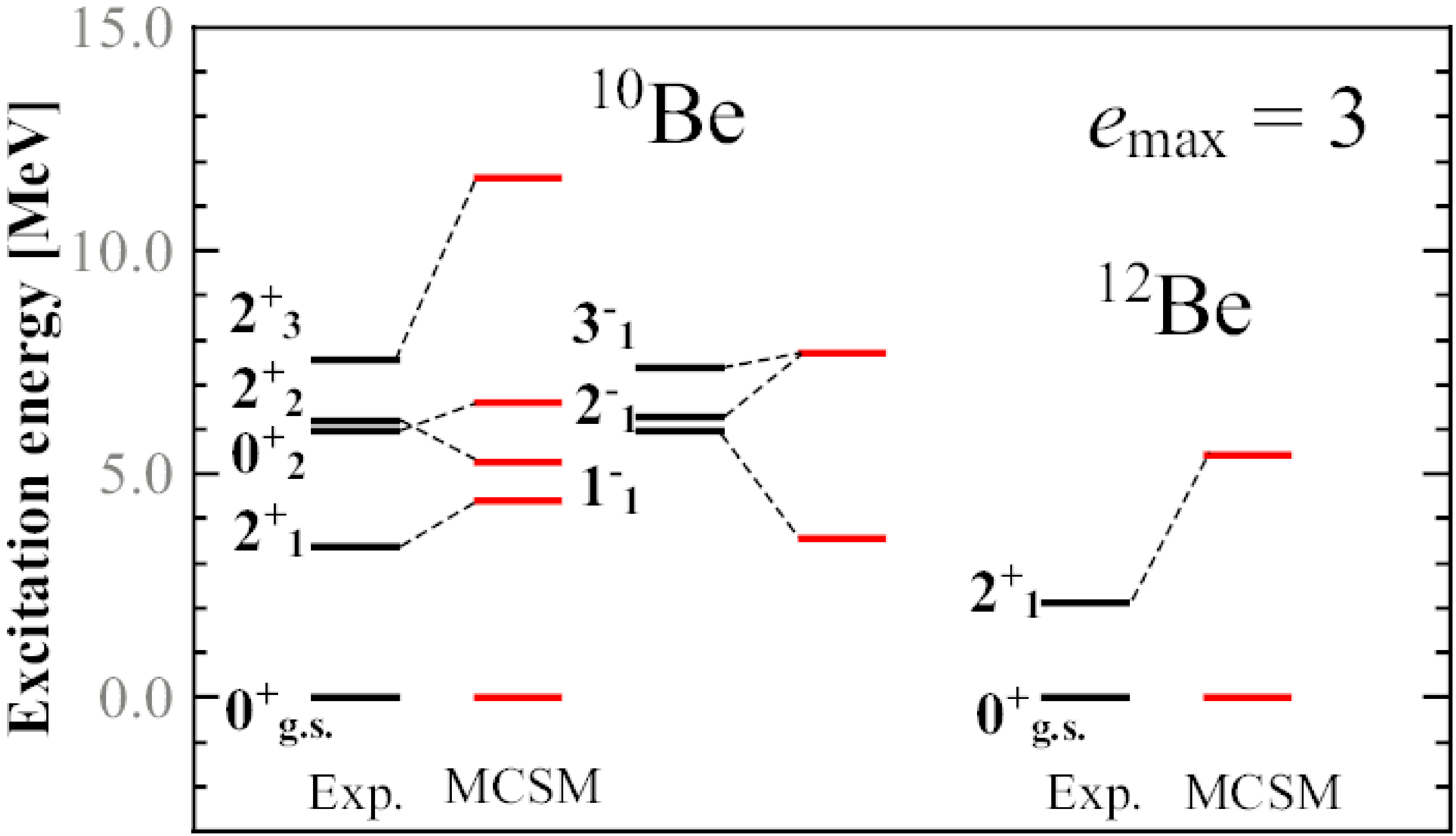
- **The convergence of excited energy for $^{10}$Be as the function of MCSM dimension.**

$$\epsilon = |E_n - E_{n-1}|$$



# Beryllium low-lying spectra

- The excited states of $^{10}$Be and $^{12}$Be without treatment of spurious COM motion.



# Beryllium low-lying spectra

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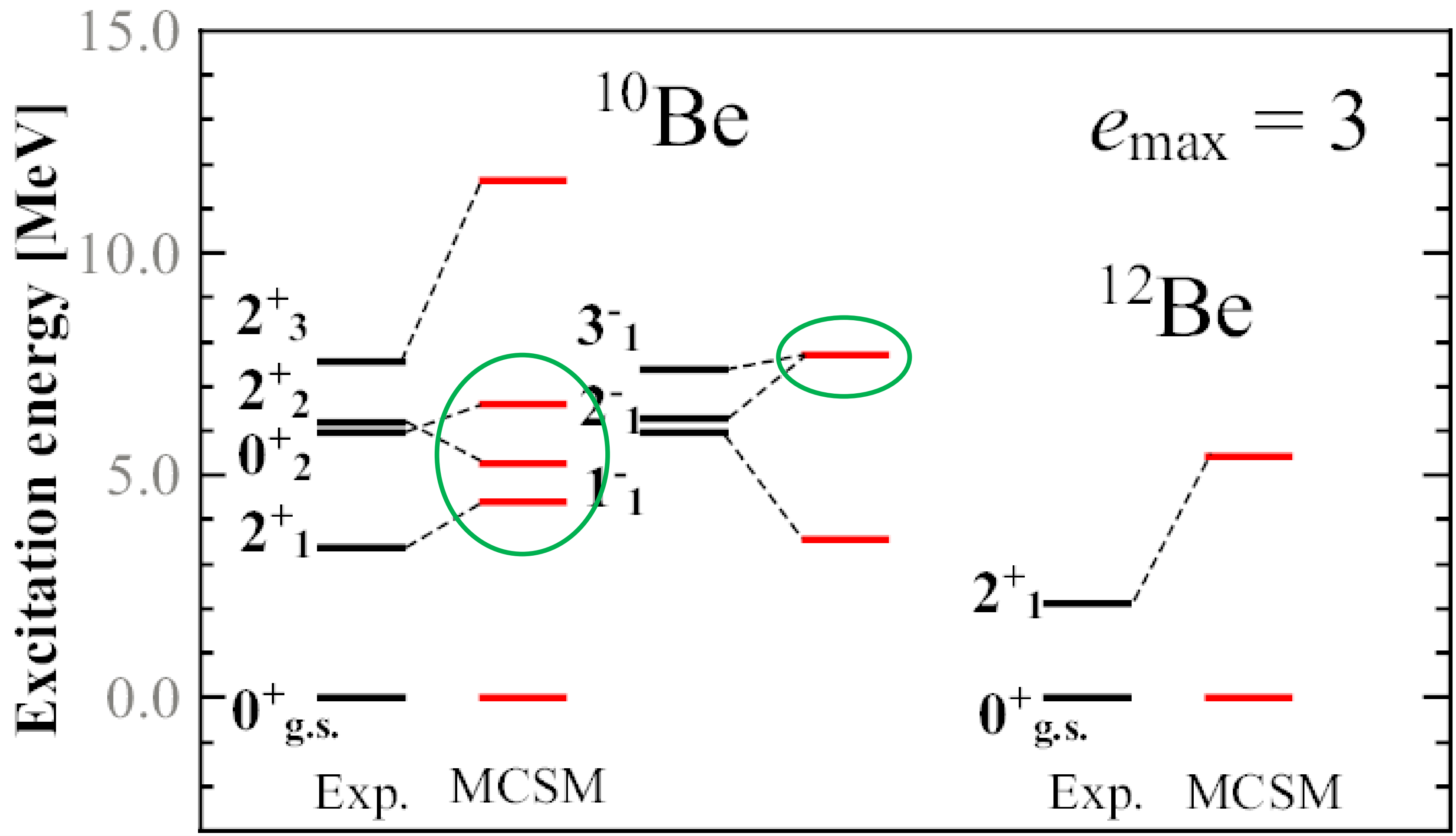
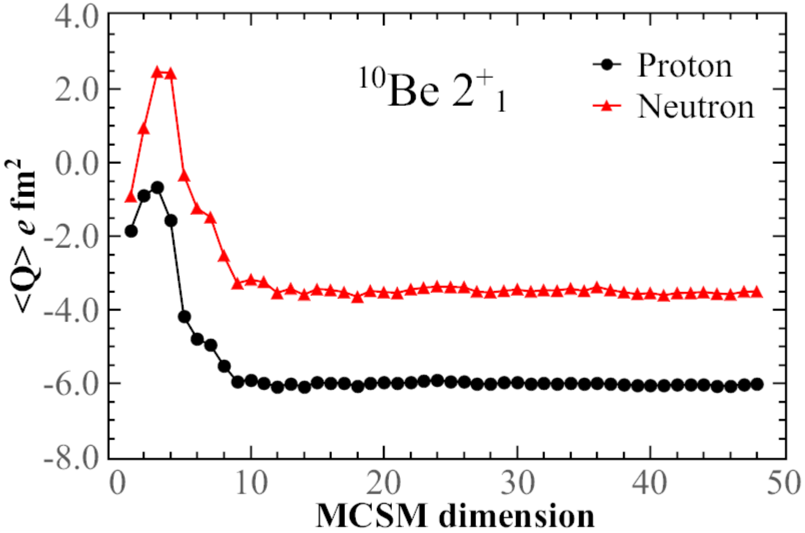
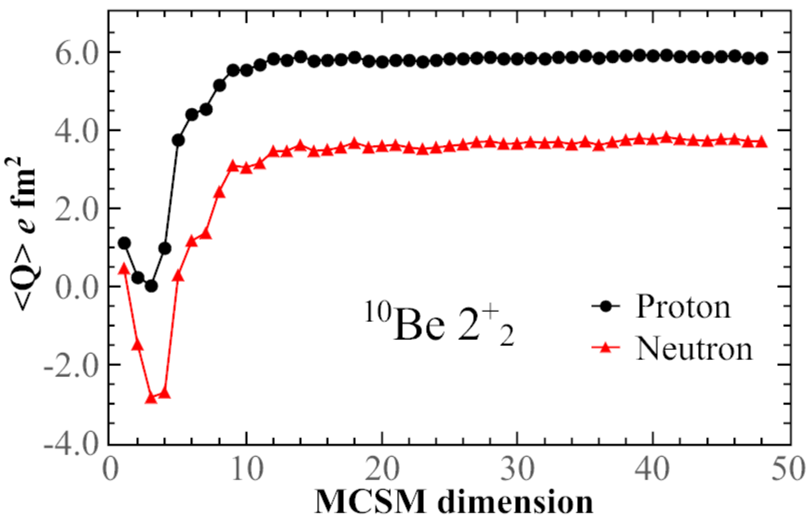
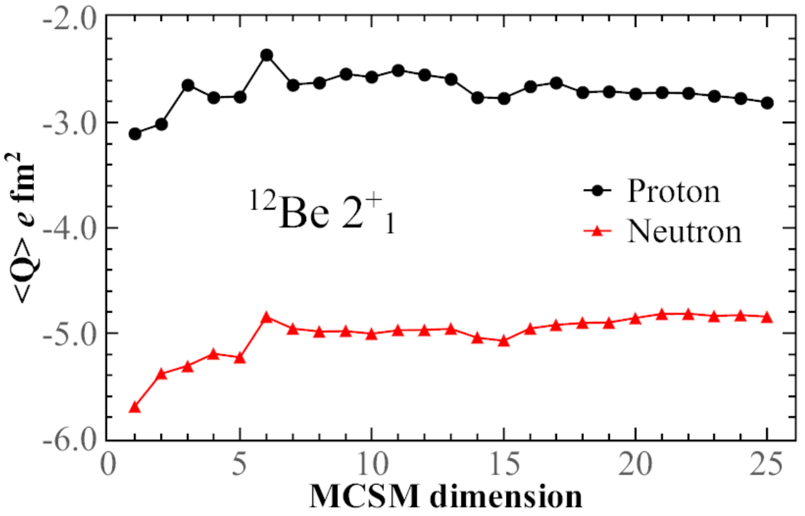


# Quadrupole moment

- The expectation value of quadrupole moments of $2^+_1$ and $2^+_2$ for $^{10}$Be and $2^+_1$ for $^{12}$Be



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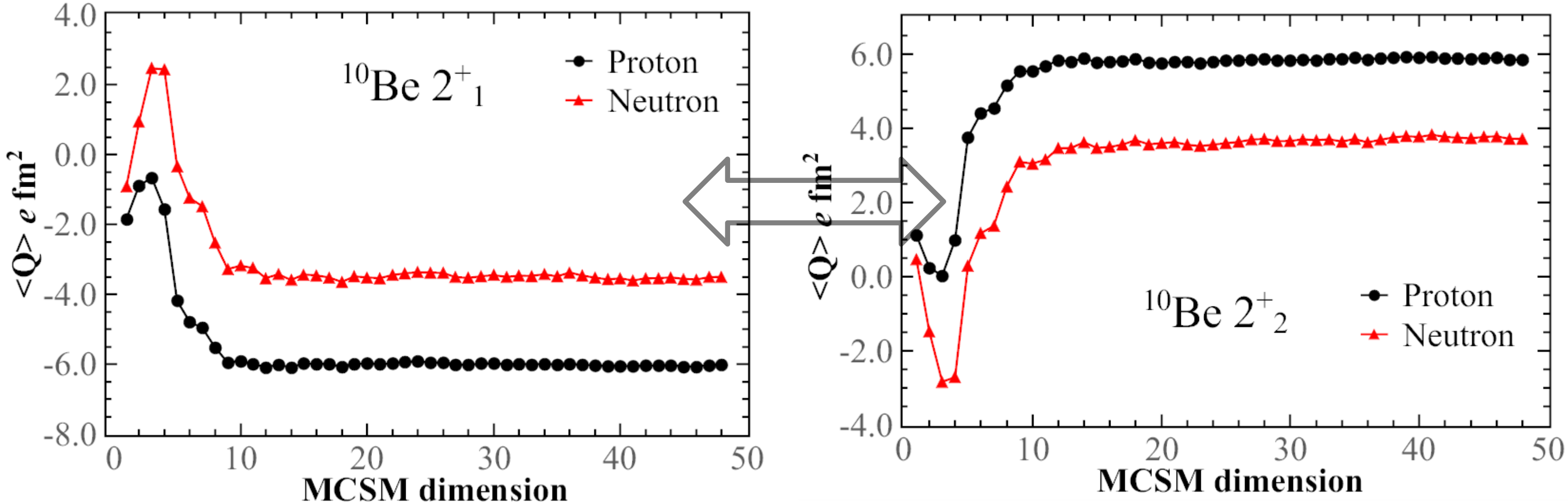


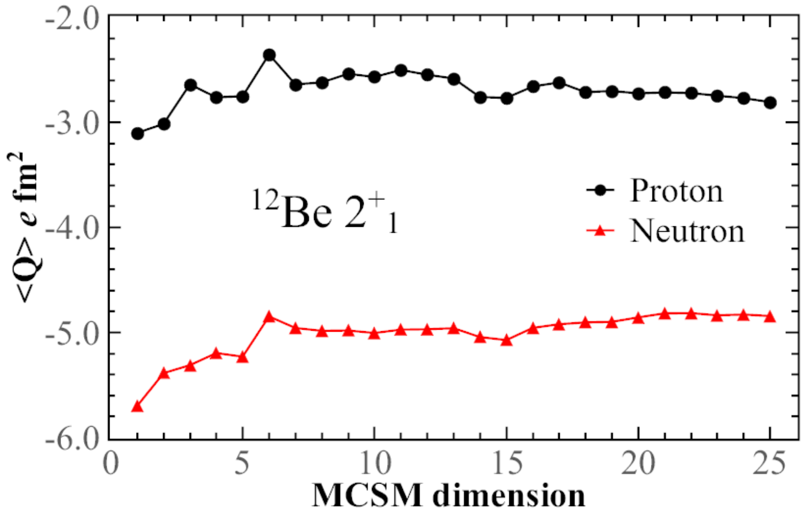


- **Opposite deformation**

# Quadrupole moment

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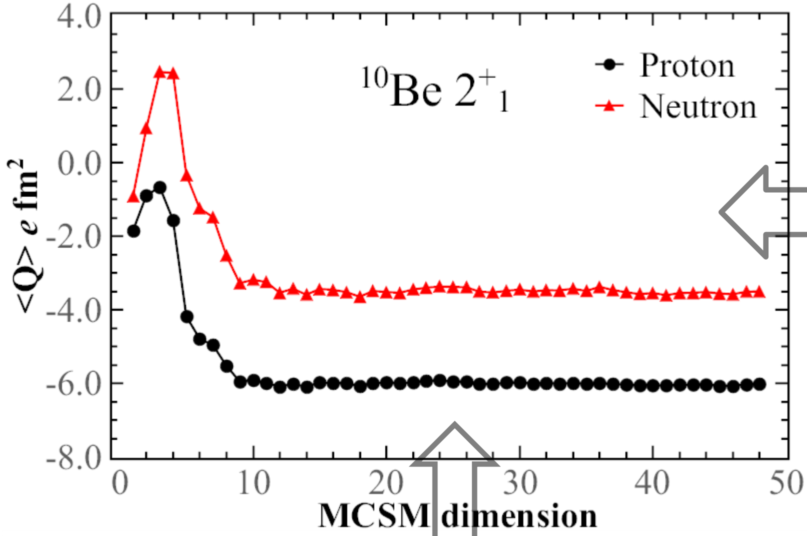
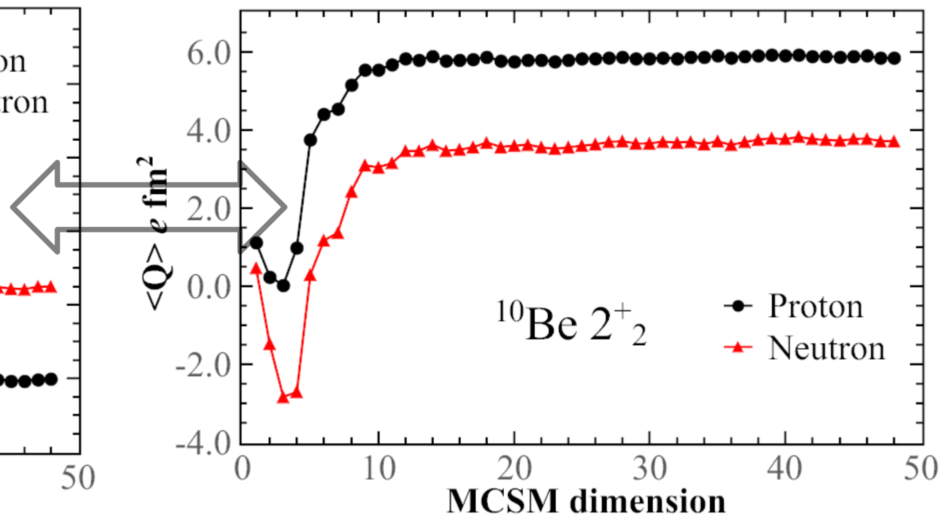
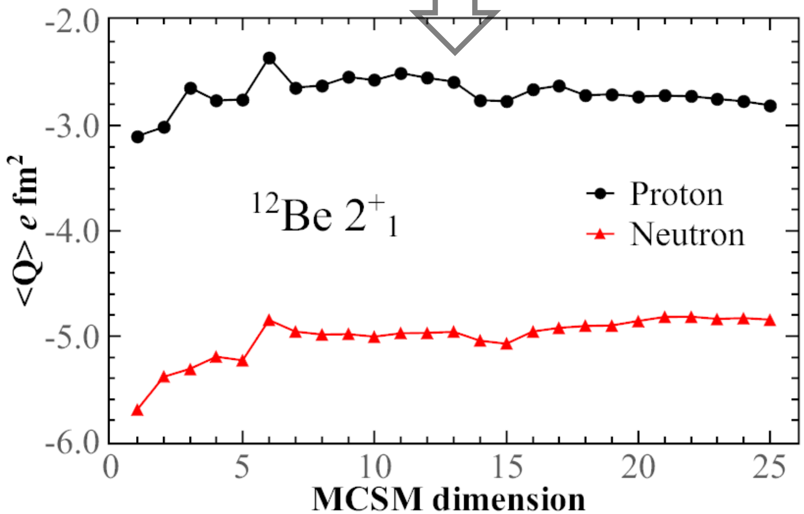


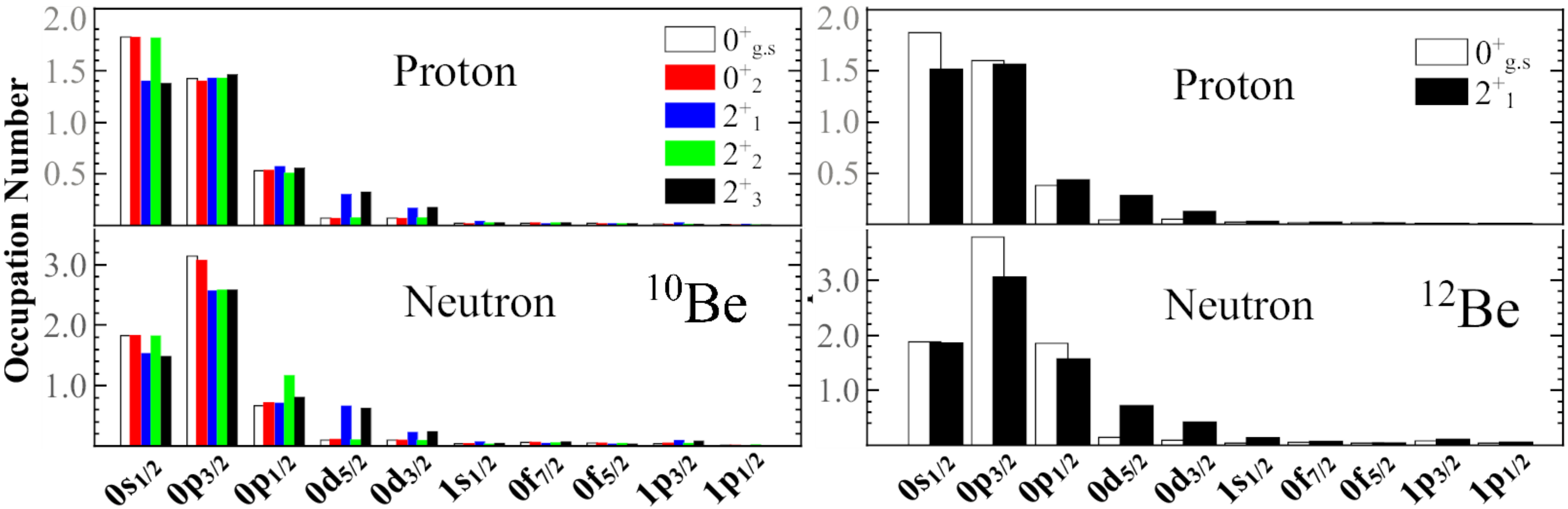




- **Opposite deformation**
- **$^{10}$Be $2^+_1$ , P > N**
  **$^{12}$Be $2^+_1$ , N > P**

# Occupation probabilities

- The single particle orbit occupation number of $0^+_1$ $0^+_2$ $2^+_1$ $2^+_2$ $2^+_3$ state for $^{10}$Be and $0^+_1$ $2^+_1$ for $^{12}$Be.




- **$2^+_1$**

**P:** *s*-shell "core" (~1.8) + *p*-shell "valence"

**N:** NO *sp*-shell "core"

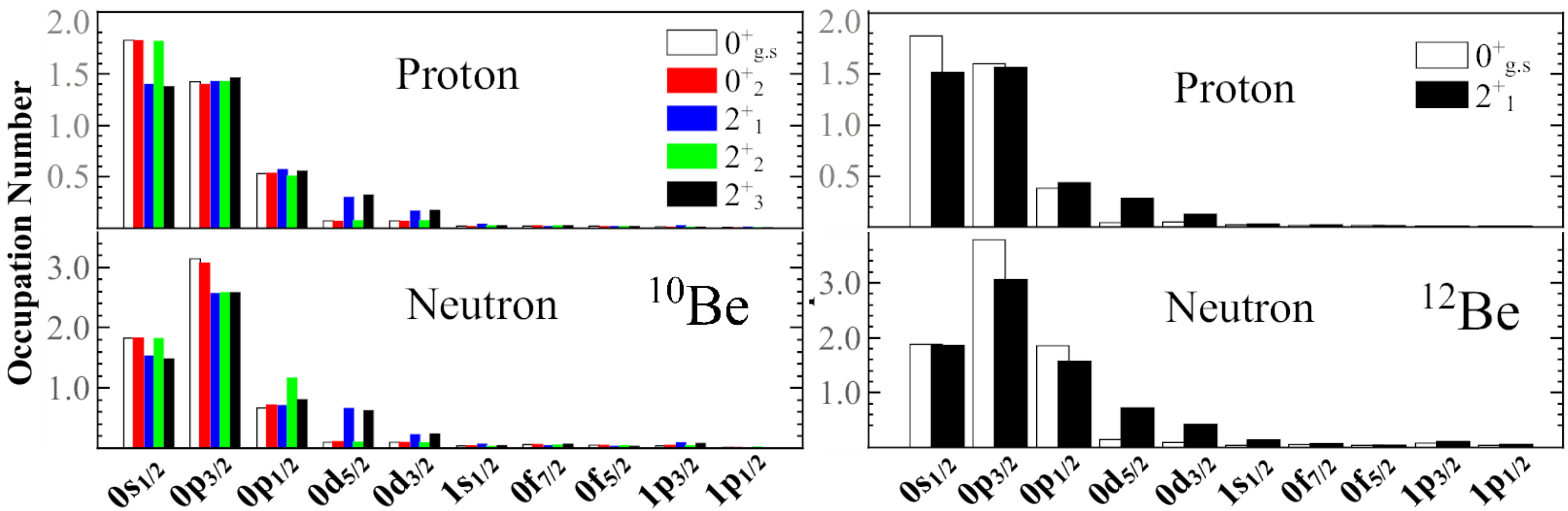
- **$2^+_1$**

**P:** *s*-shell (~ 1.5) + *p*-shell (~ 2.0)

**N:** *sp*-shell "core" + *sd,pf*-shell "valence"

# Occupation probabilities

- The single particle orbit occupation number of $0^+_1$ $0^+_2$ $2^+_1$ $2^+_2$ $2^+_3$ state for $^{10}Be$ and $0^+_1$ $2^+_1$ for $^{12}Be$.

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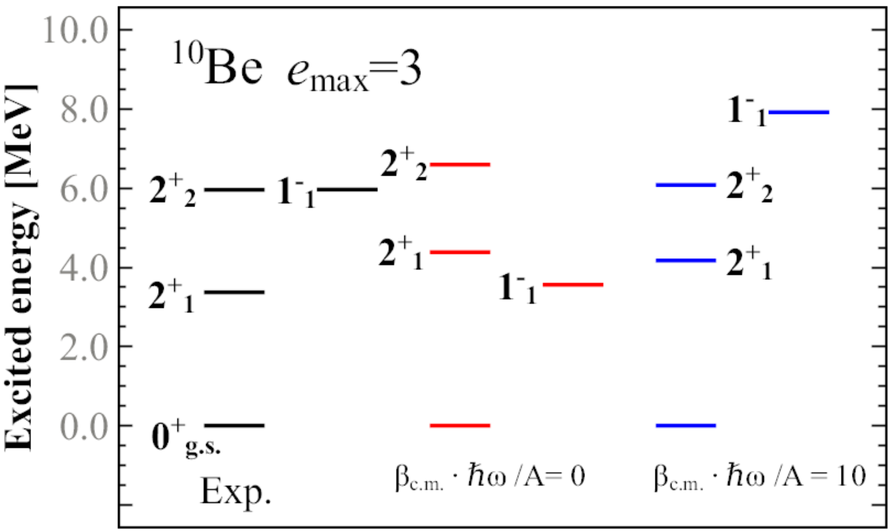
- $2^+_1$

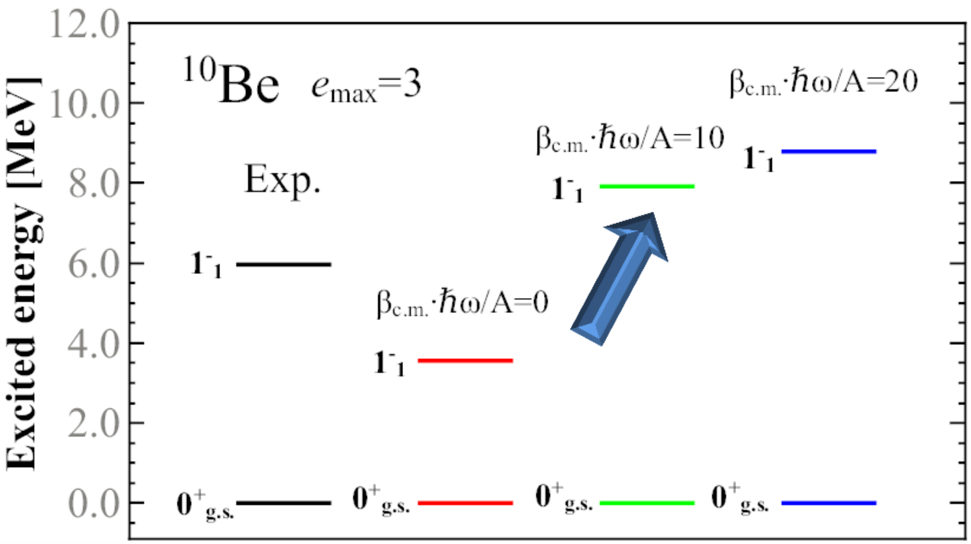
**P:** *s*-shell (~ 1.5) + *p*-shell (~ 2.0)
**N:** *sp*-shell "core" + *sd,pf*-shell "valence"

- **$0^+_2$ : 0d5/2, 0d3/2, 1s1/2 P: 4.1% N: 3.8% total: 8%**

**If the sd-shell is important, NCSM approach may have some difficulty because the full sd-shell configurations cannot be included at 8 ħ Ω truncation.**

# Treatment of Spurious COM motion



# E2 transition

| | $^{10}$Be | | | |
|---|---|---|---|---|
| | Q | $B(E2;2^+_1\rightarrow0^+_1)$ | $B(E2;2^+_2\rightarrow0^+_1)$ | $B(E2;2^+_2\rightarrow2^+_1)$ |
| **Exp.** | | 9.2(3) | 0.11(2) | |
| **MCSM** | -7.71 | 9.29 | 0.32 | 3.28 |

Unit: Q($e$ fm$^2$), B(E2) ($e^2$ fm$^4$)

- E.A. McCutchan, C. J. Lister, R. B. Wiringa, *etc.* Phys. Rev. Lett. **103**, 192501 (2009)

## ➢ GFMC

| $H$ | AV18 | AV18+UIX | AV18+IL2 | AV18+IL7 | Expt. |
|---|---|---|---|---|---|
| $\lvert E_{gs}(0^+)\rvert$ | 50.1(2) | 59.5(3) | 66.4(4) | 64.3(2) | 64.98 |
| $E_x(2^+_1)$ | 2.9(2) | 3.5(3) | 5.0(4) | 3.8(2) | 3.37 |
| $E_x(2^+_2)$ | 2.7(2) | 3.8(3) | 5.8(4) | 5.5(2) | 5.96 |
| $B(E2;2^+_1\rightarrow0^+)$ | 10.5(3) | 17.9(5) | 8.1(3) | 8.8(2) | 9.2(3) |
| $B(E2;2^+_2\rightarrow0^+)$ | 3.3(2) | 0.35(5) | 3.3(2) | 1.7(1) | 0.11(2) |
| $\Sigma B(E2)$ | 13.8(4) | 18.2(6) | 11.4(4) | 10.5(3) | 9.3(3) |

- M. Pervin, S. C. Pieper, and R.B. Wiringa, Phys. Rev. C. **76**, 064319 (2007).

➢ **NCSM** with the CD-BONN, *NN* potential:
$B(E2;\ 2^+_1\rightarrow0^+_{g.s.}) = 6.6\ e^2\ fm^4$

- E. Caurier, P. Navr´atil, W.E. Ormand, and J.P Vary, Phys. Rev. C **66**, 024314 (2002).

# $^{10}$Be: triaxial deformation ?

1) Assuming the $0^+_1$ and the $2^+_1$ states belong to the same K=0 band, the intrinsic quadrupole moment $Q_0$ can be evaluated from the B(E2) and the spectroscopic quadrupole moment
2) The $B(E2; 2^+_2 \to 2^+_1) = 0$, as the transition between $2^+_2$ and $2^+_1$ is forbidden.

$$Q_0 = \frac{(I+1)(2I+3)}{3K^2 - I(I+1)} Q$$

$Q_0 = 20.51\ e\ \mathrm{fm}^2$

$$Q_0 = \left[\frac{16\pi}{5} \cdot B(E2)\right]^{1/2}$$

$Q_0 = 21.61\ e\ \mathrm{fm}^2$

➢ **Seems to suggest axially symmetric deformation**

$B(E2; 2^+_2 \to 2^+_1) = 0.32\ e^2\ \mathrm{fm}^4$

➢ **Breaking of *K* selection rule, triaxially symmetric deformation**

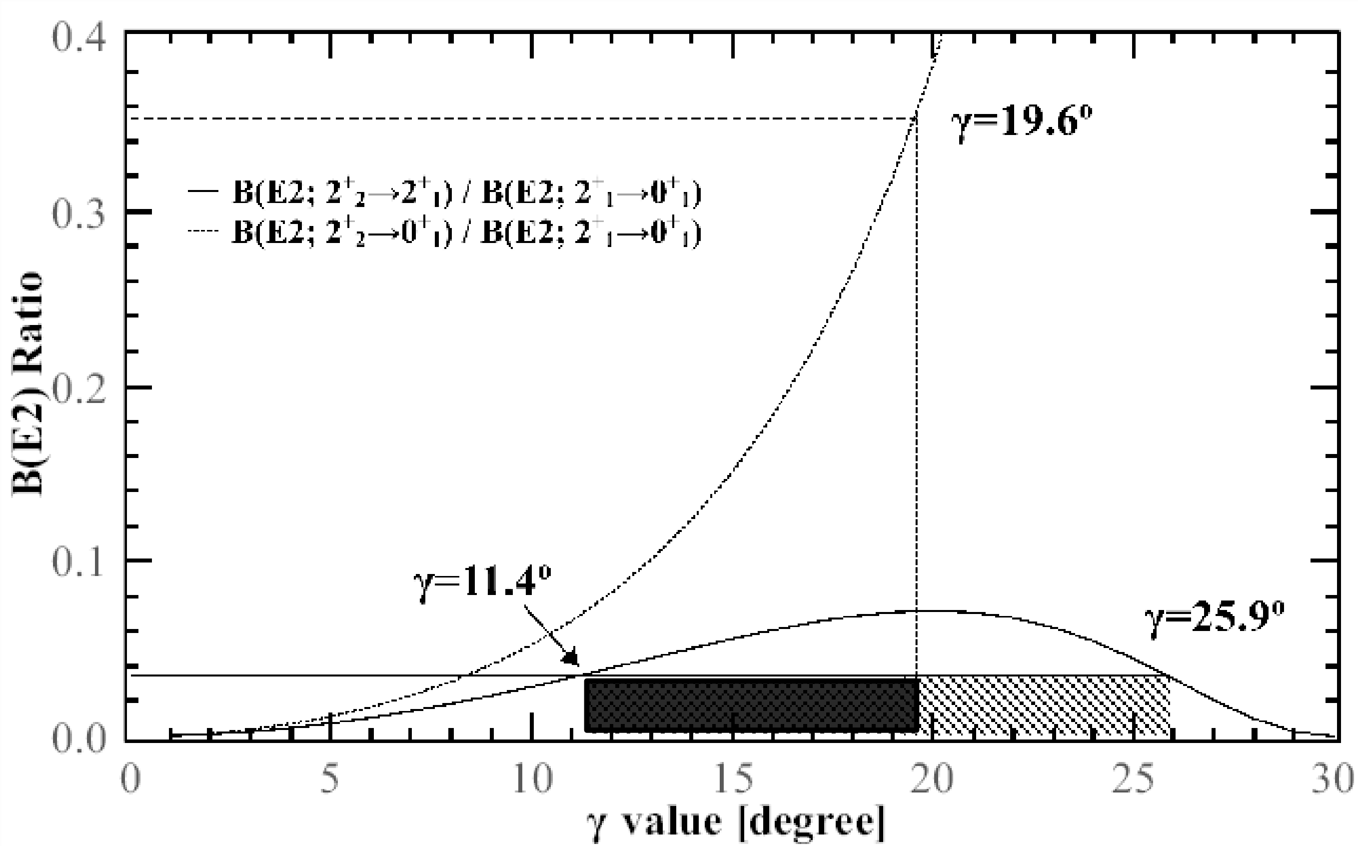
# $^{10}$Be: triaxial deformation ?

**Davydov-Filippov model:**

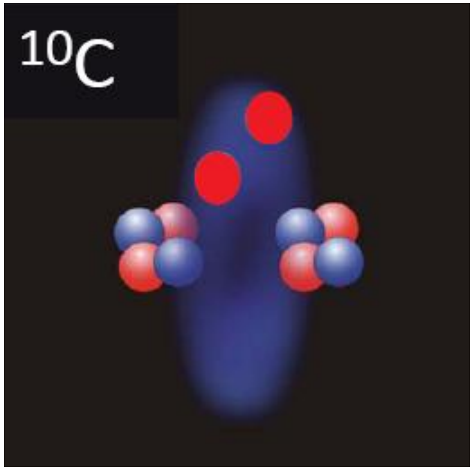
✓ A.S. Davydov and G.F. Filippov, 1958.

$$\frac{B(E2;2_2^+\to 0_1^+)}{B(E2;2_1^+\to 0_1^+)}=\frac{1-\frac{3-2\sin^2(3\gamma)}{\sqrt{9-8\sin^2(3\gamma)}}}{1+\frac{3-2\sin^2(3\gamma)}{\sqrt{9-8\sin^2(3\gamma)}}}$$

$$\frac{B(E2;2_2^+\to 2_1^+)}{B(E2;2_1^+\to 0_1^+)}=\frac{\frac{20}{7}\cdot\frac{3-2\sin^2(3\gamma)}{9-8\sin^2(3\gamma)}}{1+\frac{3-2\sin^2(3\gamma)}{\sqrt{9-8\sin^2(3\gamma)}}}$$



# B(E2) of Mirror nuclei: $^{10}$Be and $^{10}$C




- The mirror symmetry of A=10 nuclei ?
- Evidence of proton halo ?

A Sensitive test lies in the relative B(E2; $2^+ \rightarrow 0^+$)

- **Liquid drop model**

$$B(E2) \propto Q^2 \propto (ZeR_0^2\beta)^2 \Longrightarrow \frac{^{10}\mathrm{C} : B(E2; 2_1^+ \rightarrow 0_1^+)}{^{10}\mathrm{Be} : B(E2; 2_1^+ \rightarrow 0_1^+)} = \left(\frac{6}{4}\right)^2$$

**The B(E2) of $^{10}$C should be LARGER than that of $^{10}$Be**

- **Shell model**

$$B(E2; 2_1^+ \rightarrow 0_1^+) \propto [3.2 + 0.1 \times T_z]^2$$

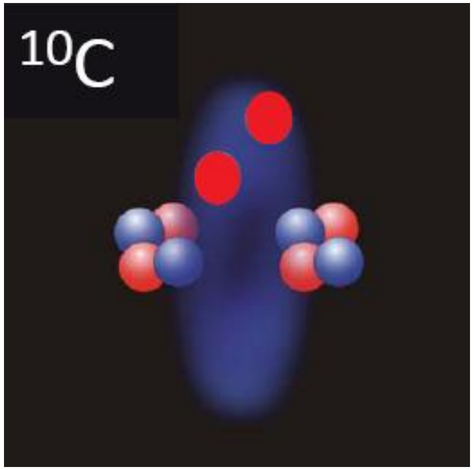
**$^{10}$C: $T_z$ = -1**
**$^{10}$Be: $T_z$=1**

- Alburger, *et al.*, Phys. Rev. 1969

**The B(E2) of $^{10}$C should be SMALLER than that of $^{10}$Be**

# B(E2) of Mirror nuclei: $^{10}$Be and $^{10}$C

- The mirror symmetry of A=10 nuclei ?
- Evidence of proton halo ?




A Sensitive test lies in the relative B(E2; $2^+ \rightarrow 0^+$)

**Expt.** B(E2; $2^+_1 \rightarrow 0^+_1$) = 8.8(3) $e^2$ fm$^4$

## GFMC (AV18)

B(E2; $2^+ \rightarrow 0^+$) ~ 4 $e^2$ fm$^4$

## (AV18+IL2)

B(E2; $2^+ \rightarrow 0^+$) ~ 15 $e^2$ fm$^4$

- priv. com. with E. A. McCutchan

## NCSM (CD Bonn)

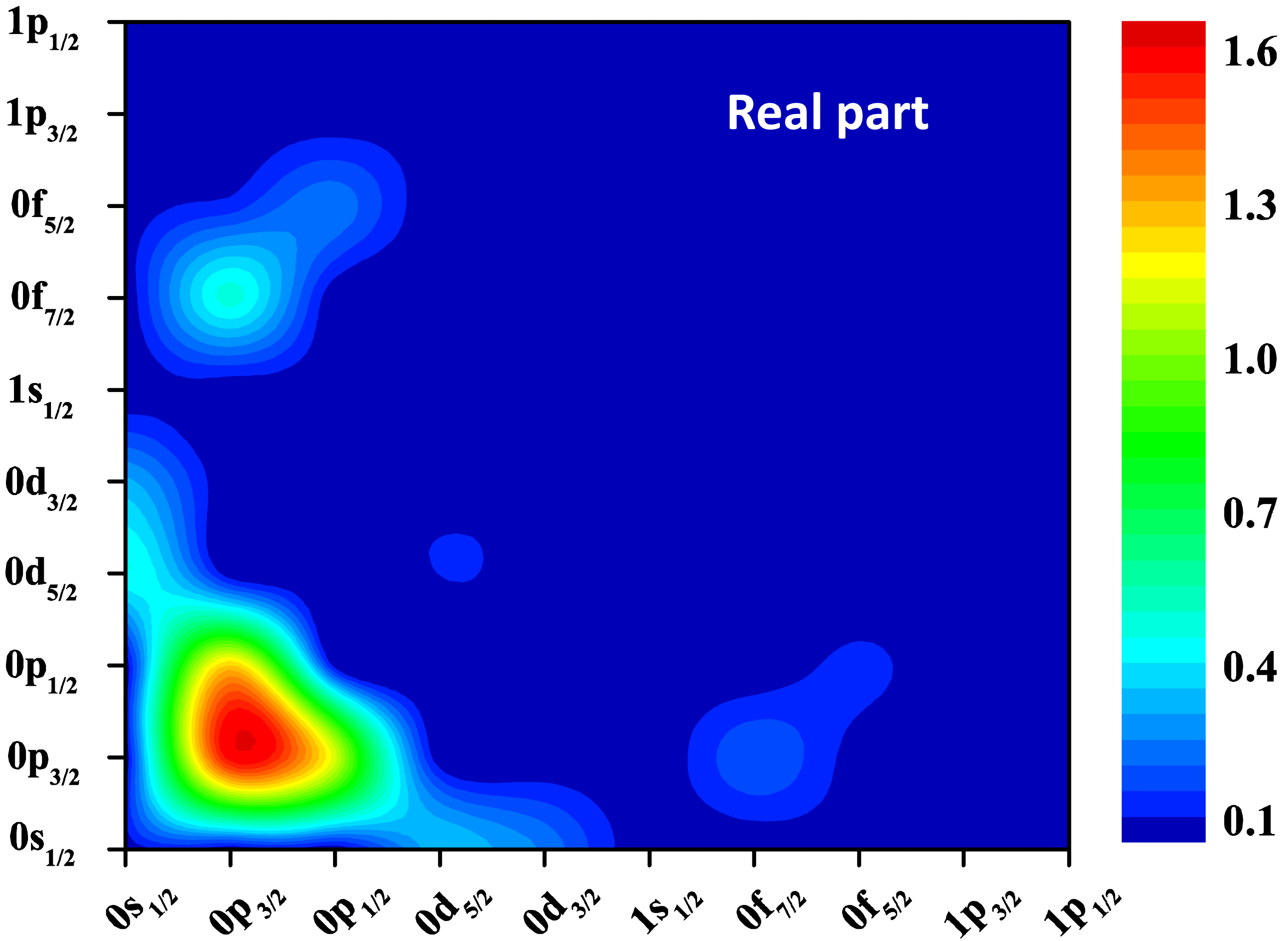
B(E2; $2^+ \rightarrow 0^+$) = 5.7 $e^2$ fm$^4$

- E. Caurier, P. Navratil, W. Ormand, and J. Vary, Phys. Rev. C **66**, 024314 (2002)

## MCSM (N$^3$LO)

B(E2; $2^+ \rightarrow 0^+$) = 9.30 $e^2$ fm$^4$

# Schematic illustration of reduced matrix elements of $^{10}C$ $B(E2;2^+_1 \rightarrow 0^+_{g.s.})$ between single particle orbits



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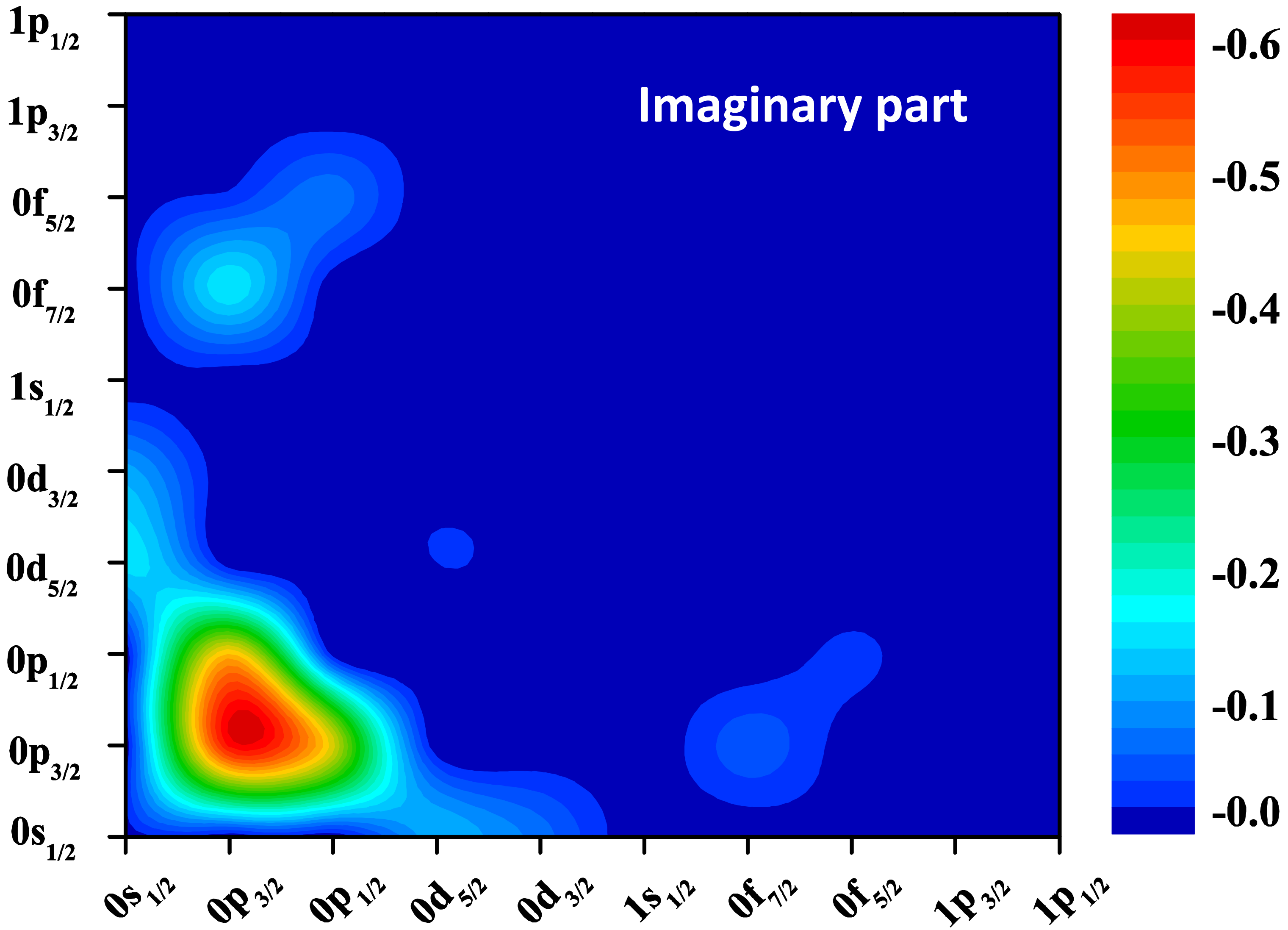

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# Summary and outlook

- **For the first time in this work, we apply the UCOM potential to the MCSM for calculating some light exotic nuclei in an *ab-initio* way.**

- **We calculate the low lying spectra of Beryllium isotopes in $e_{max}$=3 model space with and without treatment of spurious COM motion.**

**1) The results of $2^+_1$ and $2^+_2$ state excitation energies for $^{10}$Be with Lawson's prescription $\beta_{c.m.}=10\hbar\omega/A$ are closed to the experimental data;**

**2) The deformation property has been investigated in terms of the quardrupole moments, the occupation number and the E2 transition probabilities. Triaxially symmetric deformation is revealed;**

**3) The sensitivity of spurious COM has been investigated.**

# Summary and outlook

- **In *ab initio* sense, more larger model space is needed to obtain the exact the experimental data, e.g. the binding energy.**

- **Even employing unitary transformation, UCOM potential transformed from $N^3LO$ interaction is still "hard" for the MCSM calculation.**

# Thank you !