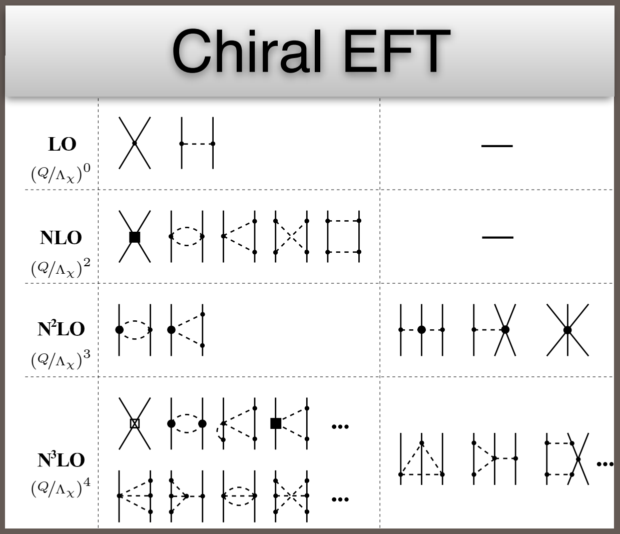
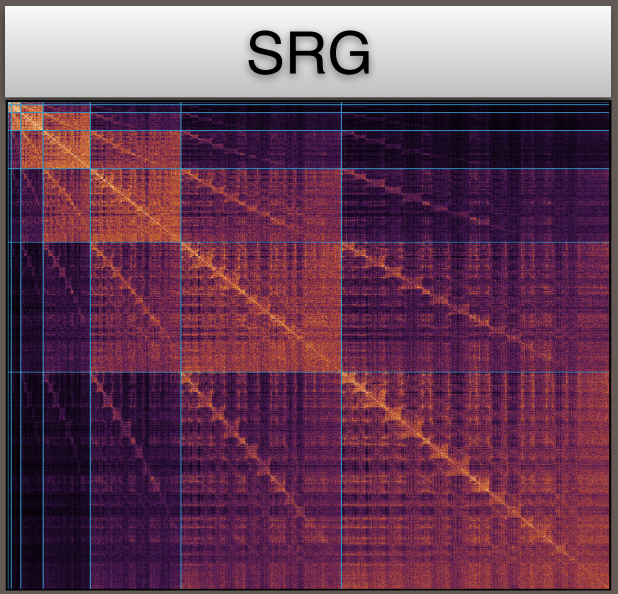
Probing Nuclear Forces in ab initio Nuclear Reactions

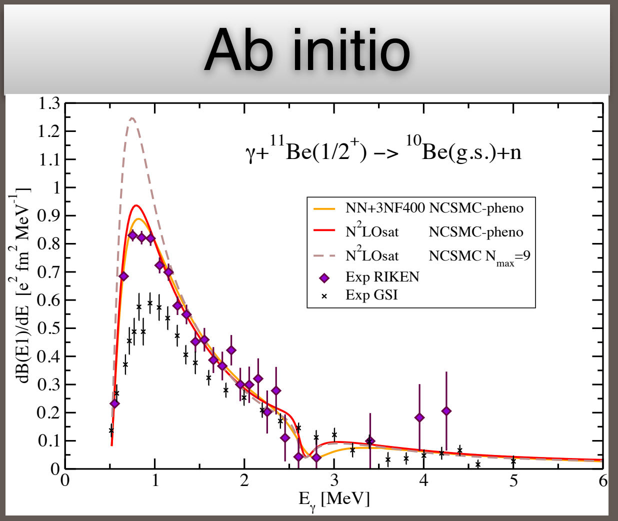
Progress in Ab Initio Techniques in Nuclear Physics

March 1 2017, TRIUMF, Vancouver

Angelo Calci | TRIUMF







Chiral NN+3N Interactions

Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs, Bernard,...

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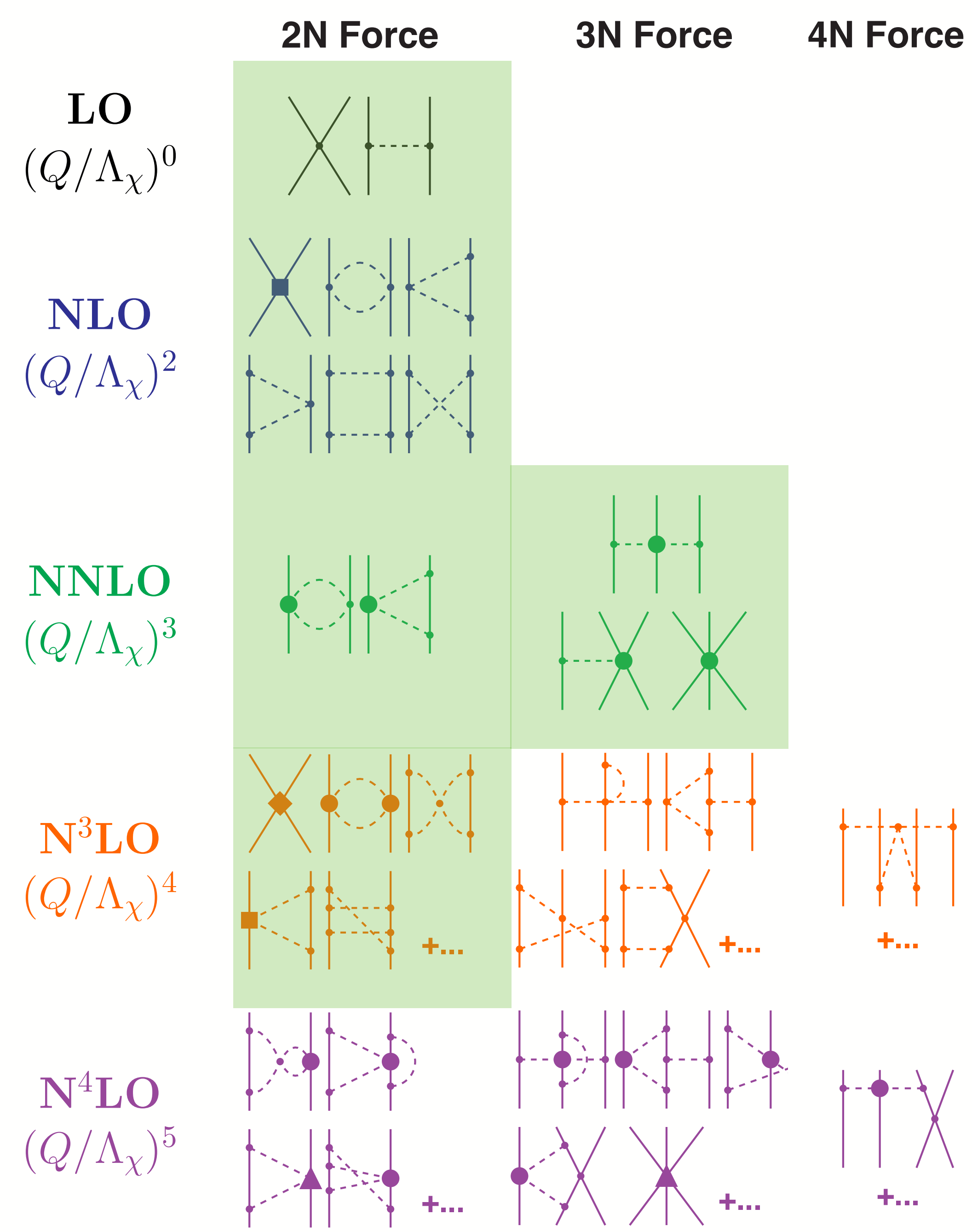
  - 3N @ N^2LO: Navrátil, local cutoff, modifications of cutoff



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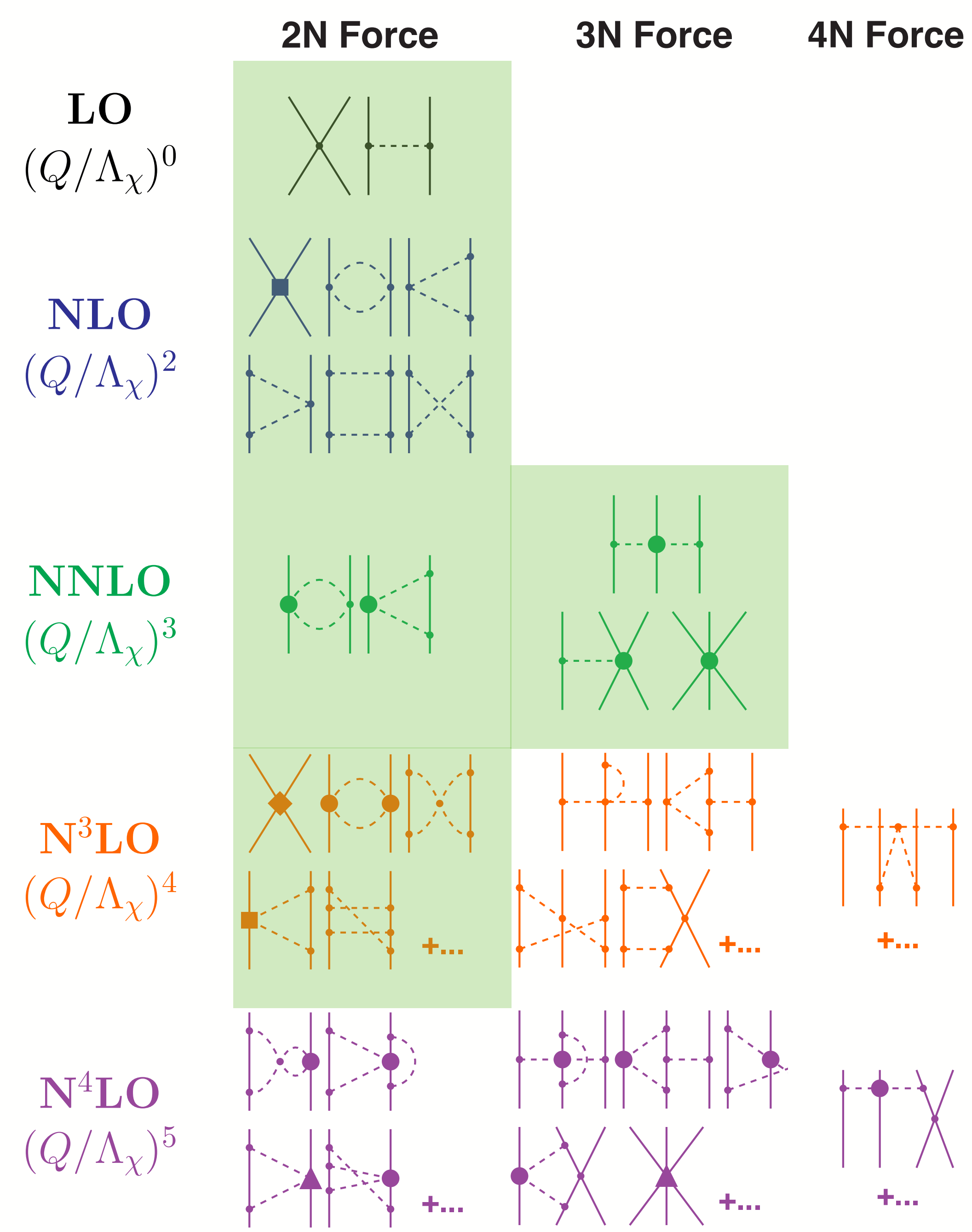

chiral interactions are not unique:

- chiral order
- regularization
- fit of LECs

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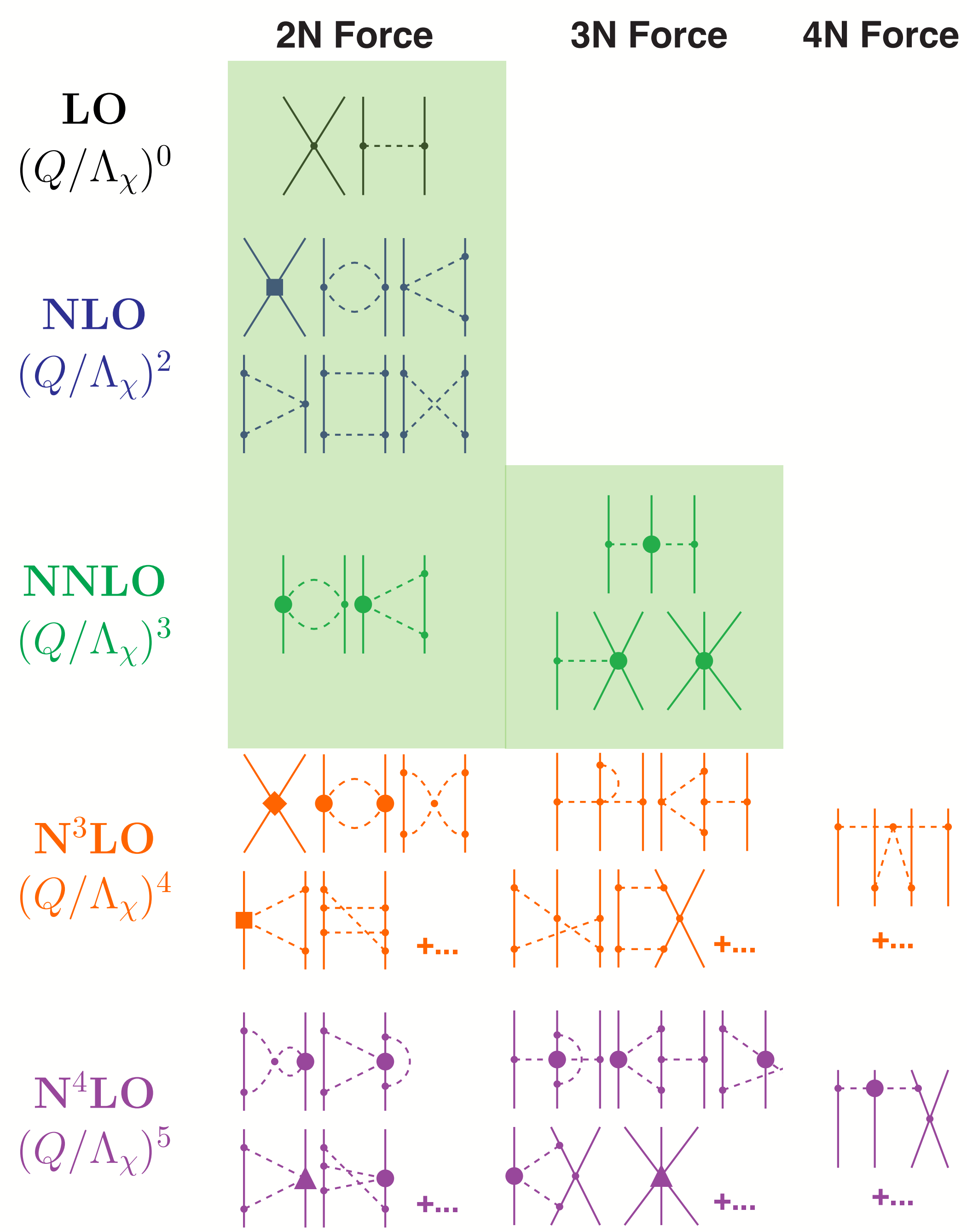

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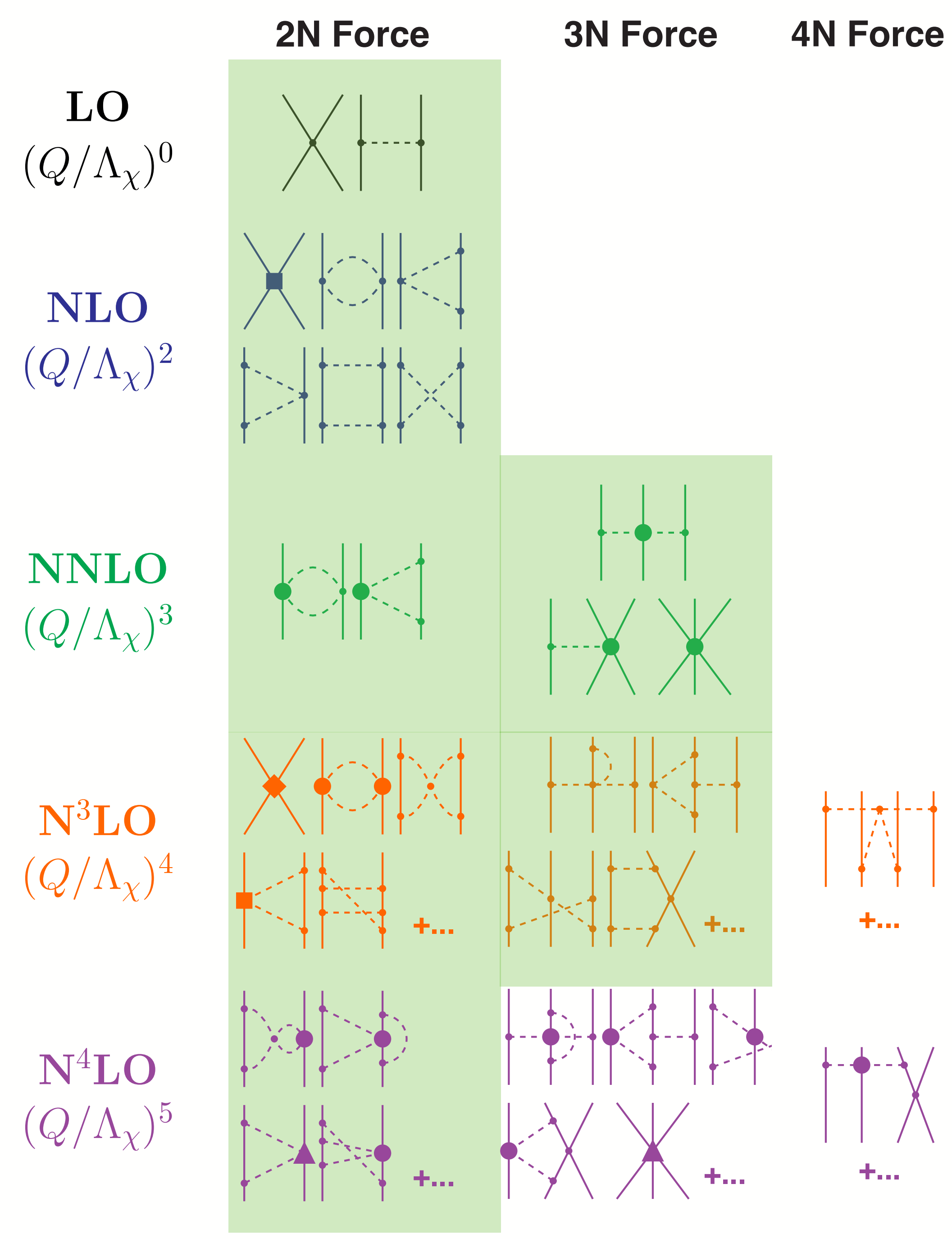

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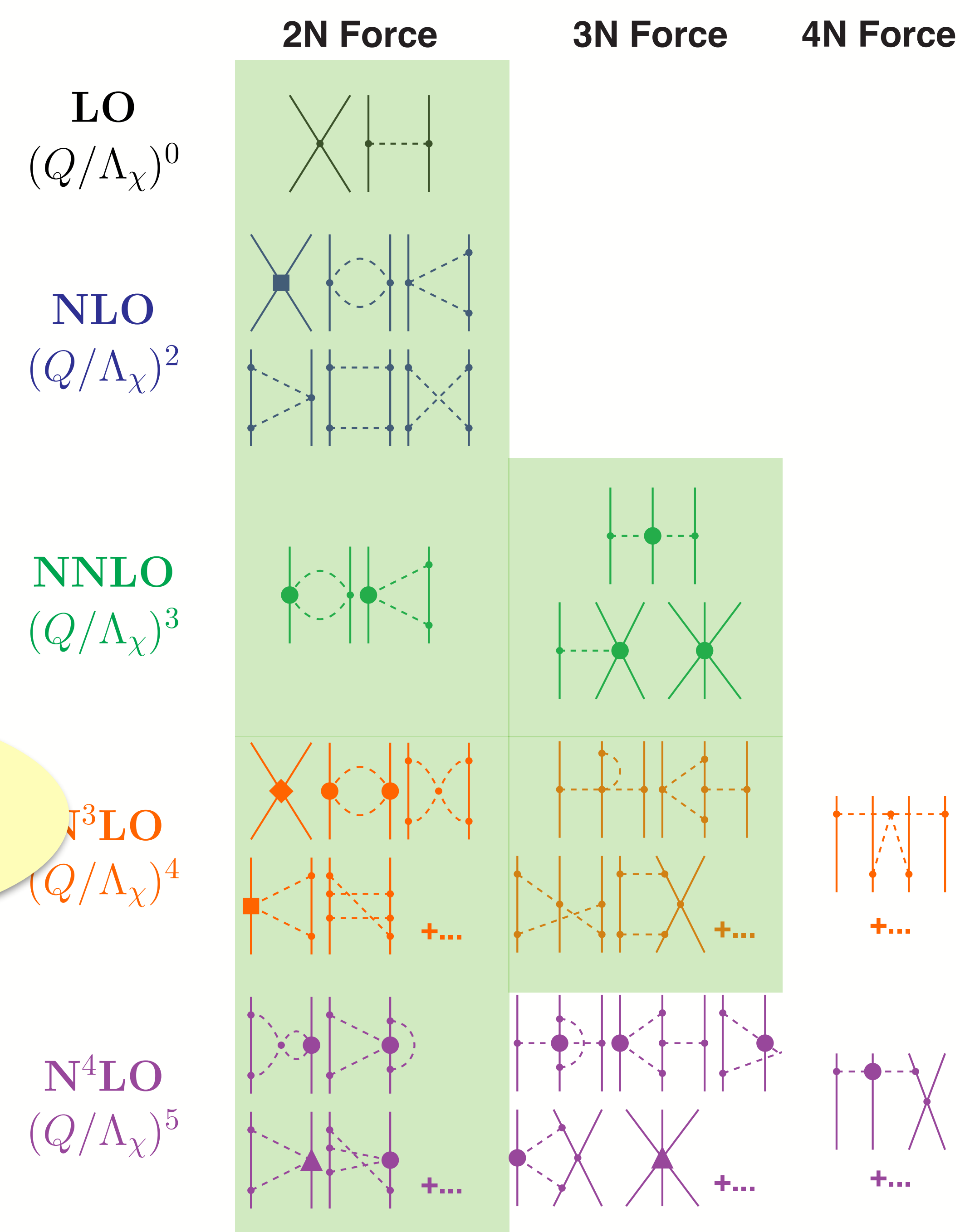
talk by Kai Hebeler



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- **$N^4LO(500)$:**
  - NN @ N^4LO: Machleidt et al., 500MeV cutoff

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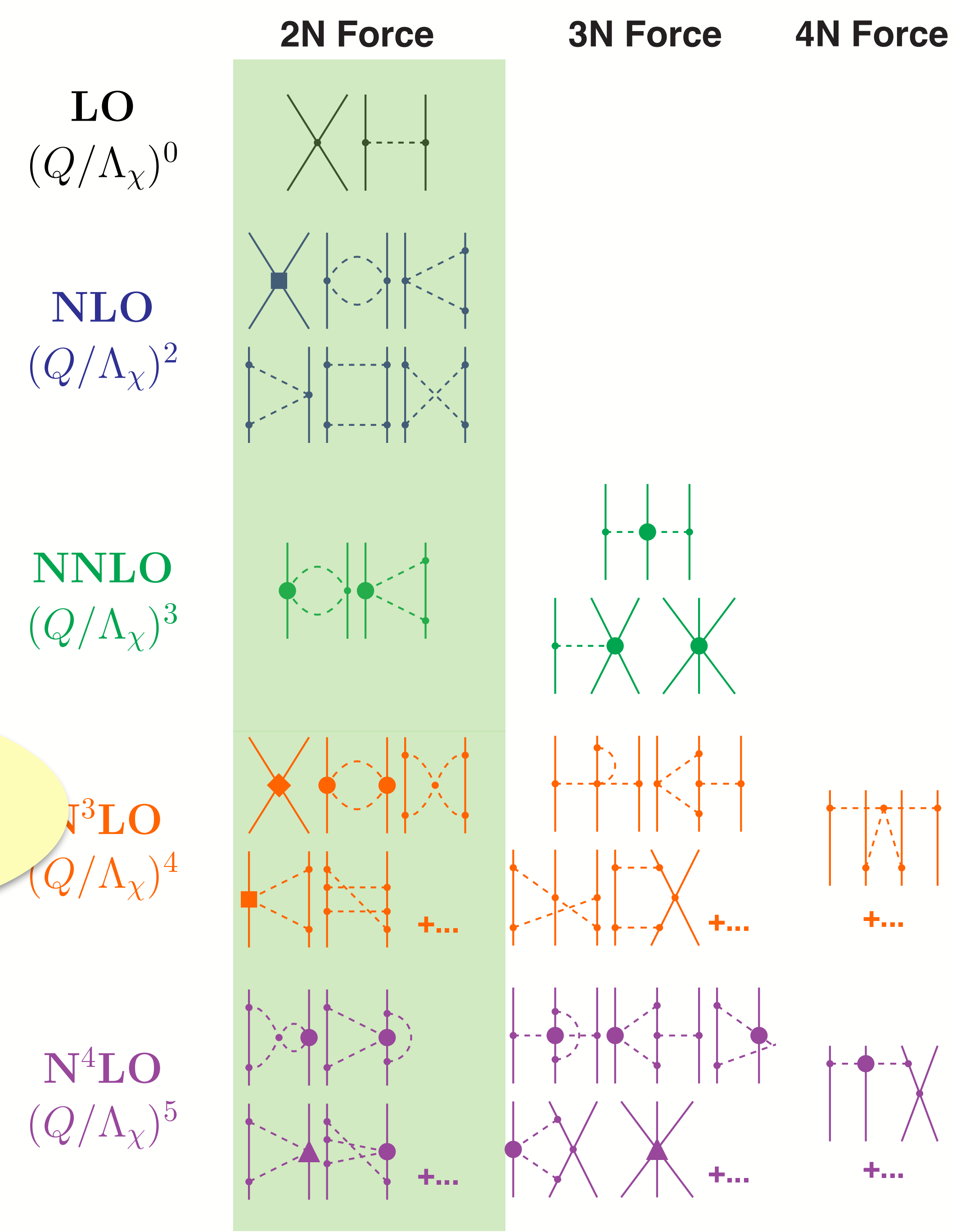


Similarity Renormalization Group (SRG)

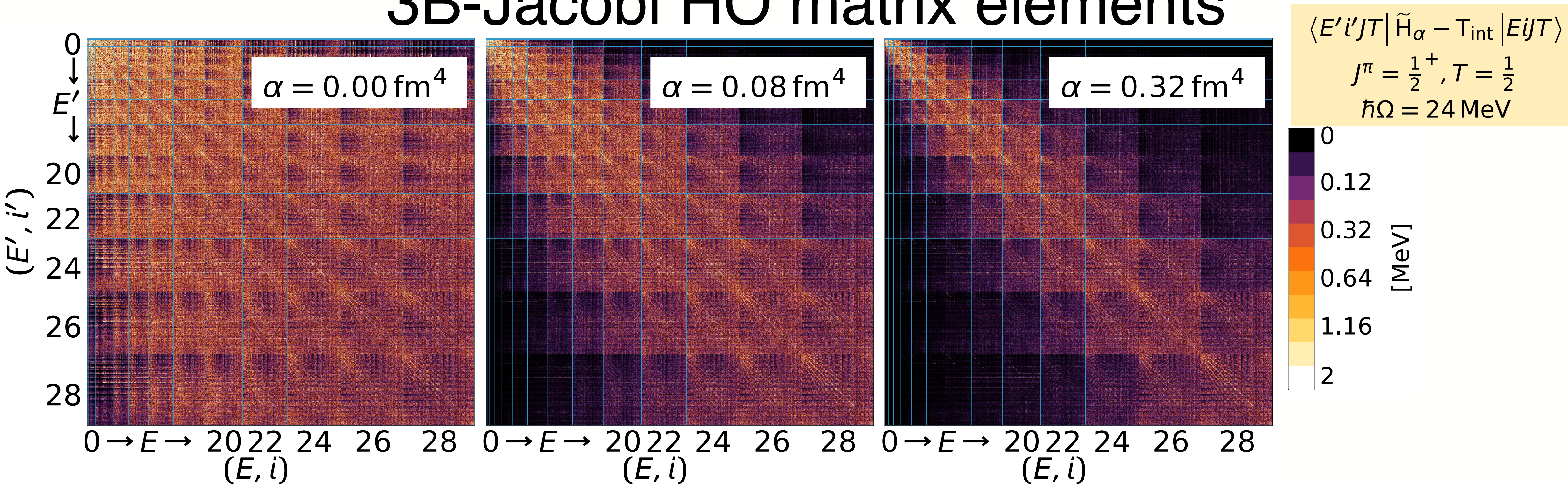
accelerate convergence by **pre-diagonalizing** the Hamiltonian with respect to the many-body basis

- **unitary transformation leads to evolution equation**

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}_\alpha = [\eta_\alpha, \widetilde{\mathrm{H}}_\alpha] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 [\mathrm{T}_{\mathrm{int}}, \widetilde{\mathrm{H}}_\alpha] = -\eta_\alpha^\dagger$$

advantages of SRG: **flexibility** and **simplicity**

3B-Jacobi HO matrix elements



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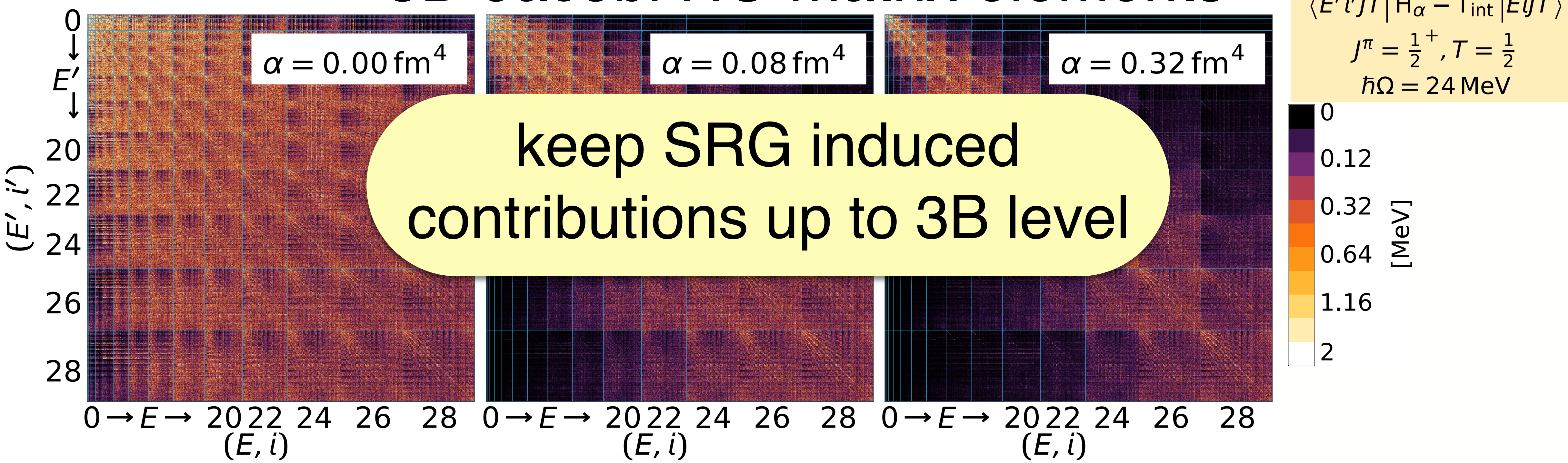
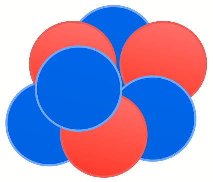


keep SRG induced contributions up to 3B level

Continuum effects in Nuclei

Baroni, Navrátil, Quaglioni *Phys. Rev. Lett. 110, 022505 (2013)*

ab initio description of nuclei



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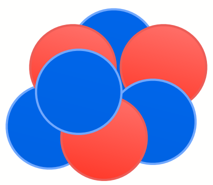

bound states & spectroscopy

(IT-)NCSM
ab initio description of nuclear clusters

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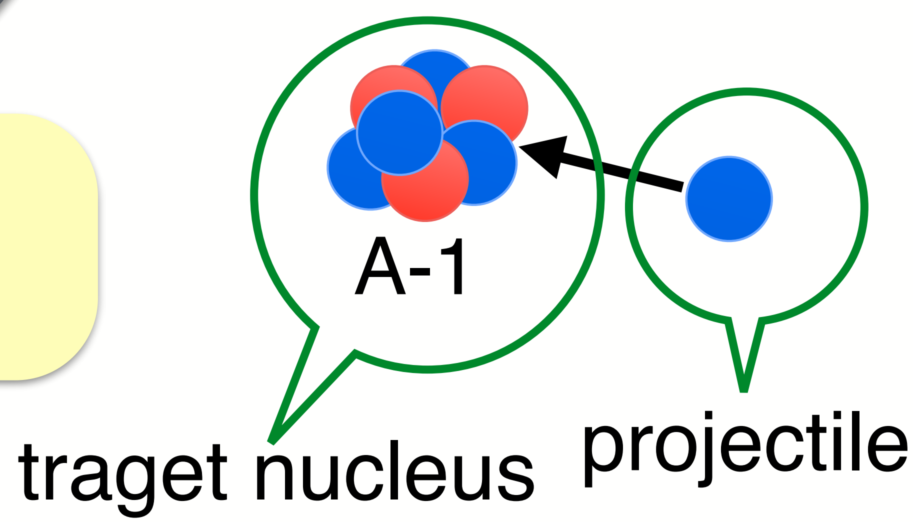

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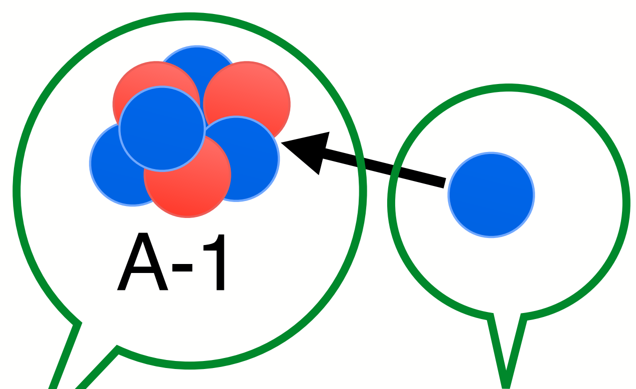

traget nucleus

projectile

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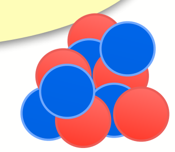
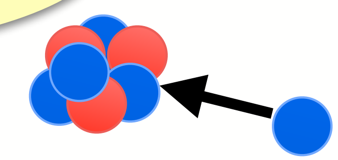
NCSM/RGM and NCSMC
continuum effects in spectroscopy

NCSM with Continuum (NCSMC)

- representing $H\left|\Psi^{J\pi T}\right\rangle = E\left|\Psi^{J\pi T}\right\rangle$ using the **over-complete basis**

$$\left|\Psi^{J\pi T}\right\rangle = \sum_{\lambda} c_{\lambda}\left|\Psi_A E_{\lambda} J^{\pi} T\right\rangle + \sum_{\nu}\int \mathrm{d}r\, r^2 \frac{\chi_{\nu}(r)}{r}\left|\xi_{\nu r}^{J\pi T}\right\rangle$$





expansion in A-body NCSM eigenstates

relative motion of clusters NCSM/RGM expansion

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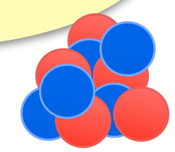

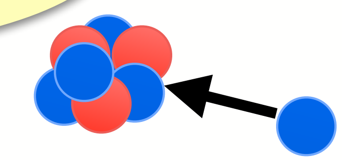

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H_{NCSM}: covered by NCSM

h: given by $\left\langle \Psi_A E_{\lambda'} J^\pi T \right| H \left|\xi_{\nu r}^{J^\pi T}\right\rangle$

$\mathcal{H}$: contains NCSM/RGM Hamiltonian kernel

Continuum effects and Nuclear Reactions

with
P. Navrátil, S. Quaglioni,
R. Roth, J. Dohet-Eraly G. Hupin

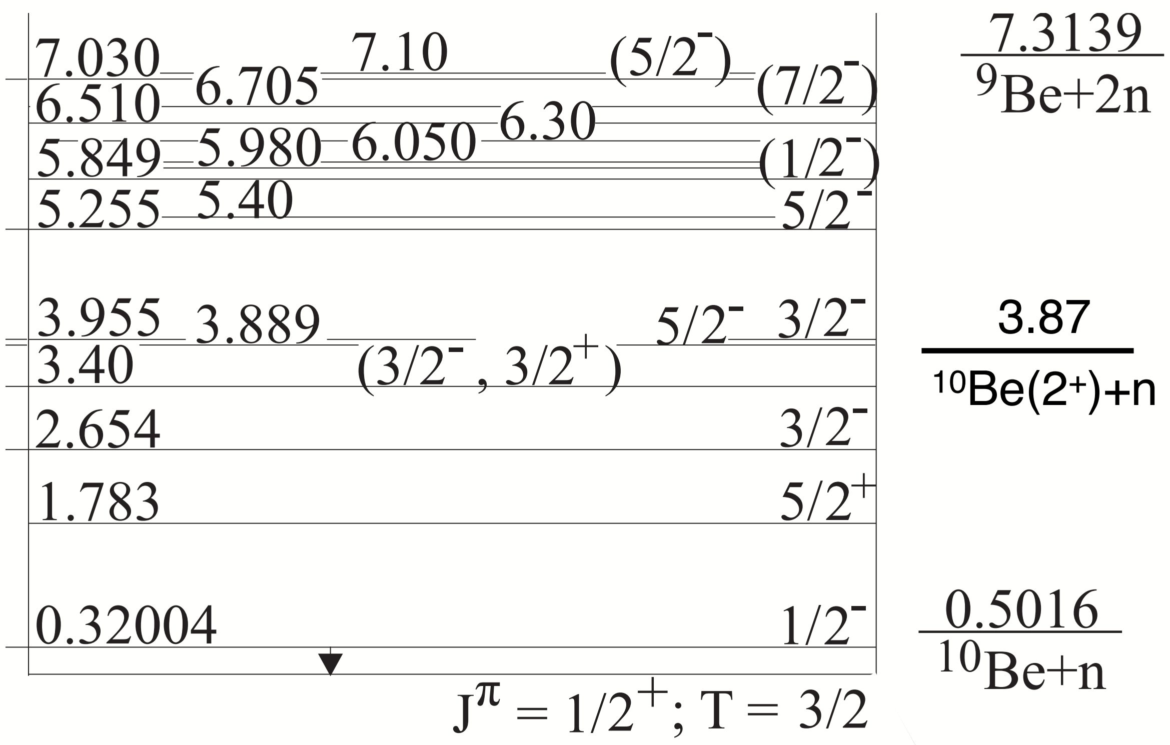
Neutron-rich halo Nucleus ^{11}Be

PRL **117,** 242501 (2016) PHYSICAL REVIEW LETTERS week ending 9 DECEMBER 2016

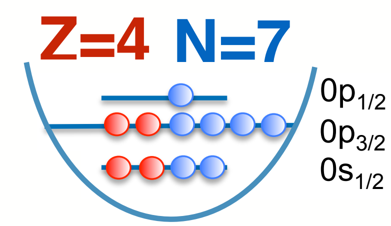
Can *Ab Initio* Theory Explain the Phenomenon of Parity Inversion in ^{11}Be?

Angelo Calci,[1,*] Petr Navrátil,[1,†] Robert Roth,[2] Jérémy Dohet-Eraly,[1,‡] Sofia Quaglioni,[3] and Guillaume Hupin[4,5]
[1]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada*
[2]*Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*
[3]*Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA*
[4]*Institut de Physique Nucléaire, Université Paris-Sud, IN2P3/CNRS, F-91406 Orsay Cedex, France*
[5]*CEA, DAM, DIF, F-91297 Arpajon, France*

Spectrum



- **parity inversion**
  shell model predicts
  g.s. to be $J^{\pi}=1/2^{-}$



- **Halo structure**
  weakly bound J=1/2 states
  spectrum dominated by n-^{10}Be

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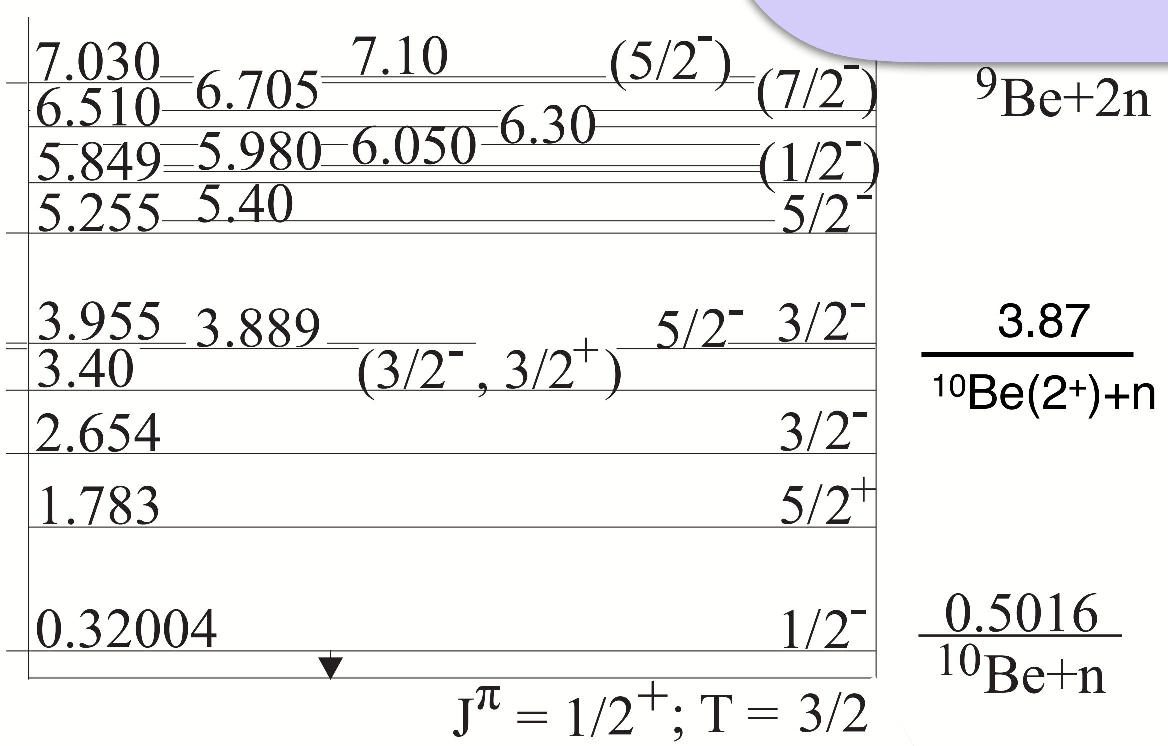
[2]Institut für … tadt, Germany
[3]Lawrence Liver… fornia 94551, USA
[4]Institut de Phy… ay Cedex, France

Can **ab initio** theory describe this complicated system?



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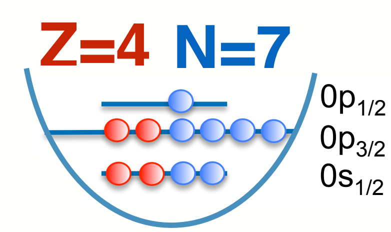

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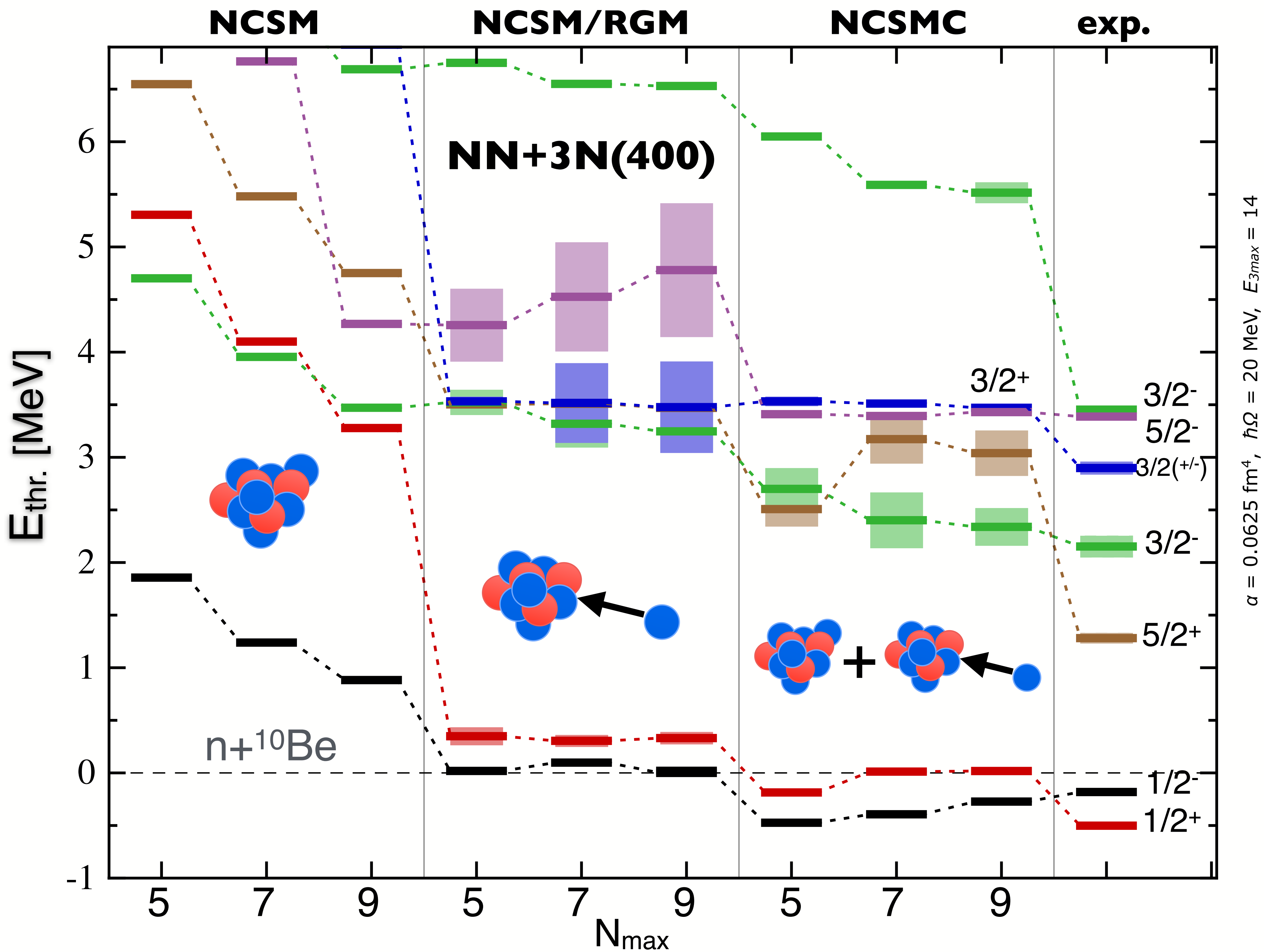
^{11}Be excitation spectrum



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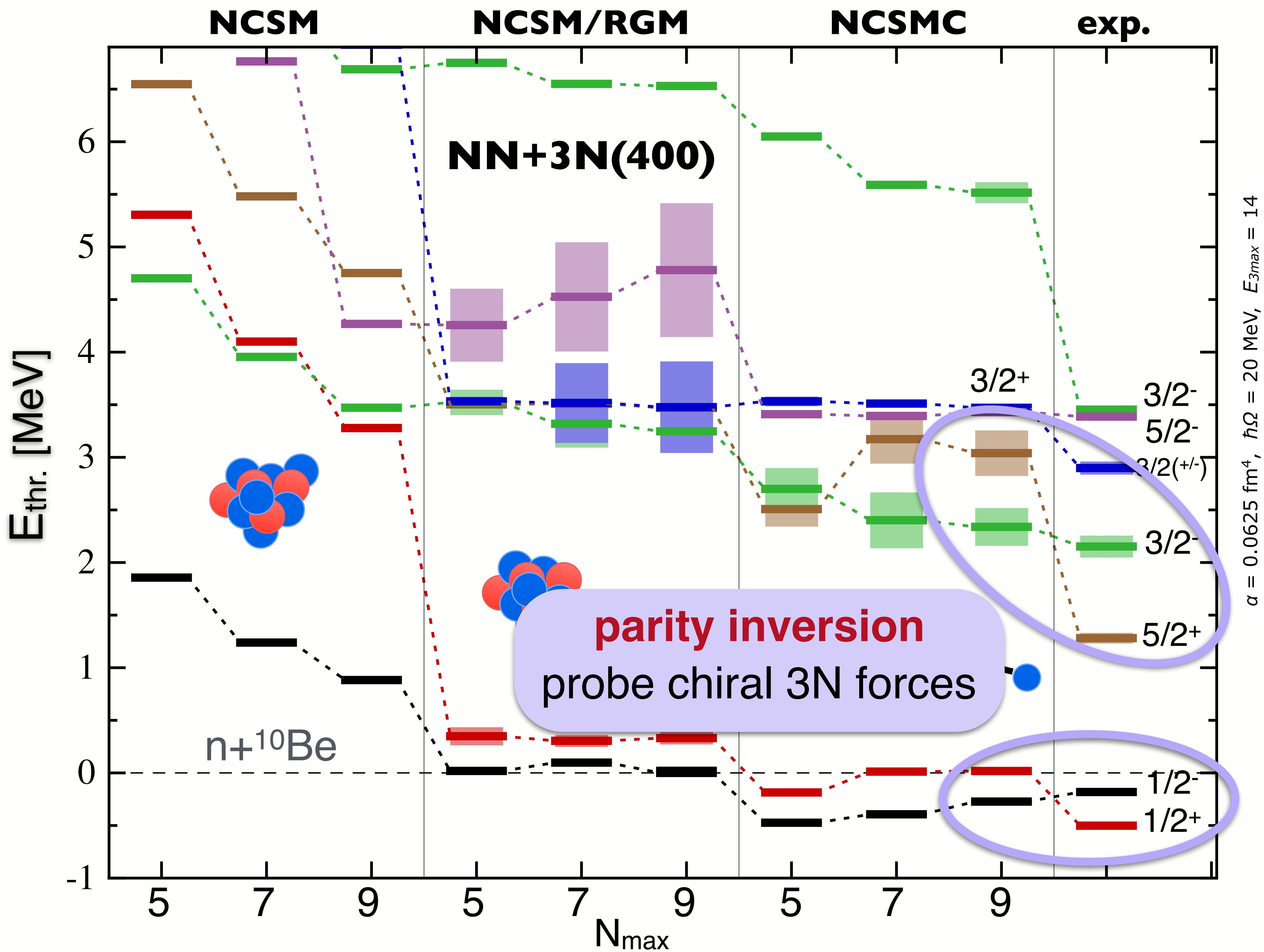

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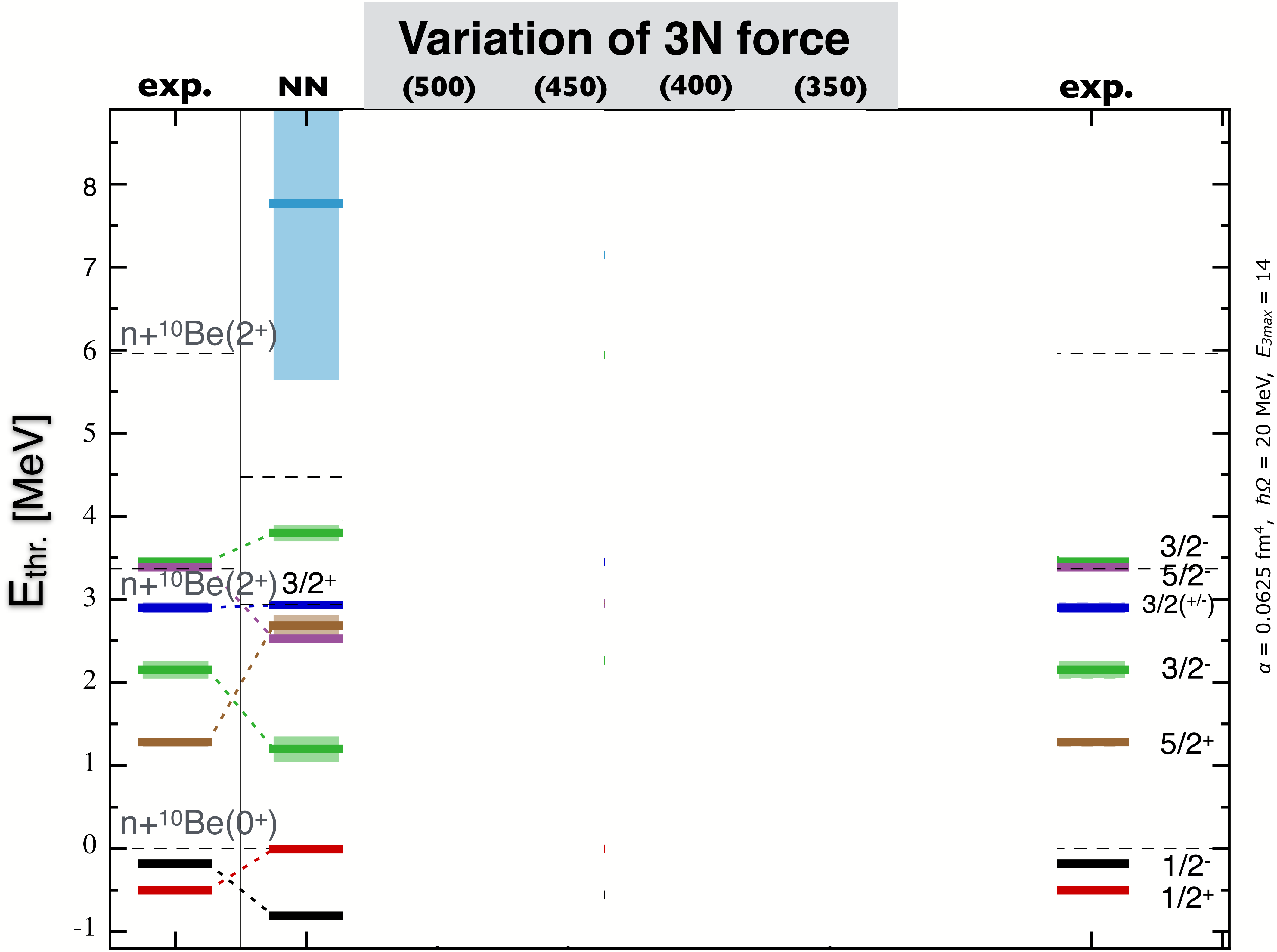

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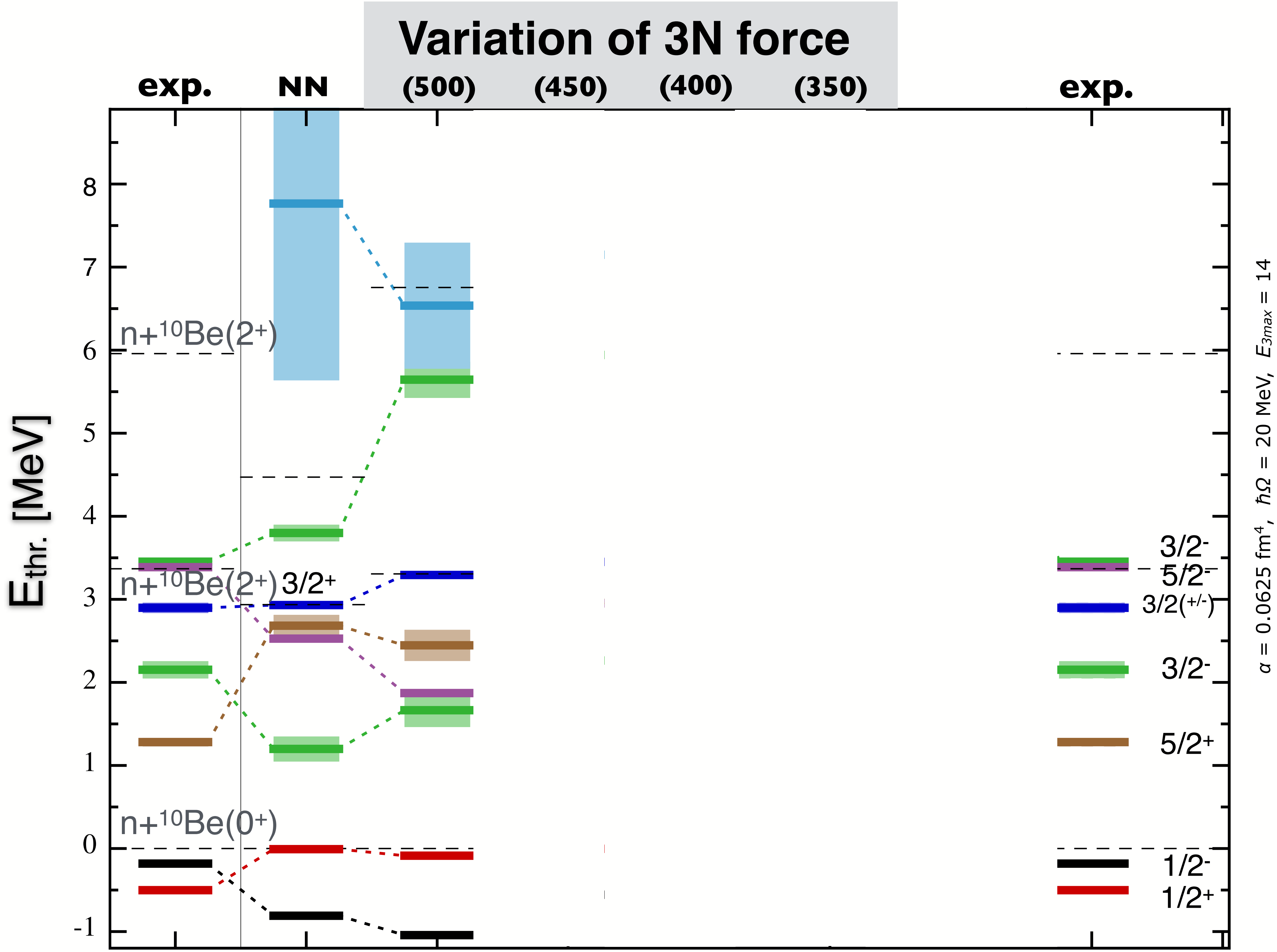

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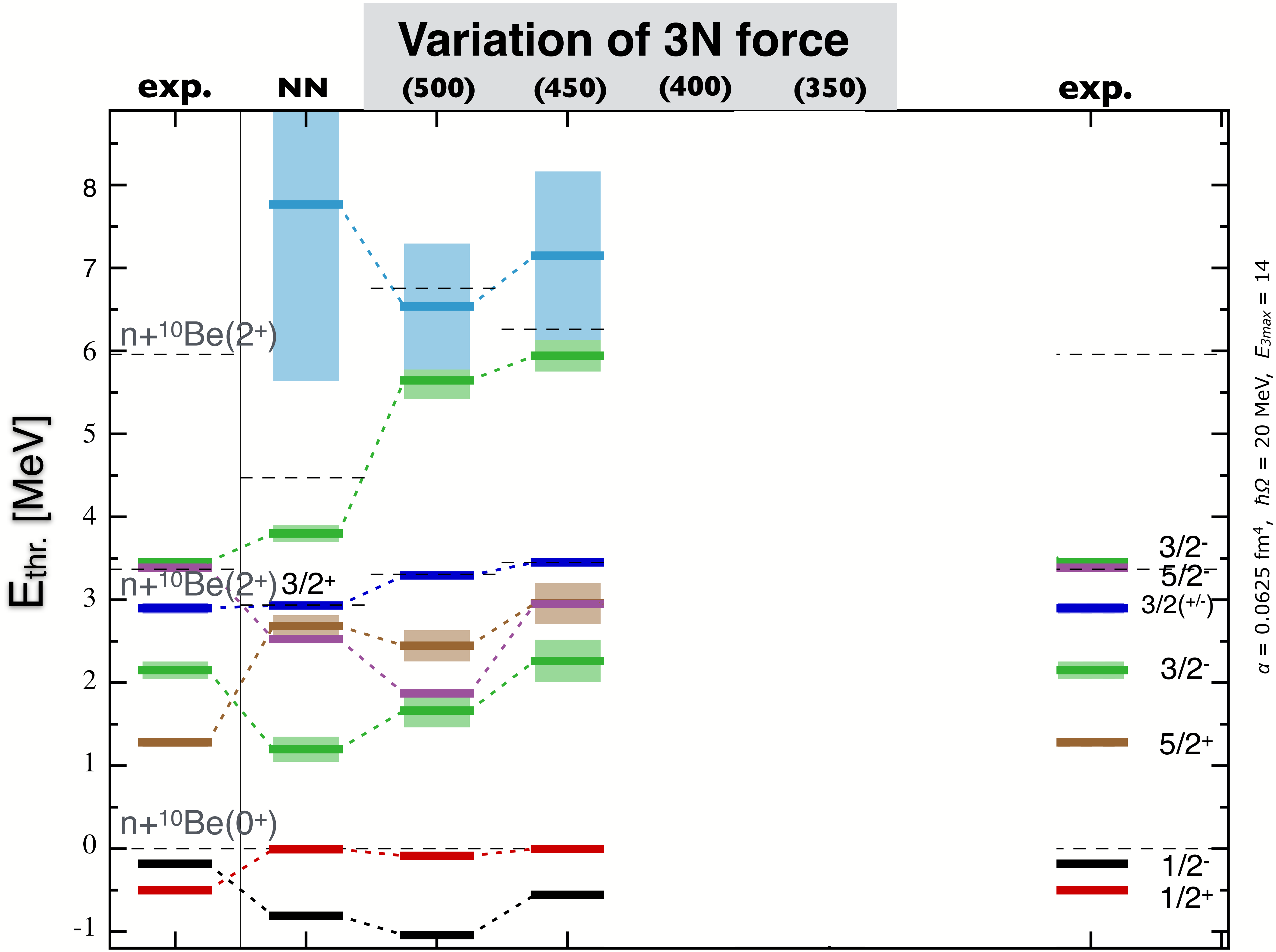

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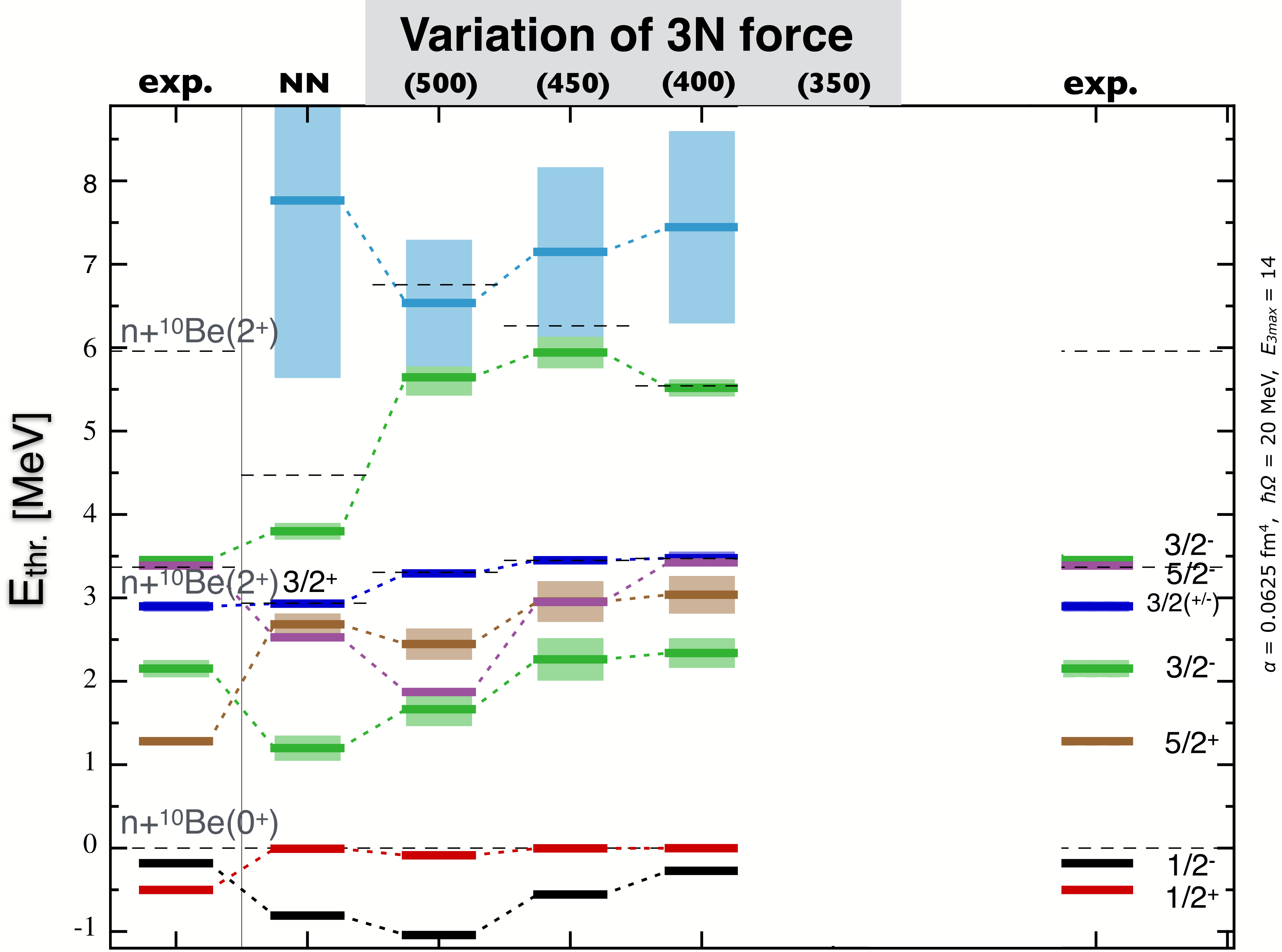

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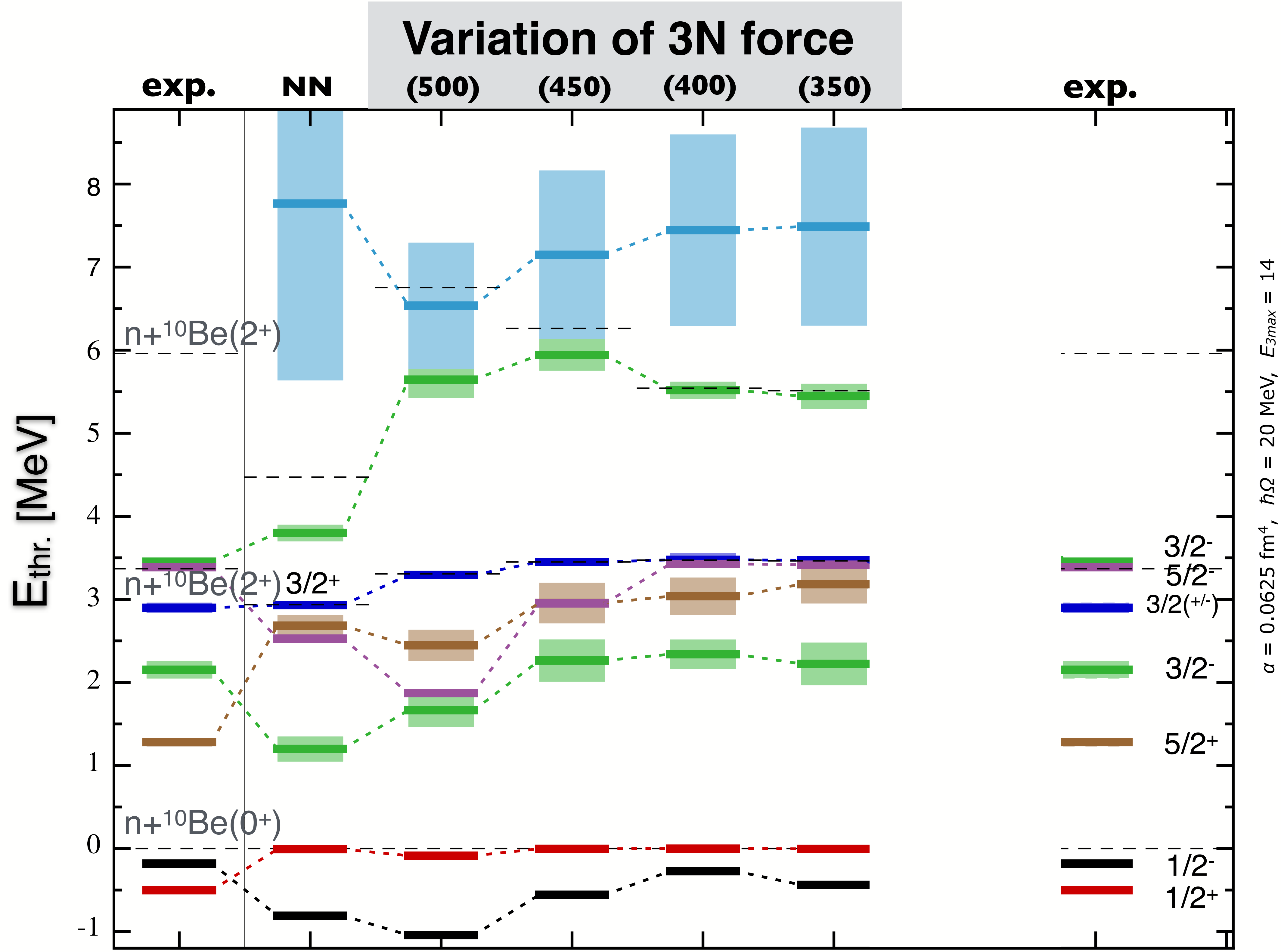

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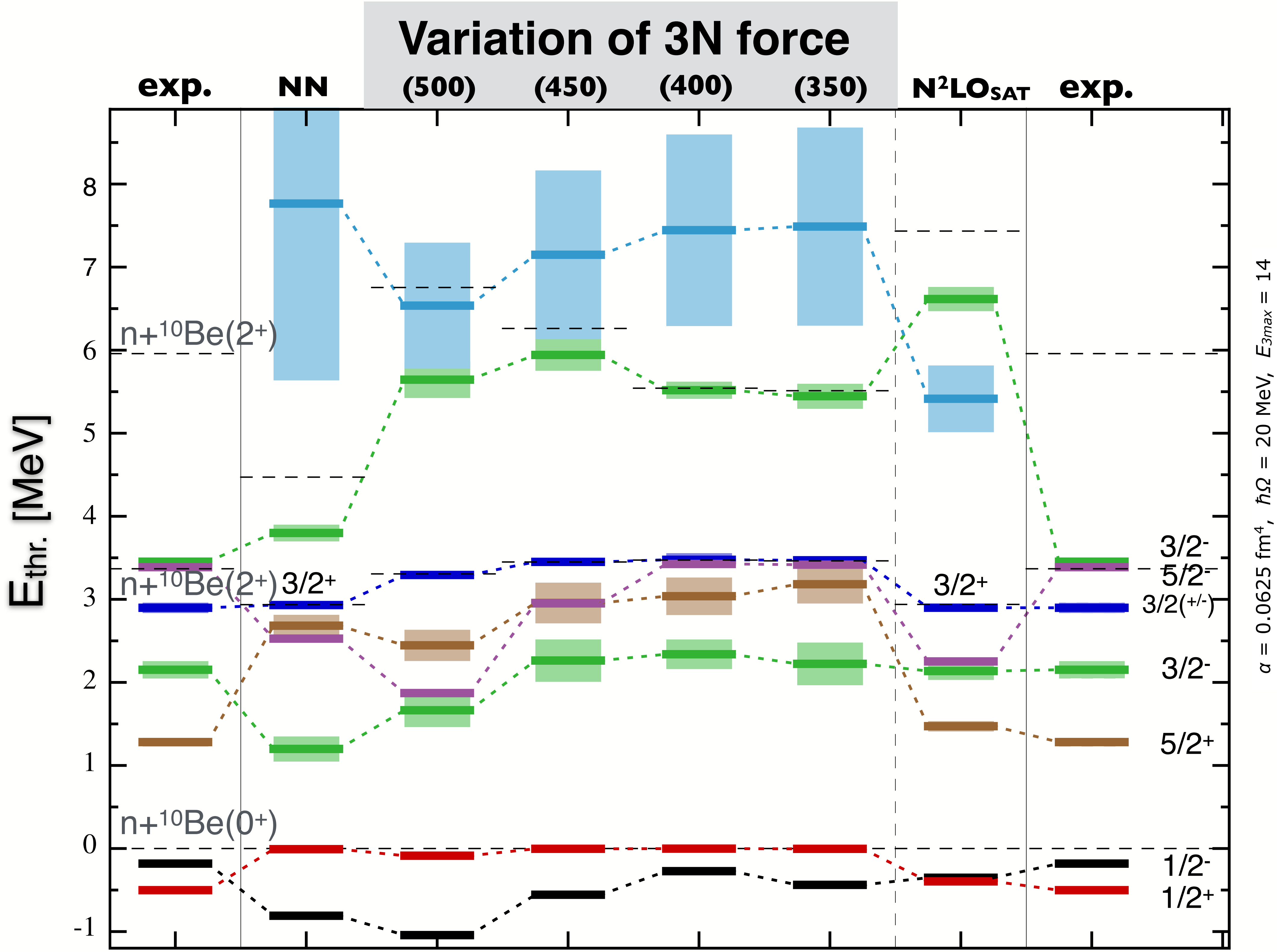

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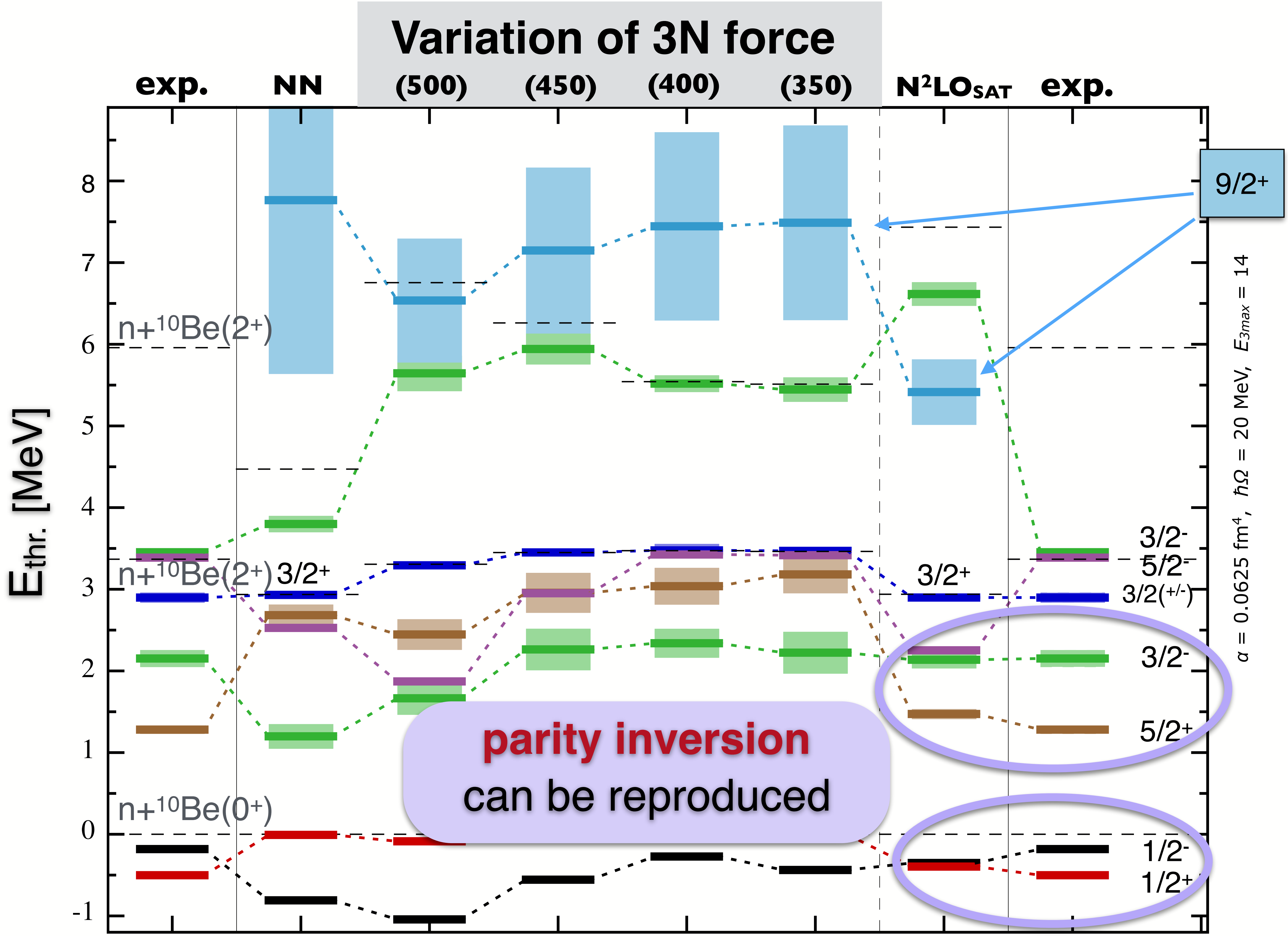

^{11}Be: Photodisintegration process & E1 transition

B(E1:1/2$^-$→1/2$^+$) [e^{2}fm^2]

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NN+3N(400)	0.0005	-	0.146	0.102(2)*
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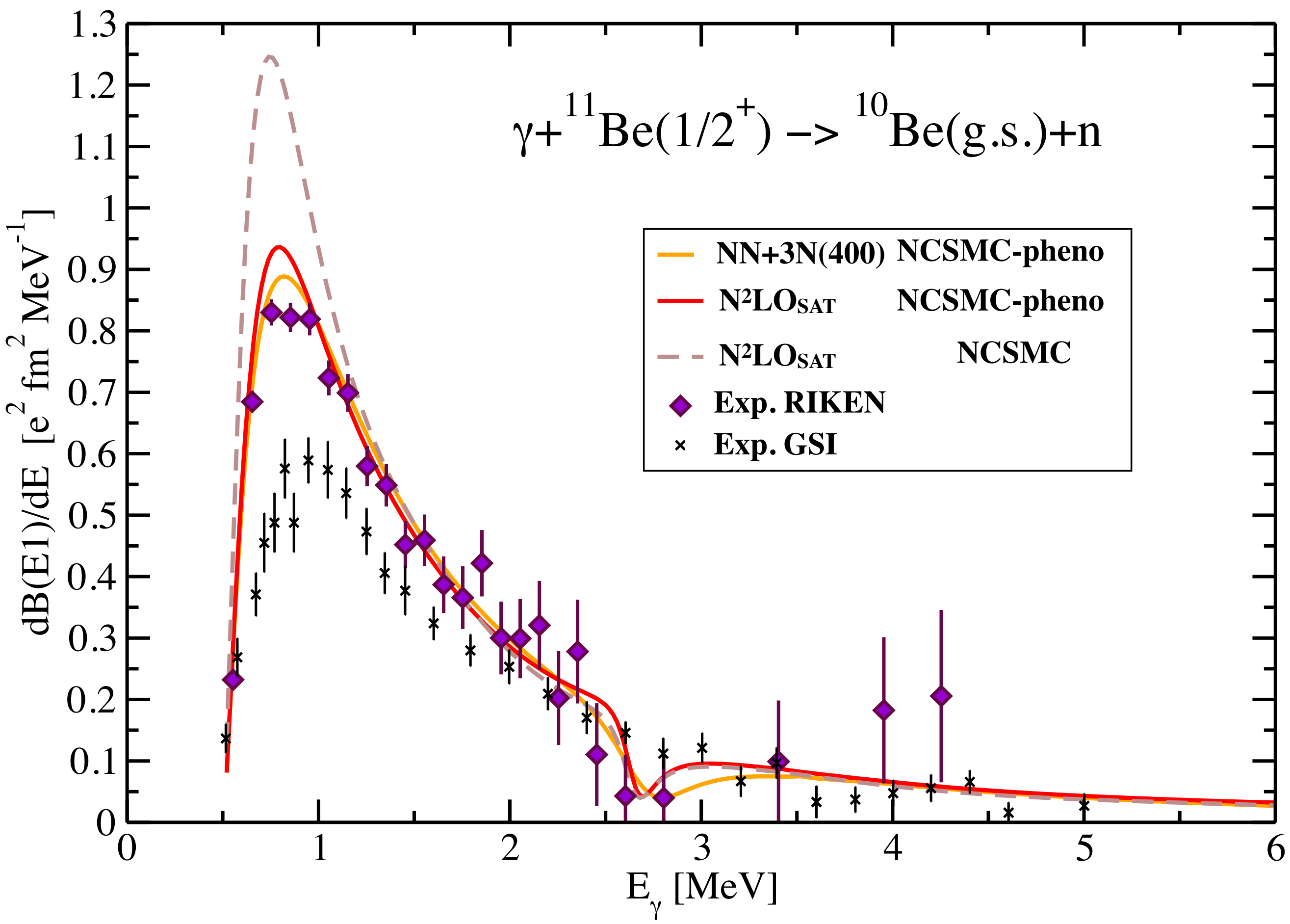

- **strongest known E1** transition between low-lying states (attributed to halo structure)
- reproduced **only** with **continuum effects**
- **conflicting** experimental **measurements**
- ab initio results:
  - **discriminate** between measurements
  - **predict dip** at 3/2$^-$ resonance energy

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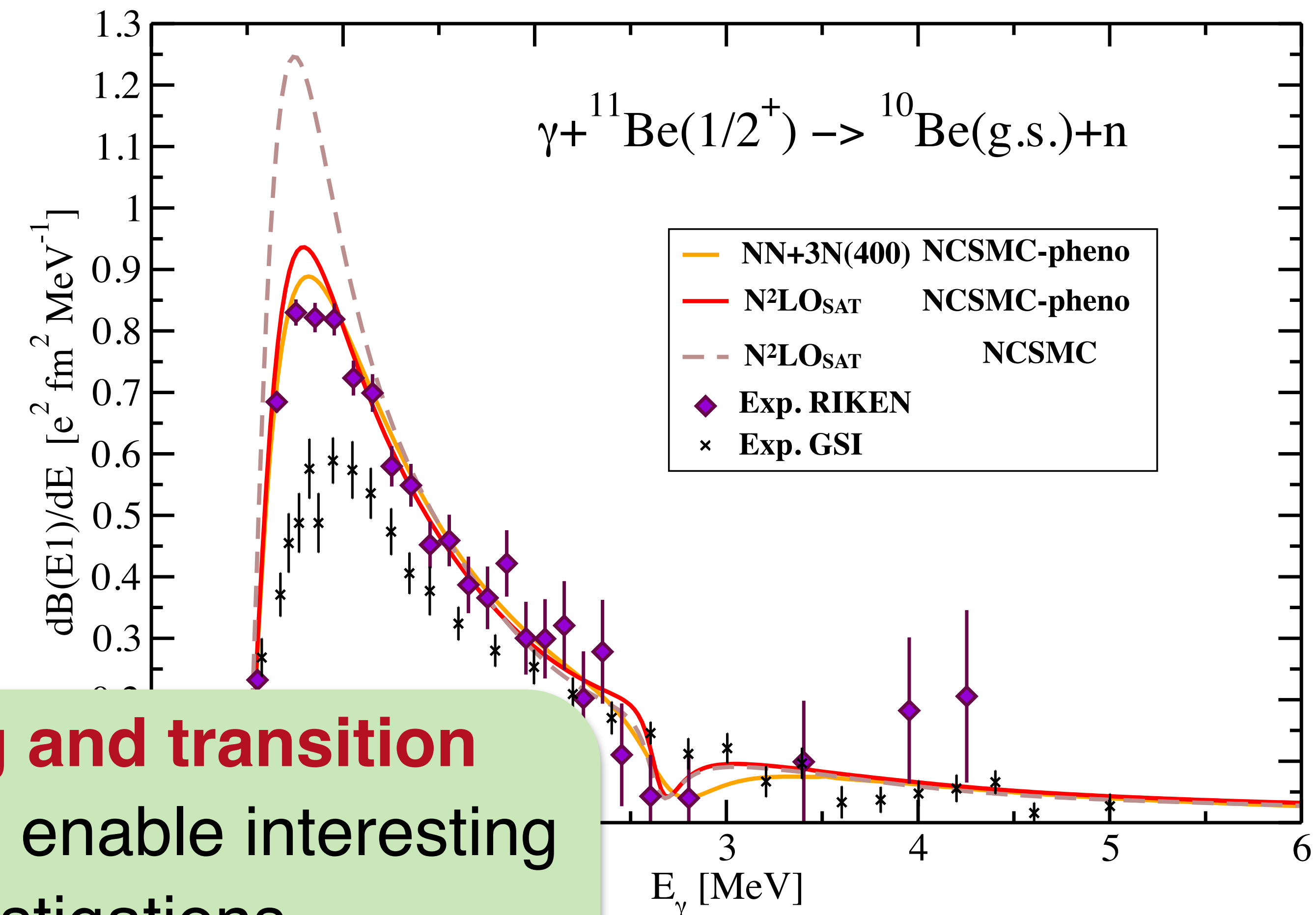

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scattering and transition observables enable interesting investigations

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NCSMC with multi-reference normal-ordered (MR-NO) 3N forces

with
P. Navrátil, R. Roth, E. Gebrerufael

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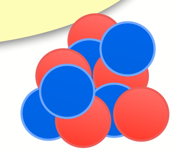

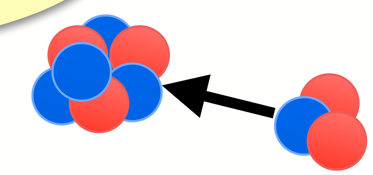

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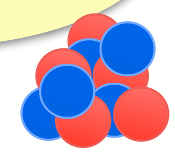

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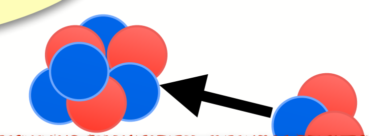

relative ... NCSM ...

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bottleneck : inclusion of 3N force

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Derive NCSM/RGM Kernels

0B kernel

$$-_{SD} < \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_{0N} \boldsymbol{T}_{A-1,A} | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD} =$$

$$= -\frac{1}{A-1} \boldsymbol{V}_{0N} \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M_1' m_j'} \sum_{M_{T_1}' m_t'} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I_1' & j' & \mathcal{J} \\ M_1' & m_j' & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1' & \frac{1}{2} & T \\ M_{T_1}' & m_t' & M_T \end{array} \right)$$

$$\times \ _{SD} < \psi'_{A-1} E_1' I_1'^{\pi_1'} M_1' T_1' M_{T_1}' | \boldsymbol{a}^\dagger_{nljm_jm_t} \boldsymbol{a}_{n'l'j'm_j'm_t'} | \psi_{A-1} E_1 I_1^{\pi_1} M_1 T_1 M_{T_1} >_{SD}$$

1B kernel

$$_{SD} < \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_A | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD}$$

$$= \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M_1' m_j'} \sum_{M_{T_1}' m_t'} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I_1' & j' & \mathcal{J} \\ M_1' & m_j' & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1' & \frac{1}{2} & T \\ M_{T_1}' & m_t' & M_T \end{array} \right)$$

$$\times \ _{SD} < \psi'_{A-1} E_1' I_1'^{\pi_1'} M_1' T_1' M_{T_1}' | \psi_{A-1} E_1 I_1^{\pi_1} M_1 T_1 M_{T_1} >_{SD}$$

$$\times < n' l' j' m_j' \frac{1}{2} m_t' | V_A | n l j m_j \frac{1}{2} m_t >$$

$$-_{SD} < \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_A \boldsymbol{T}_{A-1,A} | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD}$$

$$= -\frac{1}{A-1} \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M_1' m_j'} \sum_{M_{T_1}' m_t'} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I_1' & j' & \mathcal{J} \\ M_1' & m_j' & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1' & \frac{1}{2} & T \\ M_{T_1}' & m_t' & M_T \end{array} \right)$$

$$\times \sum_{\alpha_{A-1}} {}_{SD} < \psi'_{A-1} E_1' I_1'^{\pi_1'} M_1' T_1' M_{T_1}' | \boldsymbol{a}^\dagger_{nljm_jm_t} \boldsymbol{a}_{\alpha_{A-1}} | \psi_{A-1} E_1 I_1^{\pi_1} M_1 T_1 M_{T_1} >_{SD}$$

$$\times < n' l' j' m_j' \frac{1}{2} m_t' | \boldsymbol{V}_A | \alpha_{A-1} >$$

2B kernel

…

Derive NCSM/RGM Kernels

0B kernel

dominant 0B kernel contribution included in target eigenstates
⇒ only MR-NO 1B and 2B kernels contribute

1B kernel

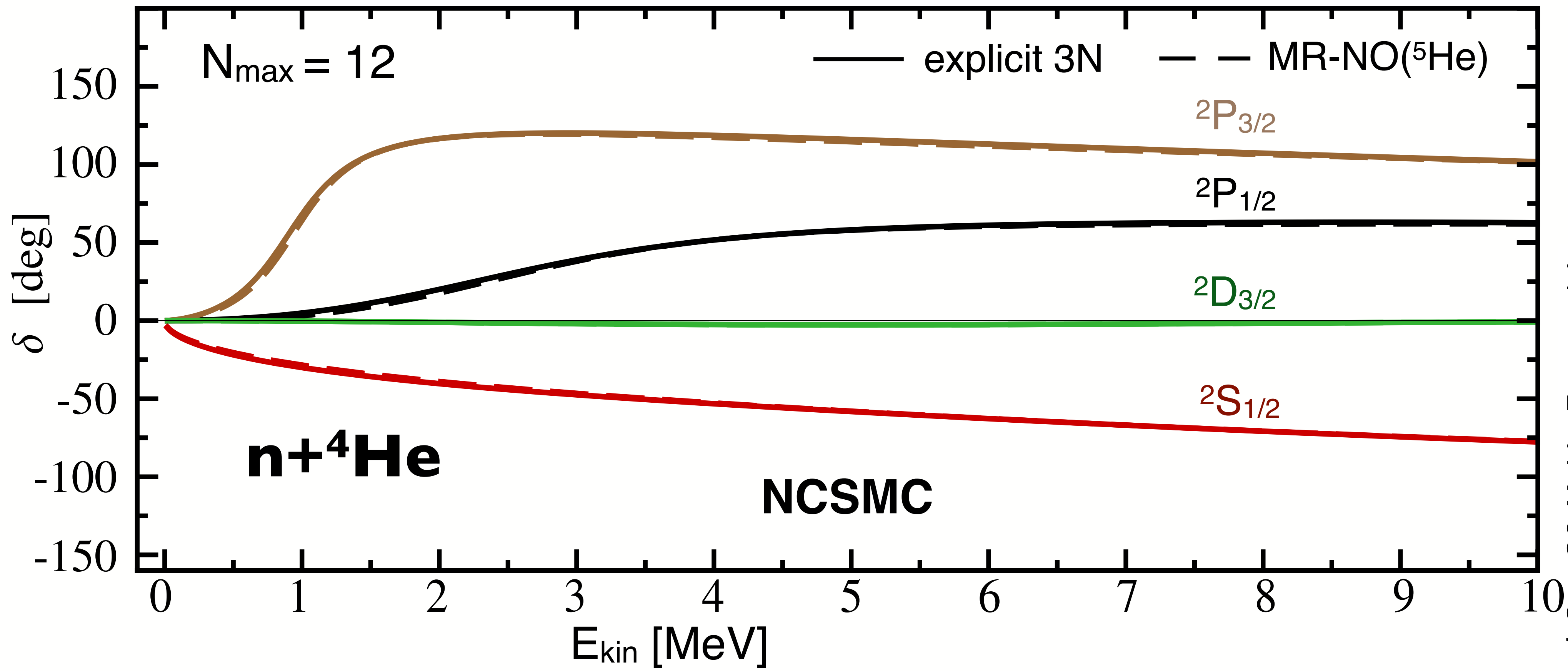
$$
\begin{aligned}
&{}_{SD}< \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_A | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD} \\
= & \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M_1' m_j'} \sum_{M_{T_1}' m_t'} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I_1' & j' & \mathcal{J} \\ M_1' & m_j' & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1' & \frac{1}{2} & T \\ M_{T_1}' & m_t' & M_T \end{array} \right) \\
\times & {}_{SD}< \psi_{A-1}' E_1' I_1'^{\pi_1'} M_1' T_1' M_{T_1}' | \psi_{A-1} E_1 I_1^{\pi_1} M_1 T_1 M_{T_1} >_{SD} \\
\times & < n' l' j' m_j' \frac{1}{2} m_t' | V_A | n l j m_j \frac{1}{2} m_t >
\end{aligned}
$$

$$
\begin{aligned}
&-{}_{SD}< \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_A \boldsymbol{T}_{A-1,A} | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD} \\
= & -\frac{1}{A-1} \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M_1' m_j'} \sum_{M_{T_1}' m_t'} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I_1' & j' & \mathcal{J} \\ M_1' & m_j' & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1' & \frac{1}{2} & T \\ M_{T_1}' & m_t' & M_T \end{array} \right) \\
\times & \sum_{\alpha_{A-1}} {}_{SD}< \psi_{A-1}' E_1' I_1'^{\pi_1'} M_1' T_1' M_{T_1}' | \boldsymbol{a}^{\dagger}_{n l j m_j m_t} \boldsymbol{a}_{\alpha_{A-1}} | \psi_{A-1} E_1 I_1^{\pi_1} M_1 T_1 M_{T_1} >_{SD} \\
\times & < n' l' j' m_j' \frac{1}{2} m_t' | \boldsymbol{V}_A | \alpha_{A-1} >
\end{aligned}
$$

2B kernel

…

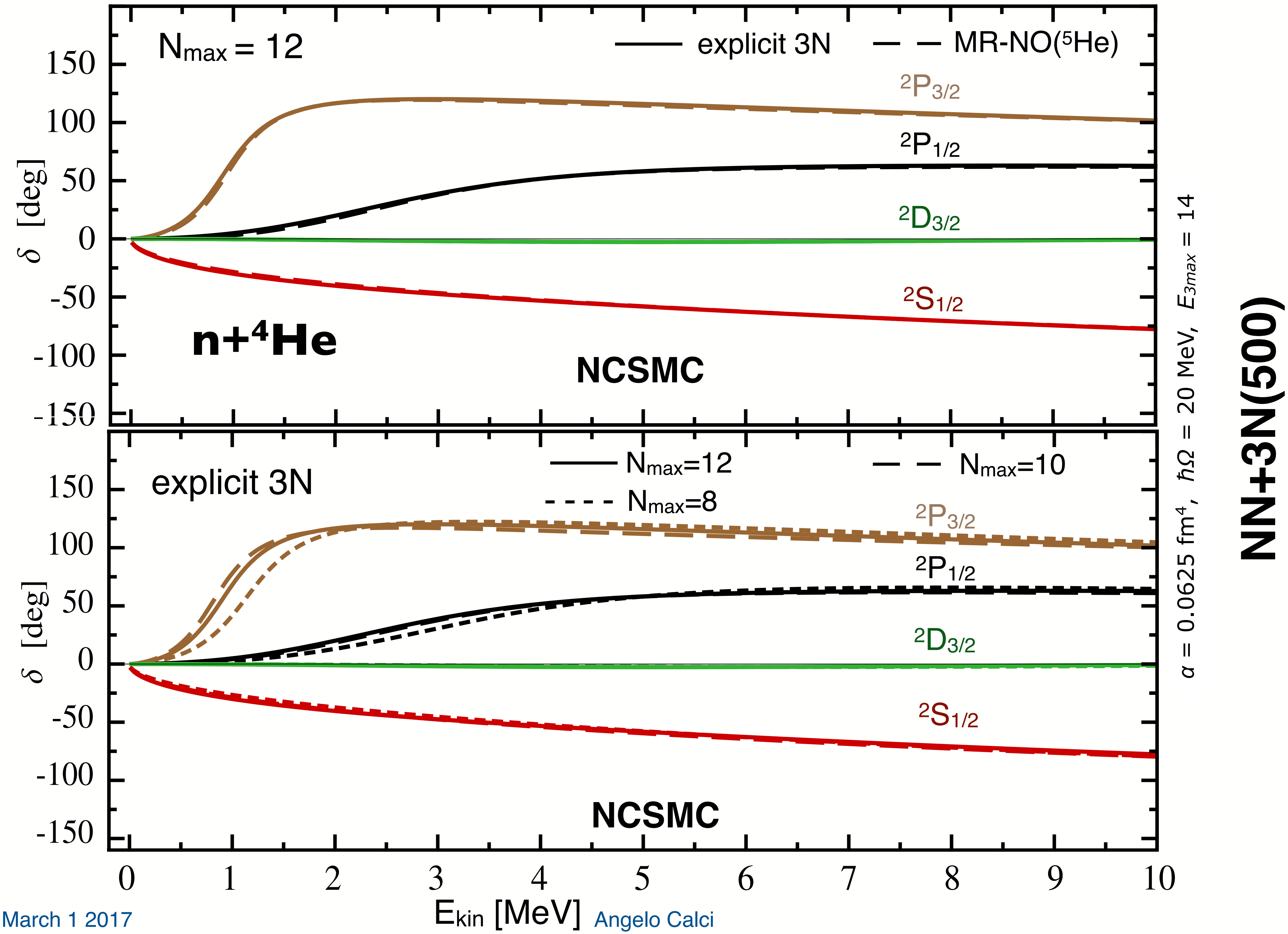
NCSMC: Impact of 3N in Kernels



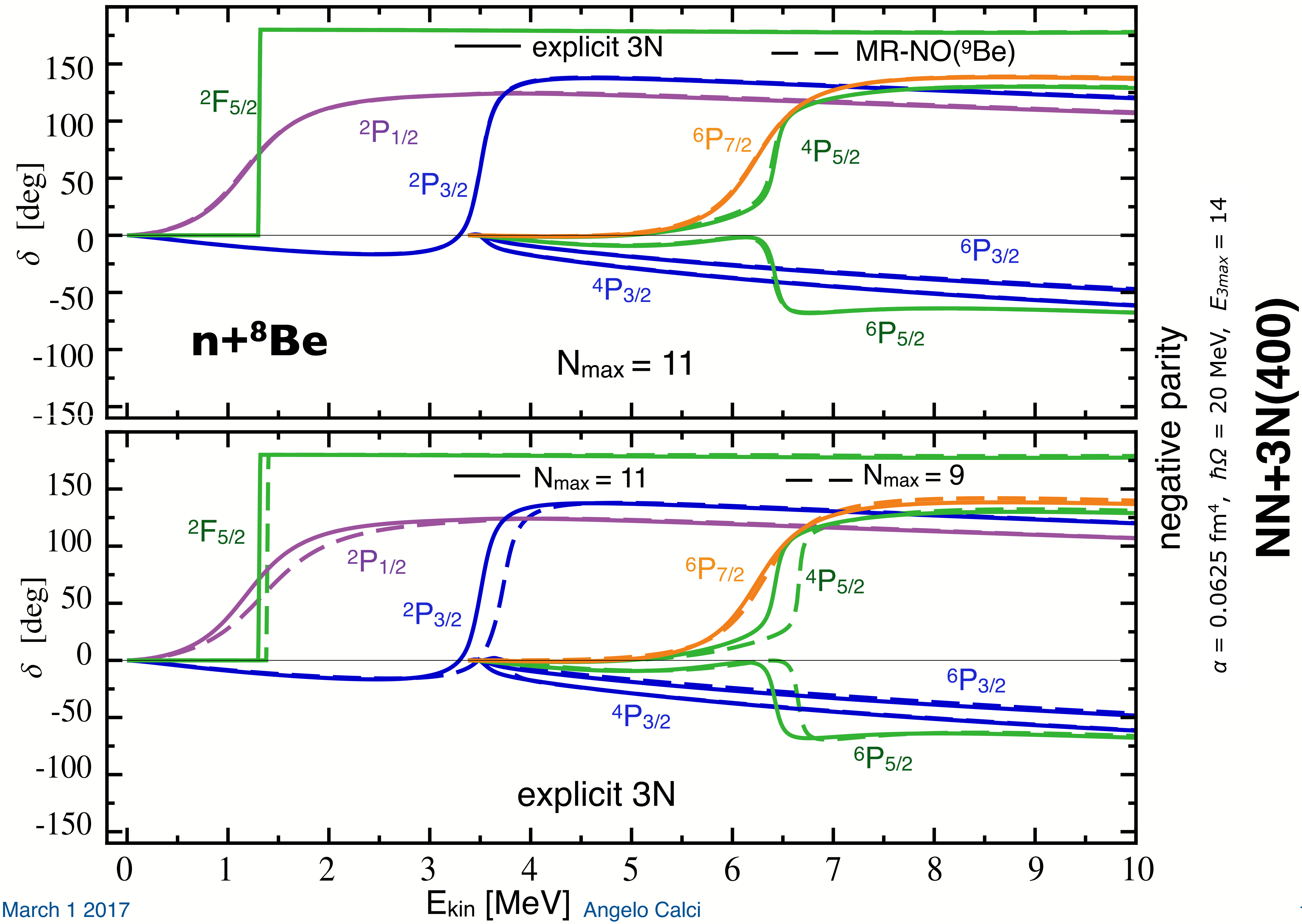
$\alpha = 0.0625\ \text{fm}^4,\ \hbar\Omega = 20\ \text{MeV},\ E_{3max} = 14$

NN+3N(500)

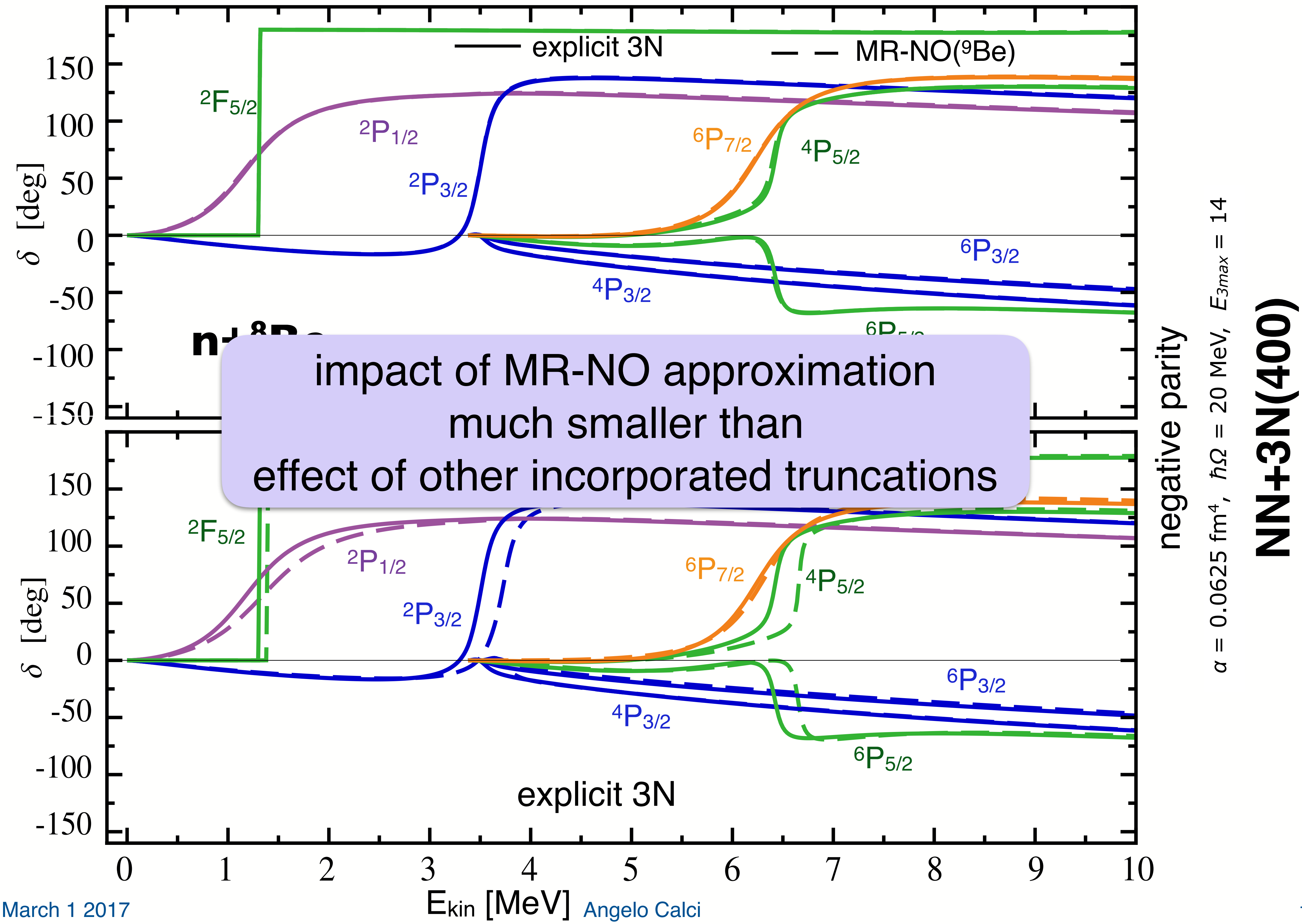
NCSMC: Impact of 3N in Kernels



NCSMC: Impact of 3N in Kernels



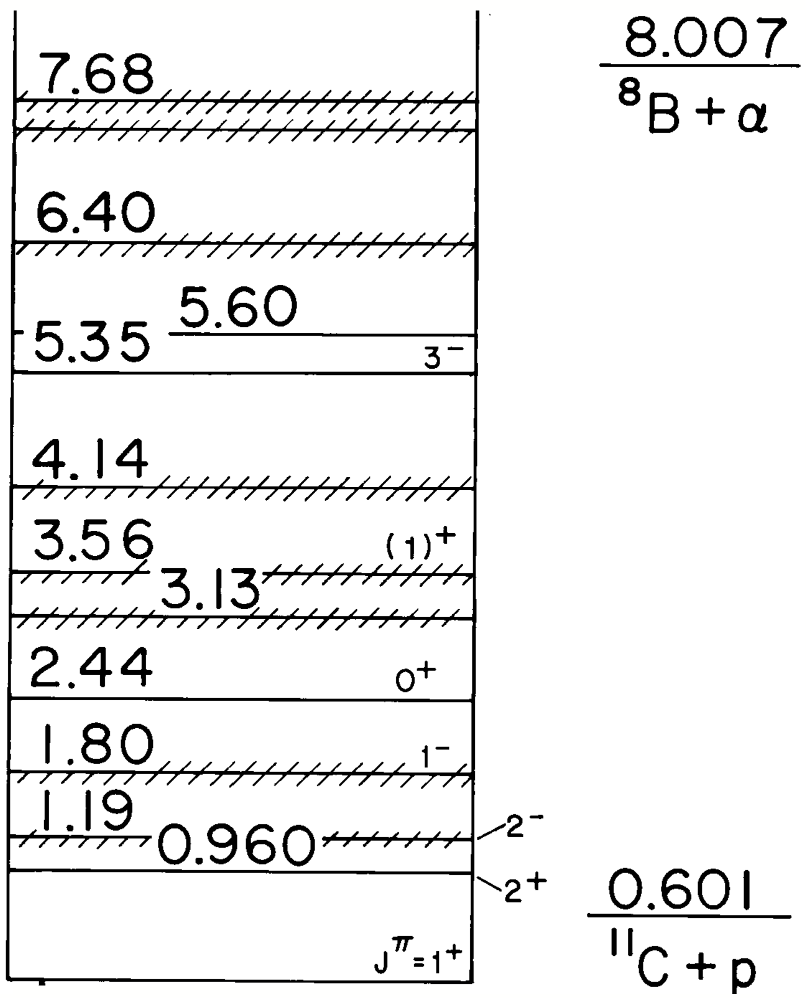
NCSMC: Impact of 3N in Kernels



impact of MR-NO approximation
much smaller than
effect of other incorporated truncations

First application: ^{12}N

- **ideal candidate**
  weakly bound $J=1^+$ state
  dominated by p-^{11}C



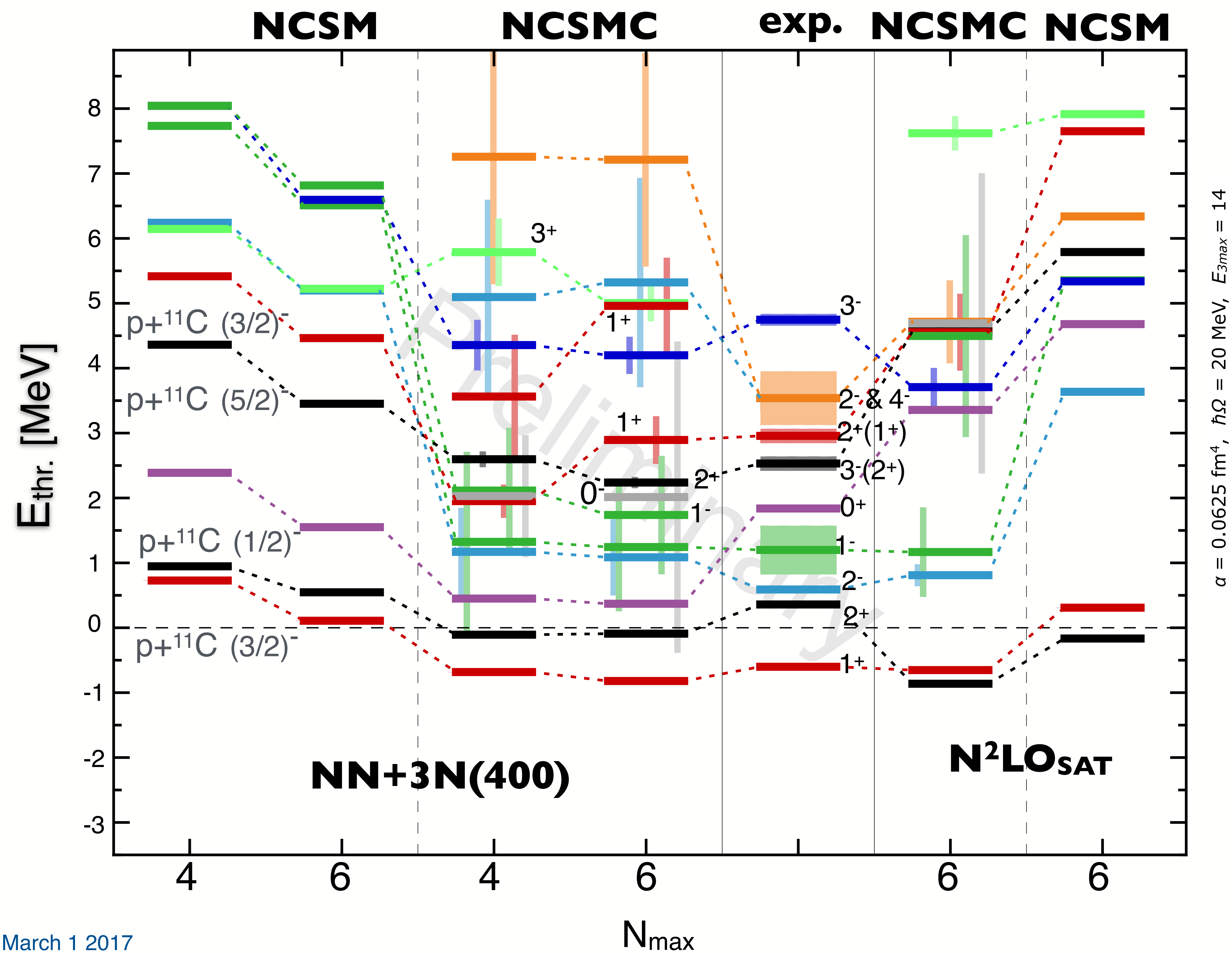
^{12}N

- some low lying resonances not measured precisely
- $^{11}C(p,\gamma)^{12}N$ can bypass triple-alpha process
- planed experiment at TUDA facility at TRIUMF

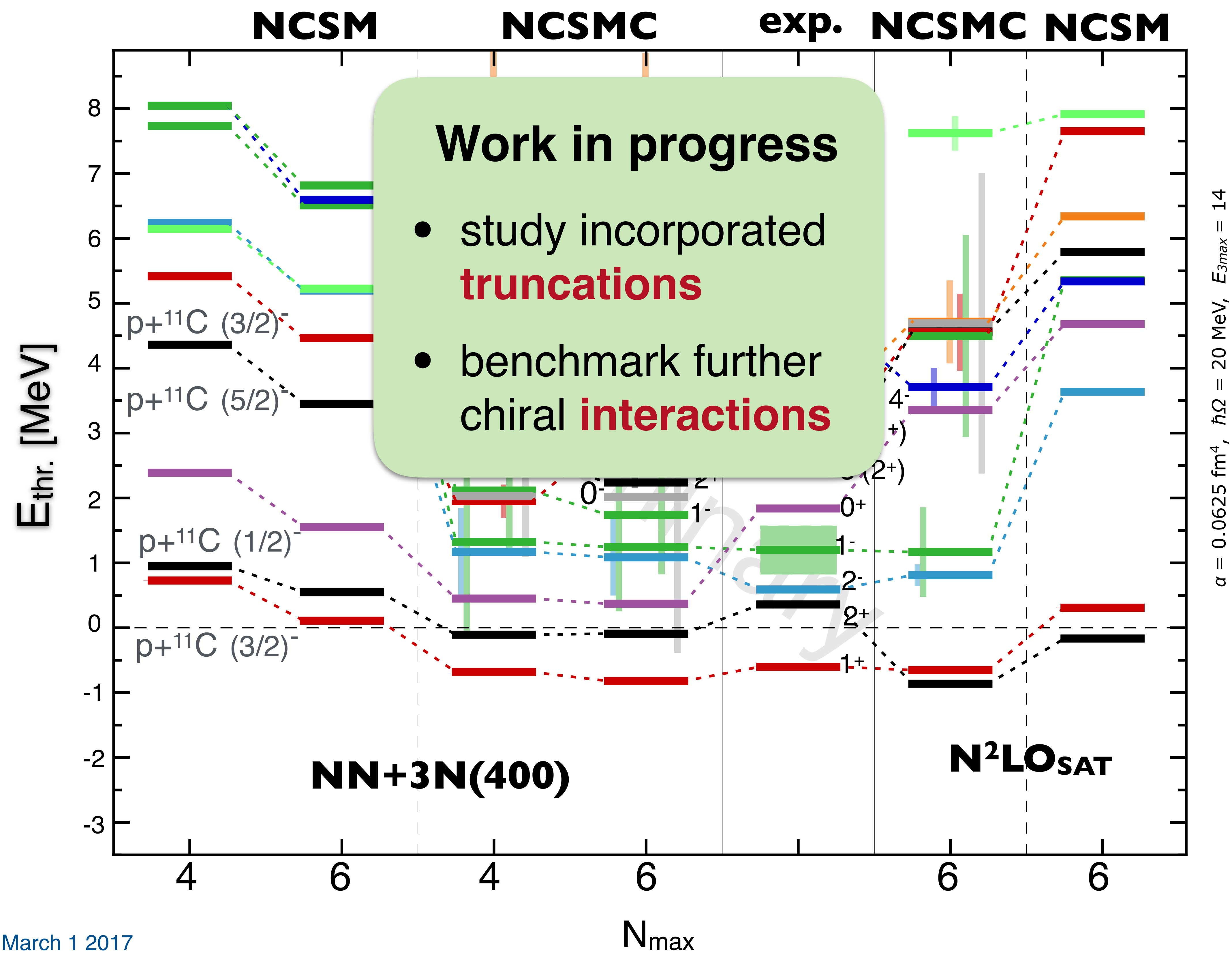
ab initio NCSMC

- include p-^{11}C continuum ($3/2^-$,$1/2^-$,$5/2^-$,$3/2^-$ states of ^{11}C)
- include 4 negative and 6 positive parity states of ^{12}N
- MR-NO with respect to $N_{max}=0$ eigenstate of ^{12}N

^{12}N spectrum with continuum effects



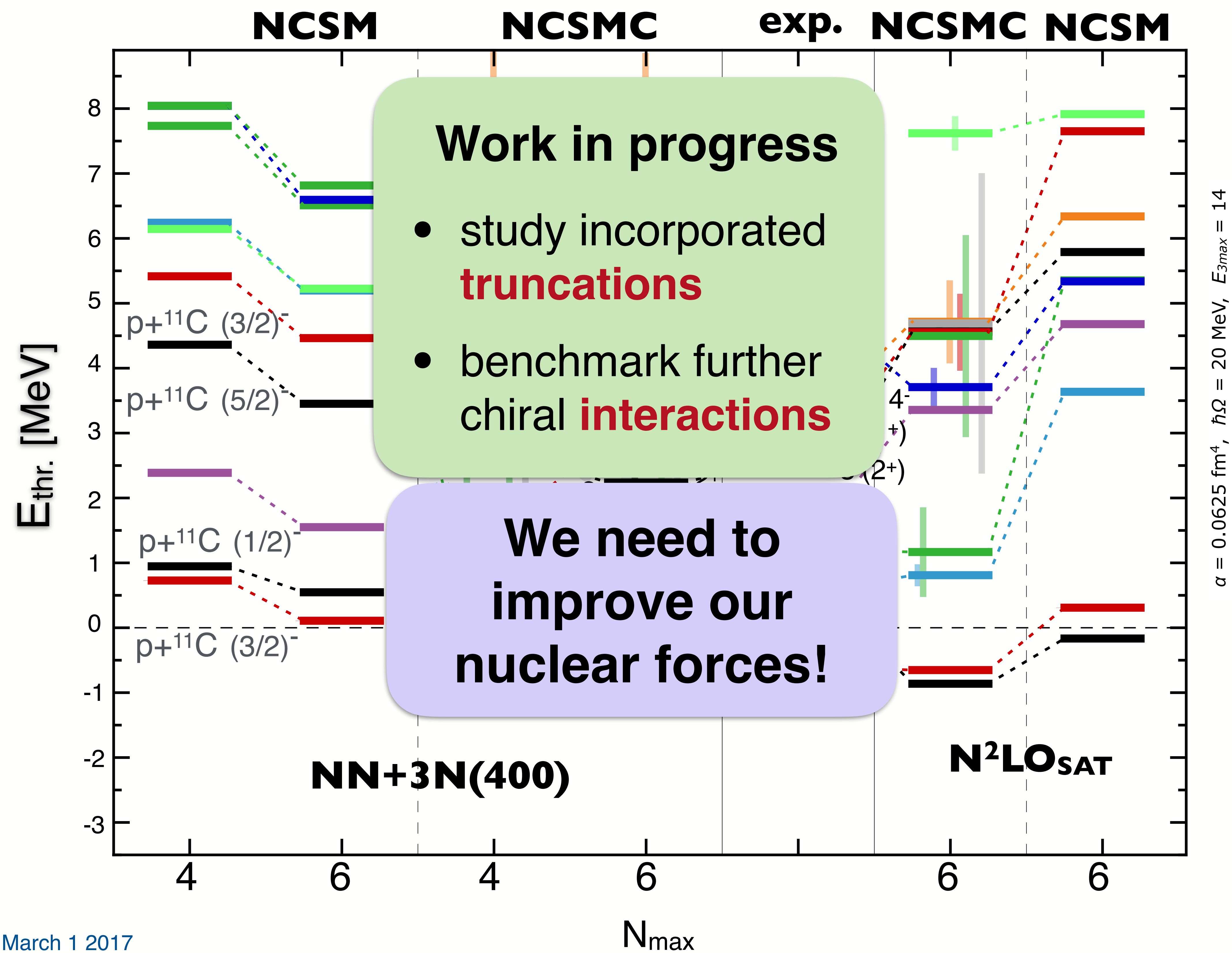
^{12}N spectrum with continuum effects



Work in progress

- study incorporated **truncations**
- benchmark further chiral **interactions**

^{12}N spectrum with continuum effects



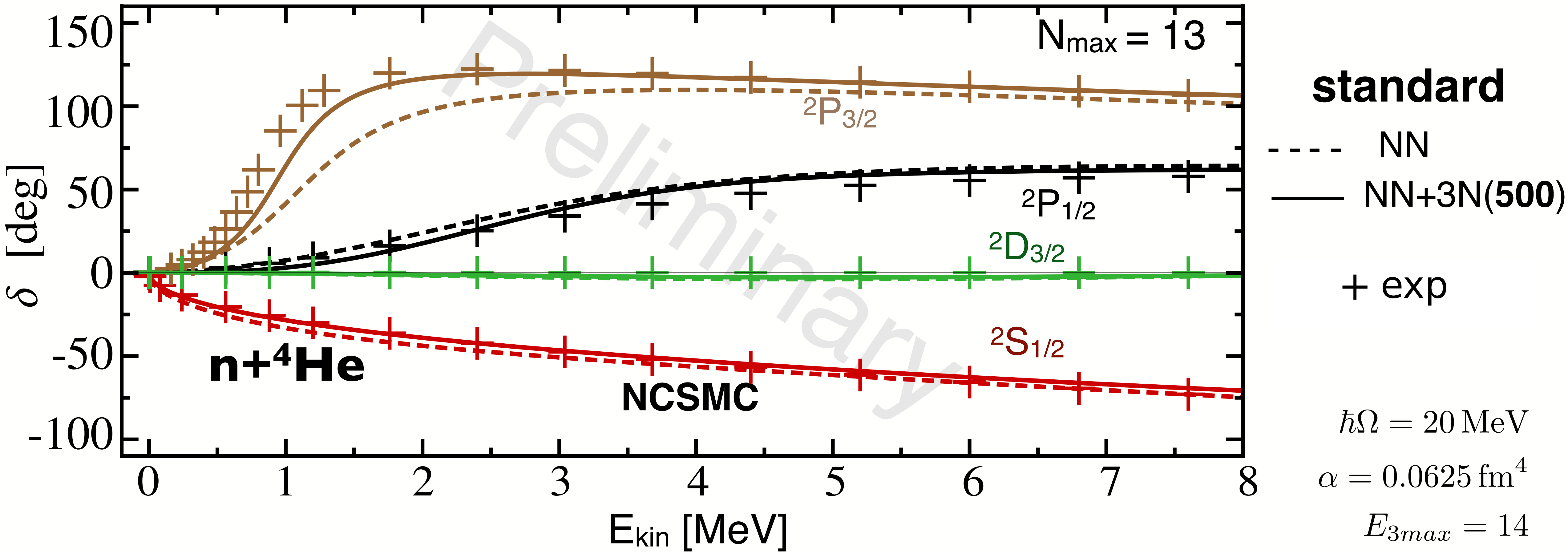
Work in progress

- study incorporated **truncations**
- benchmark further chiral **interactions**

We need to improve our nuclear forces!

Probe chiral interaction in light nuclear scattering

n-^{4}He: Standard interaction

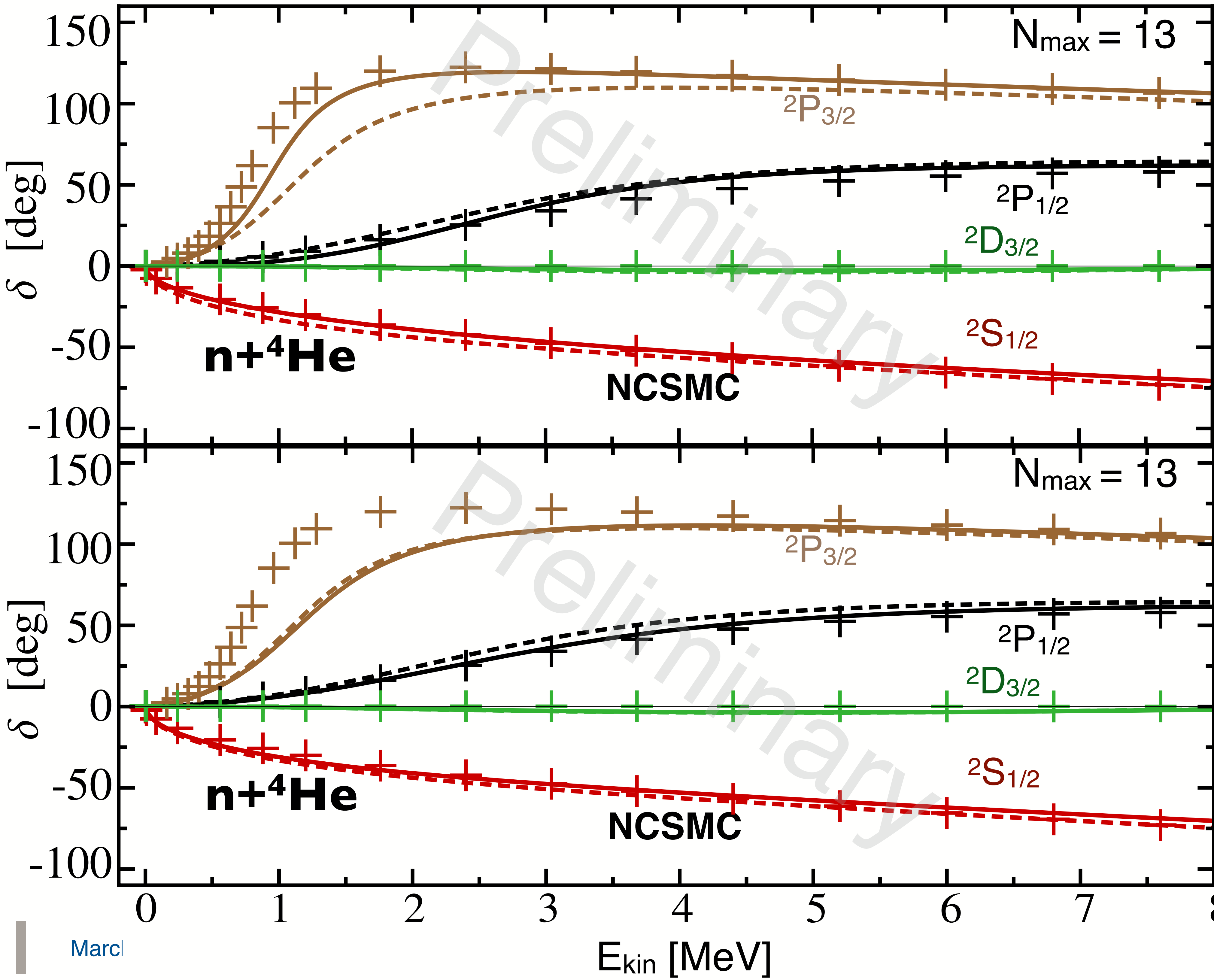


$\hbar\Omega = 20\,\mathrm{MeV}$

$\alpha = 0.0625\,\mathrm{fm}^4$

$E_{3max} = 14$

n-^{4}He: Standard interaction



standard

- - - NN

— NN+3N(**500**)

+ exp

$\hbar\Omega = 20\,\mathrm{MeV}$

$\alpha = 0.0625\,\mathrm{fm}^4$

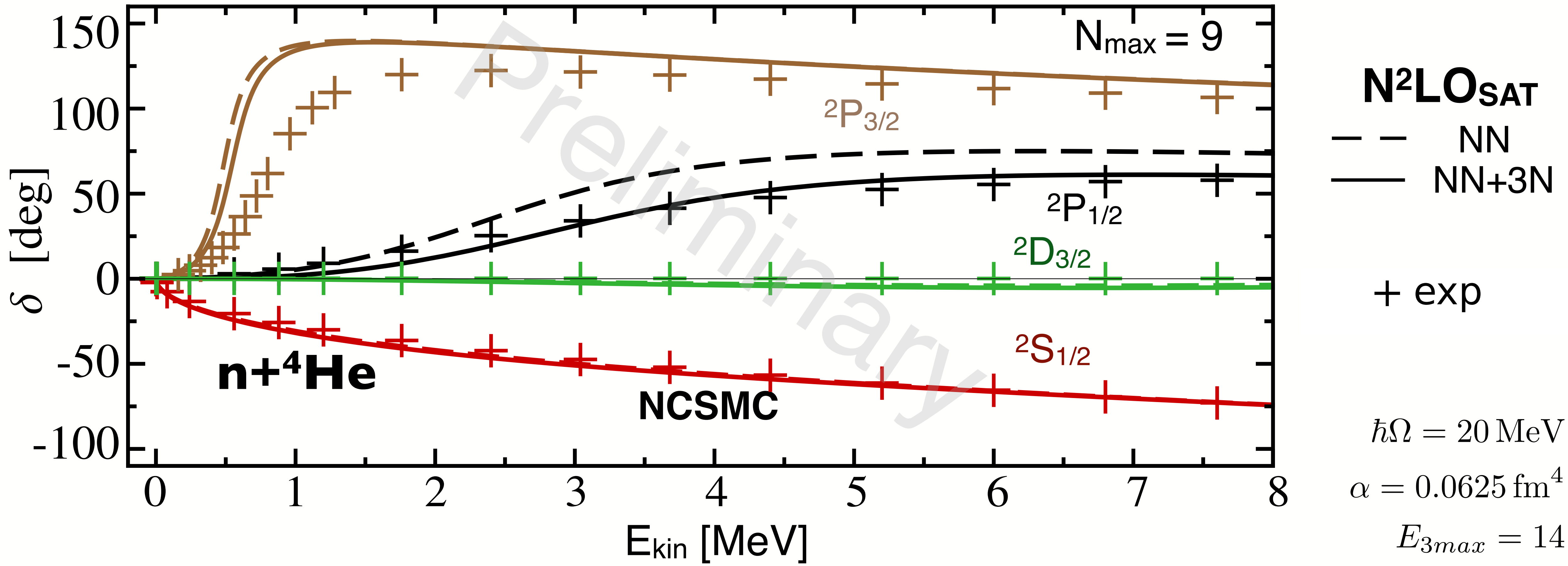
$E_{3max} = 14$

standard

- - - NN

— NN+3N(**400**)

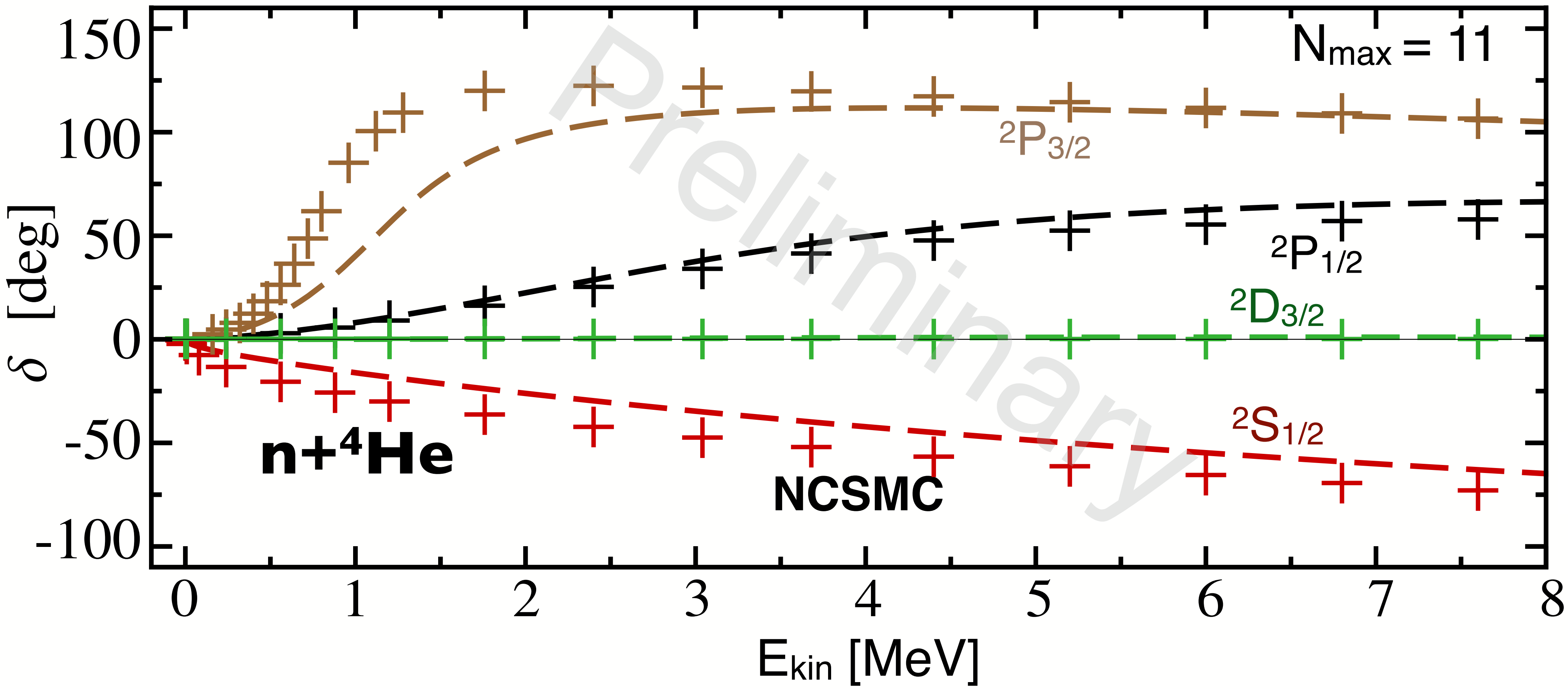
n-^{4}He with N^{2}LO$_{SAT}$



- $P_{3/2}$ - $P_{1/2}$ splitting sensitive to details of nuclear force
- under- or overestimated by NN+3N(400) or N^{2}LO$_{SAT}$ interaction

TRIUMF

n-^{4}He with LENPIC interaction



LENPIC interaction

N^{2}LO

$R = 1.0\,\mathrm{fm}$

– – NN

+ exp

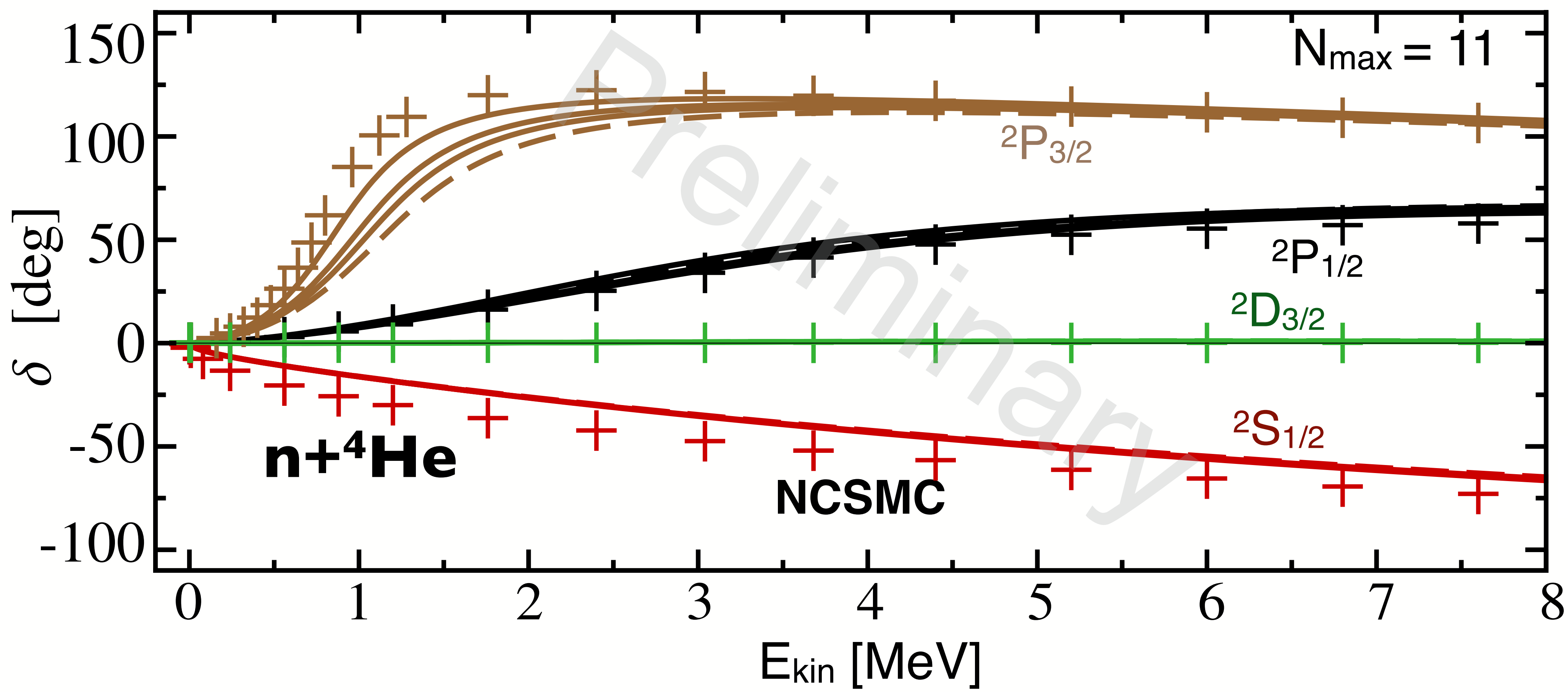
- splitting underestimated without 3N interaction

$\hbar\Omega = 24\,\mathrm{MeV}$

$\alpha = 0.08\,\mathrm{fm}^4$

$E_{3max} = 14$

n-^{4}He with LENPIC interaction



LENPIC interaction

N^{2}LO

$R = 1.0\,\mathrm{fm}$

– – NN

—— NN+3N

+ exp

$c_D = 2,4,6$

c_E fittet to Triton g.s.

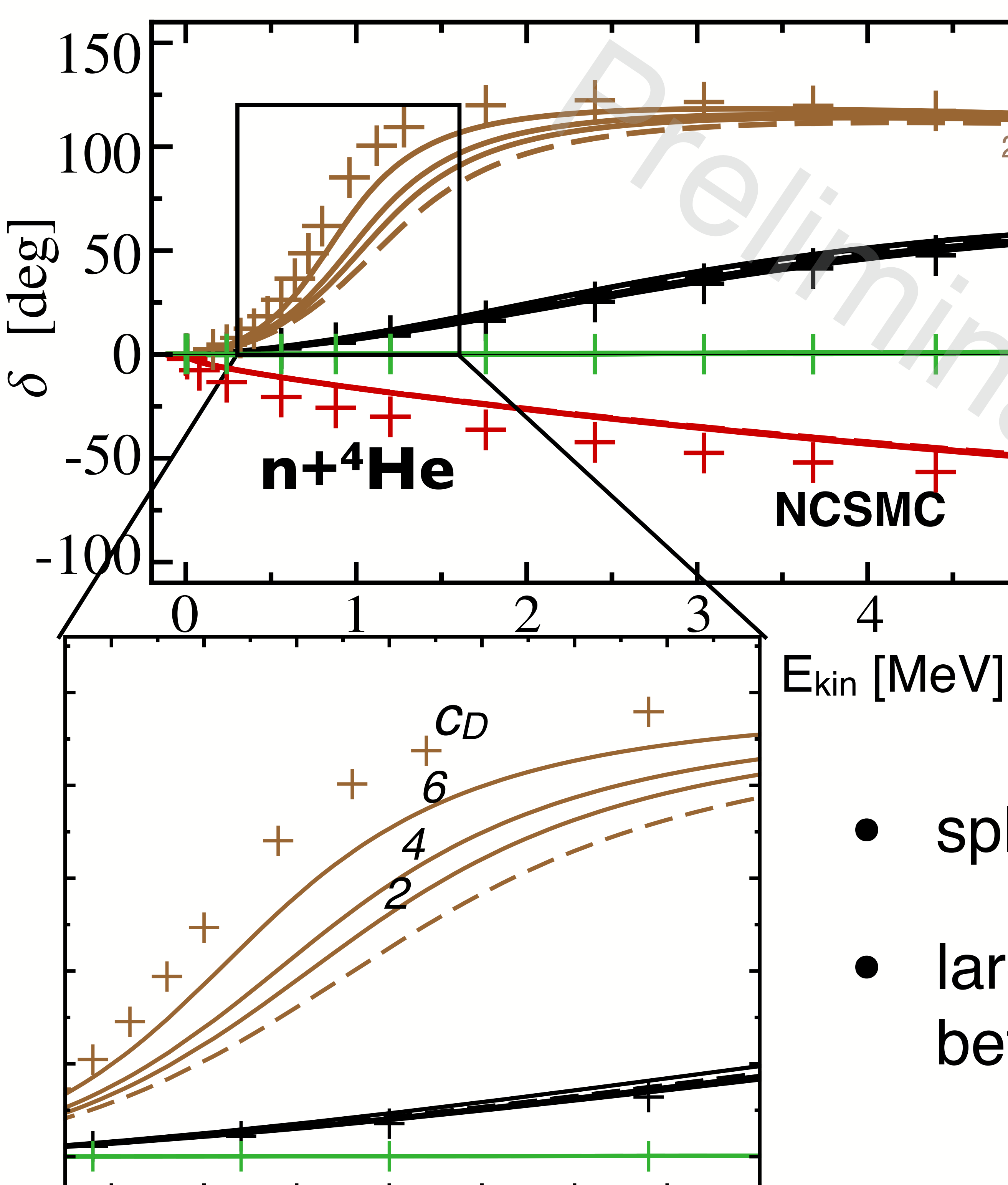
$\hbar\Omega = 24\,\mathrm{MeV}$

$\alpha = 0.08\,\mathrm{fm}^4$

$E_{3max} = 14$

- splitting underestimated without 3N interaction

n-^{4}He with LENPIC interaction



LENPIC interaction

N^{2}LO

$R = 1.0\,\text{fm}$

– – NN

—— NN+3N

+ exp

$c_D = 2,4,6$

c_E fittet to Triton g.s.

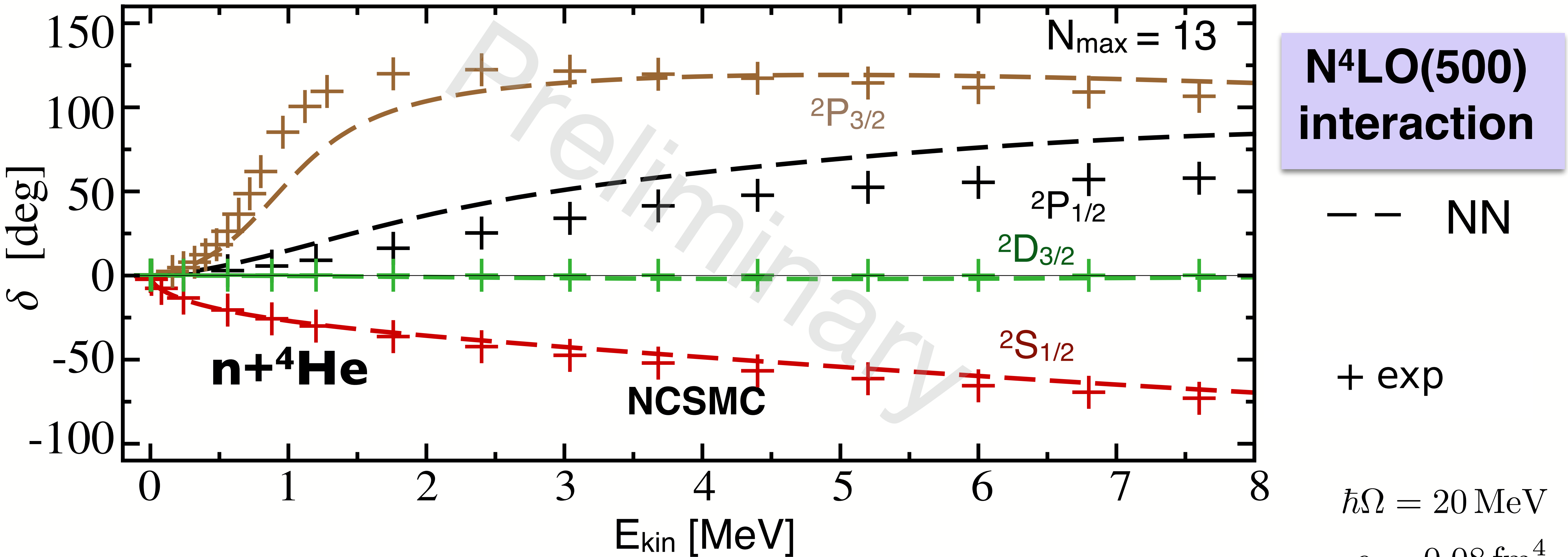
- splitting sensitive to c_D
- larger c_D values provide better reproduction

$\hbar\Omega = 24\,\text{MeV}$

$\alpha = 0.08\,\text{fm}^4$

$E_{3max} = 14$

n-^{4}He with N^{4}LO(500) interaction



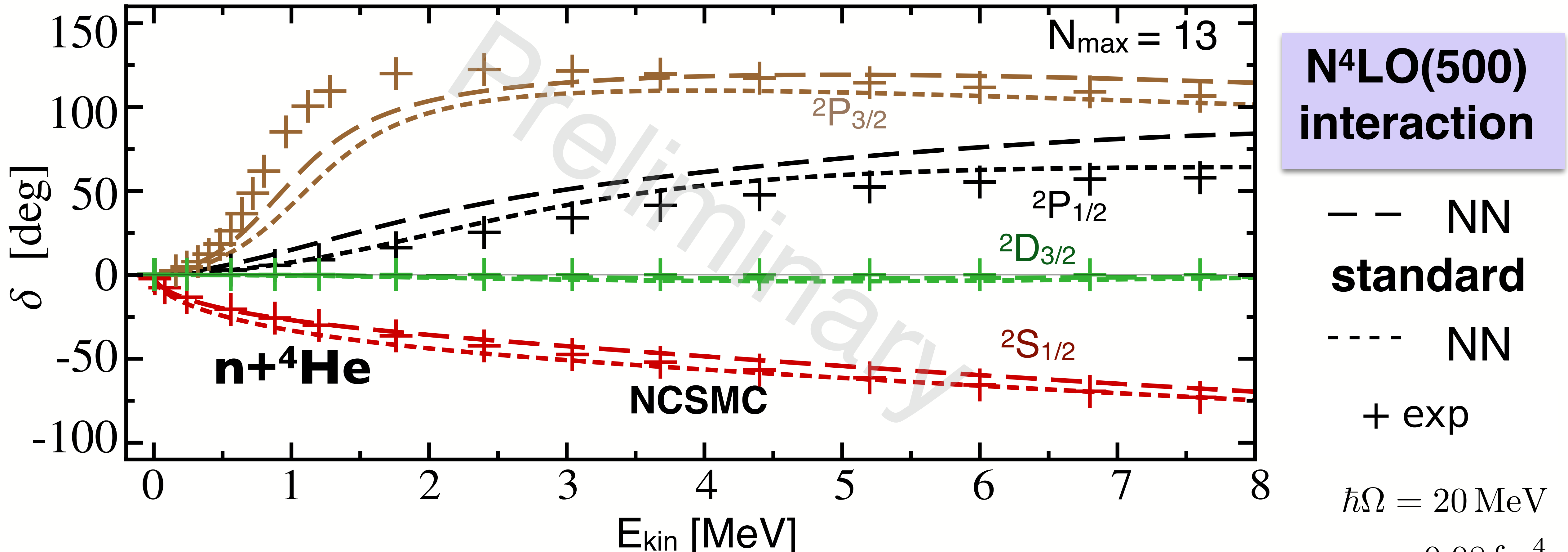
$\hbar\Omega = 20\,\mathrm{MeV}$

$\alpha = 0.08\,\mathrm{fm}^4$

$E_{3max} = 14$

- promising splitting properties of N^{4}LO NN interaction

n-^{4}He with N^{4}LO(500) interaction



$\hbar\Omega = 20\,\mathrm{MeV}$

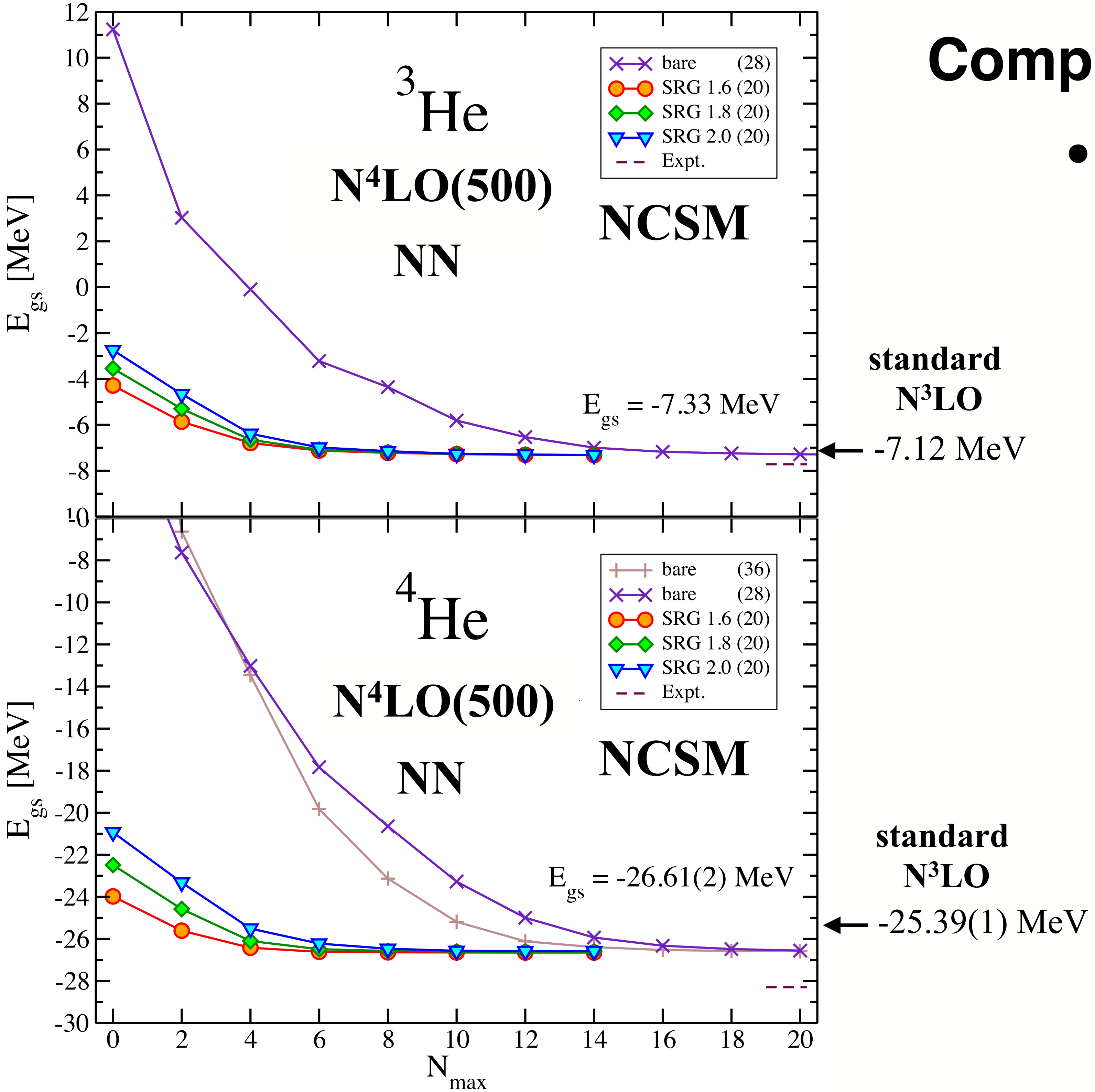
$\alpha = 0.08\,\mathrm{fm}^4$

$E_{3max} = 14$

- promising splitting properties of N^{4}LO(500) NN interaction

$N^4LO(500)$ NN interaction for other observables?

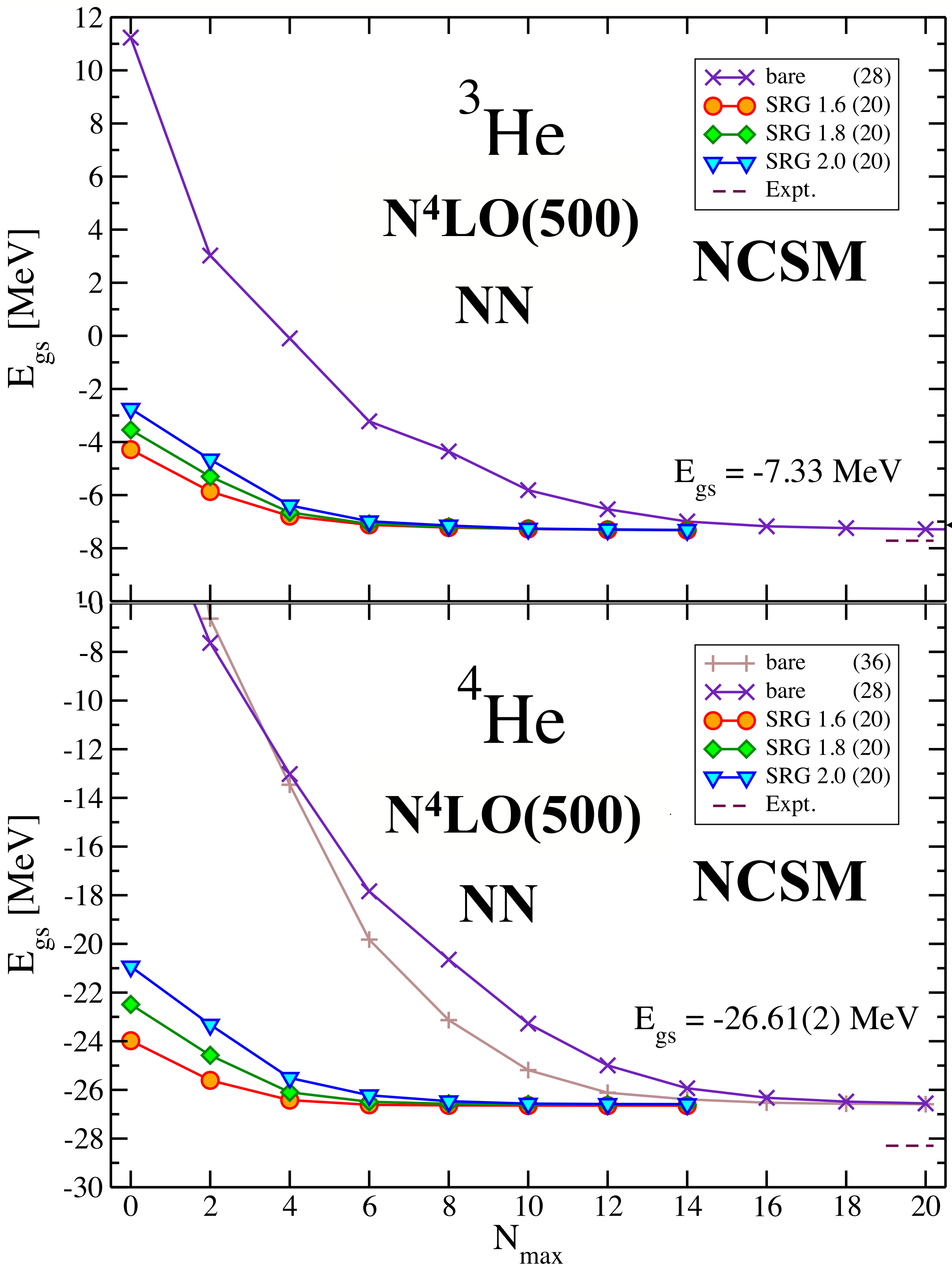
Ground-State Energies in s-Shell



Compared to standard N³LO:

- 3N force needs to be less attractive

Ground-State Energies in s-Shell

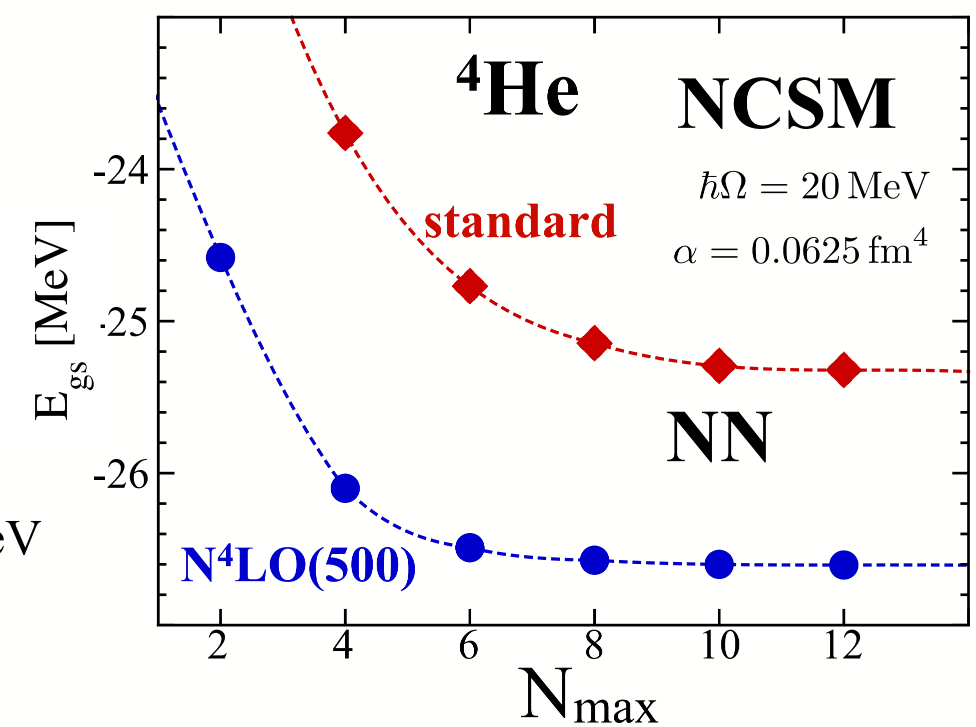


standard N^{3}LO
-7.12 MeV

standard N^{3}LO
-25.39(1) MeV

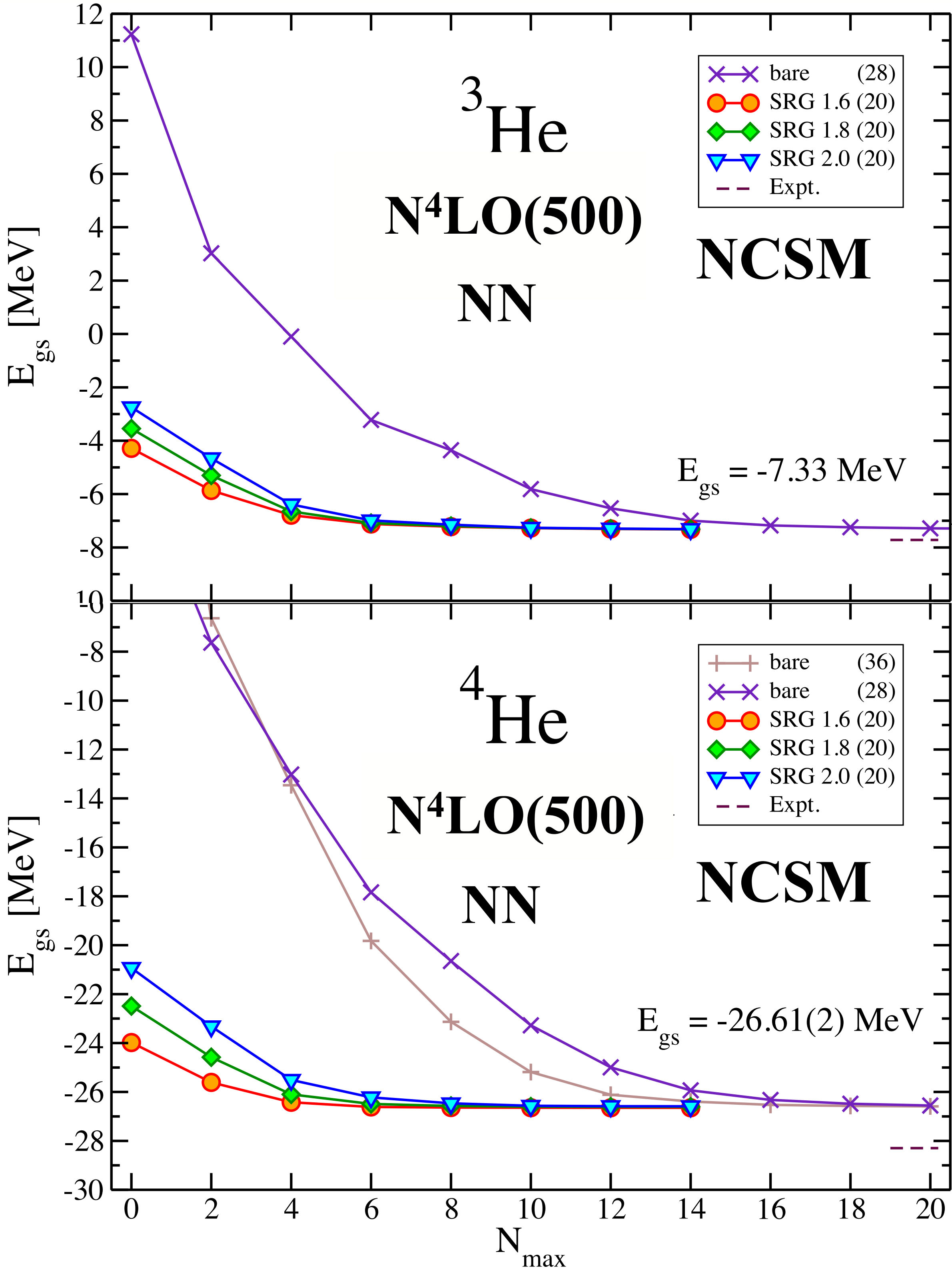
Compared to standard N^{3}LO:

- 3N force needs to be less attractive



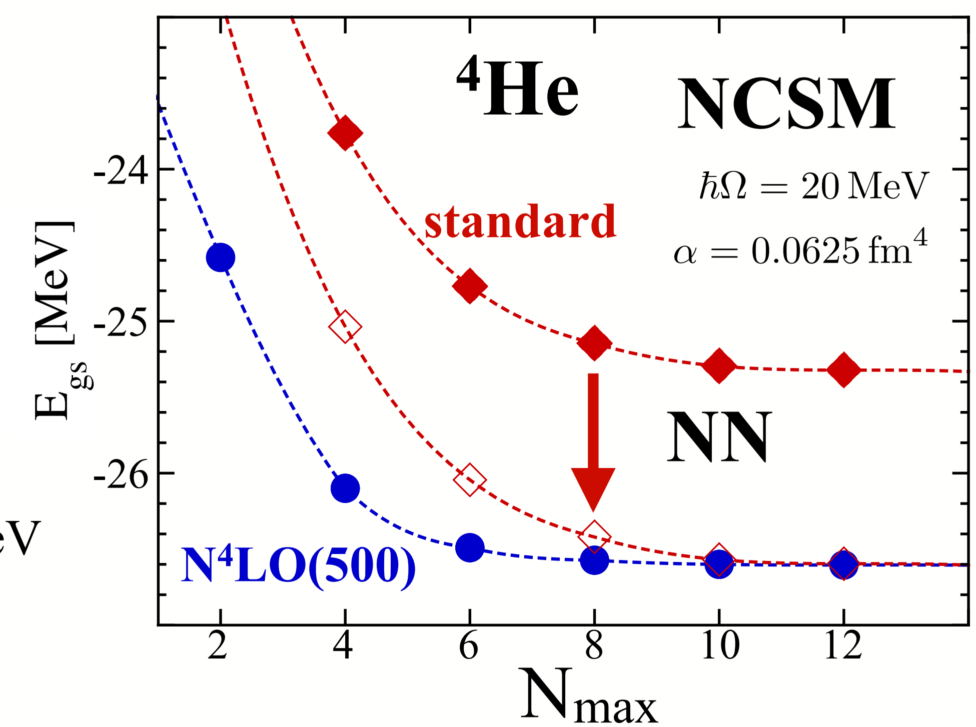
TRIUMF

Ground-State Energies in s-Shell

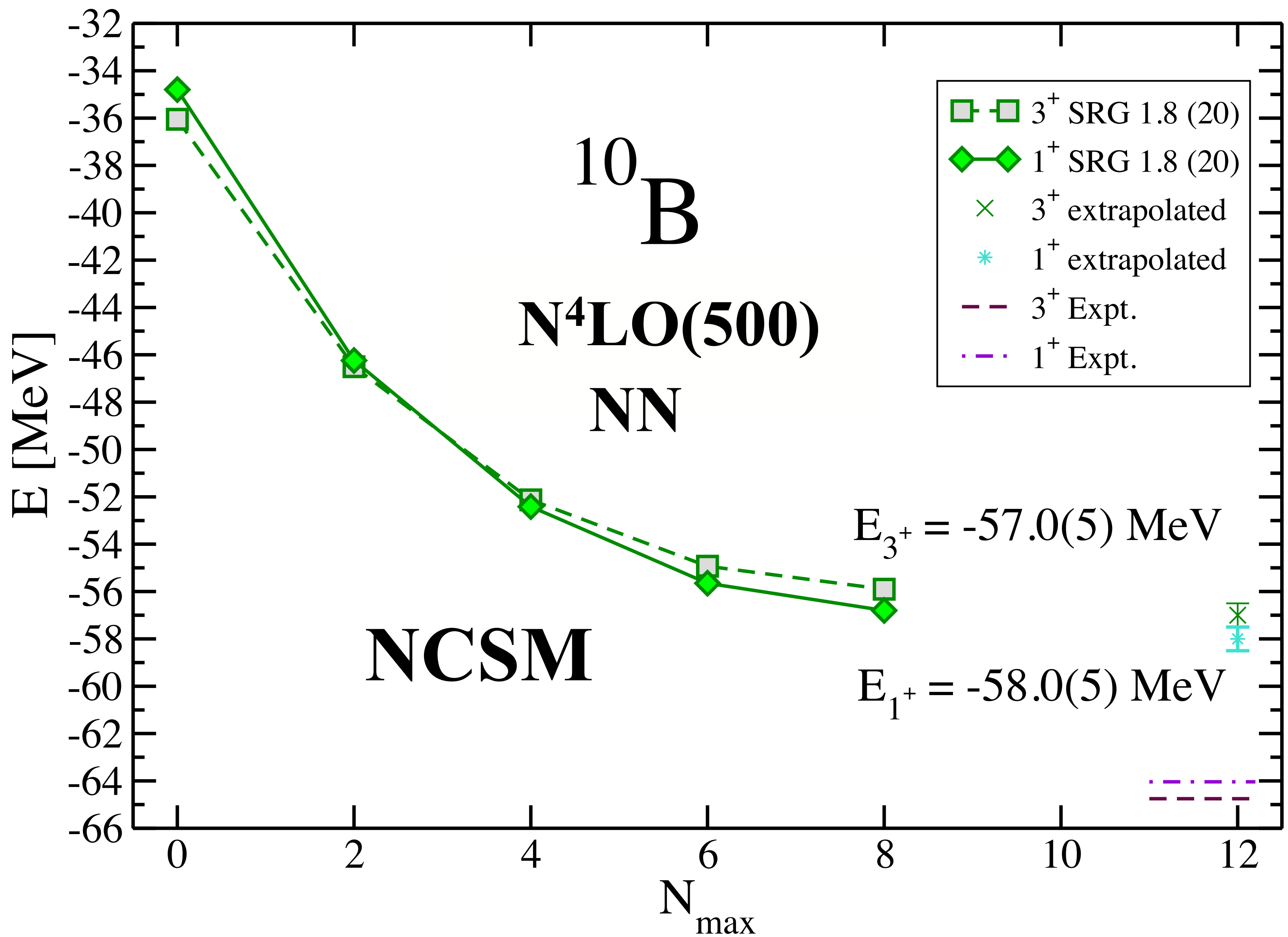


Compared to standard N³LO:

- 3N force needs to be less attractive
- N⁴LO(500) NN seems to be softer!



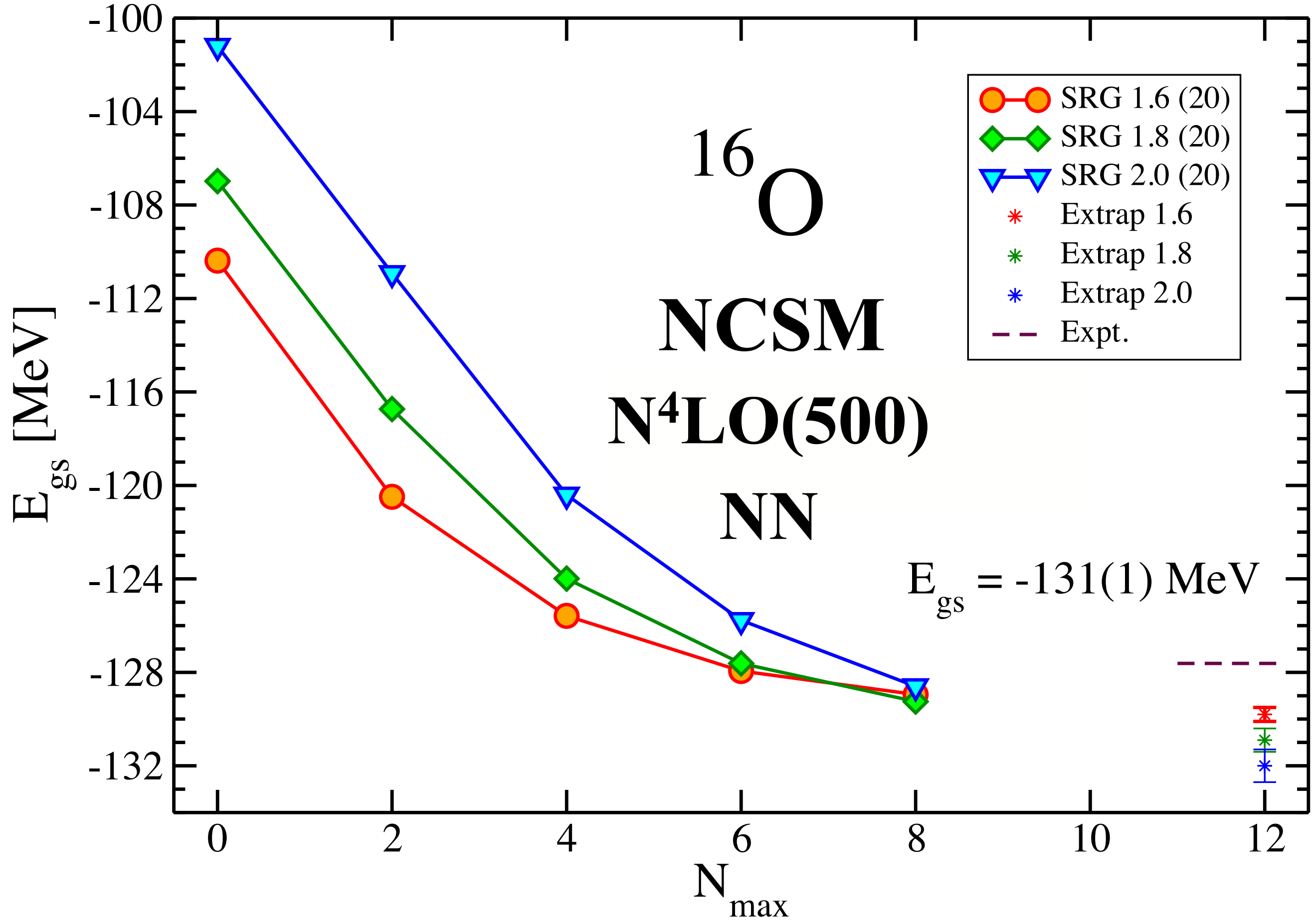
^{10}B Ground-State

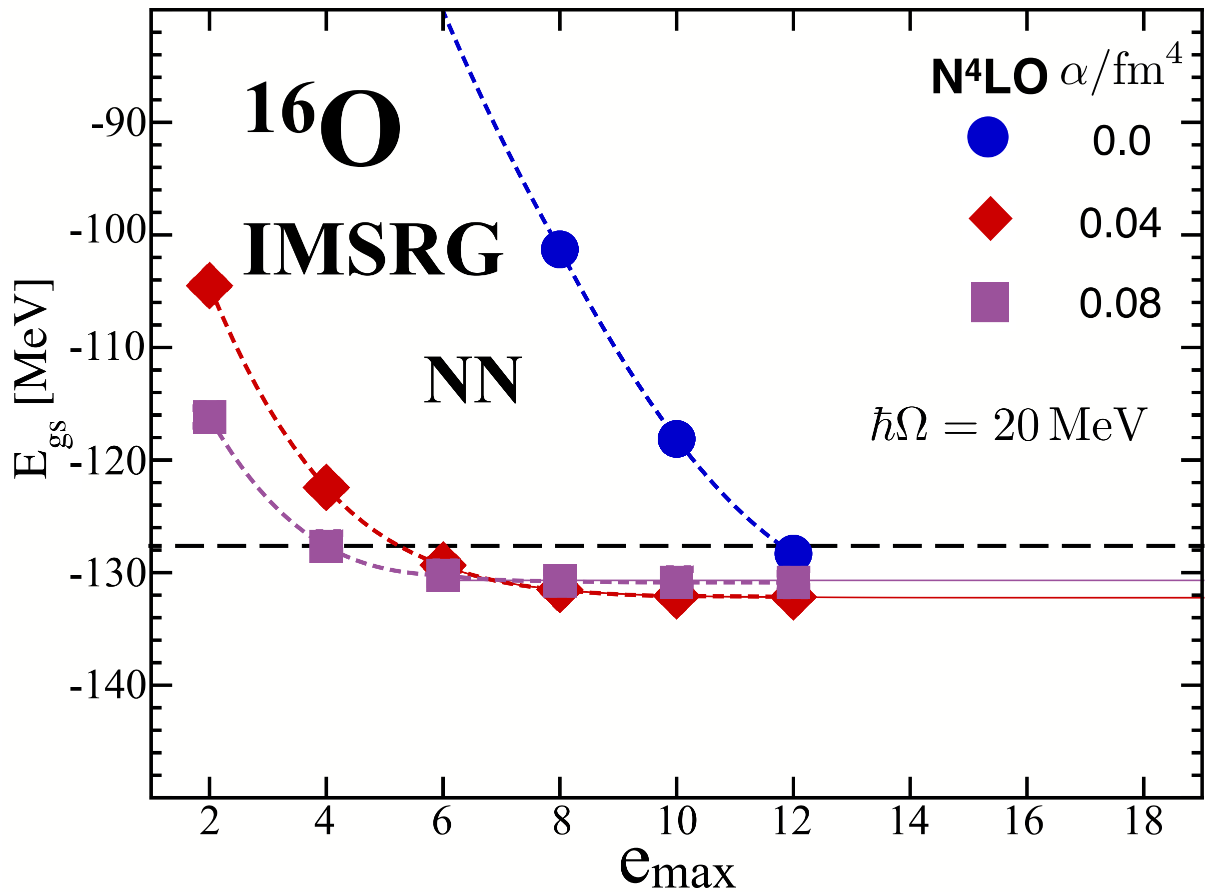


- requires 3N force to describe right ground-state similar to standard N^{3}LO

TRIUMF

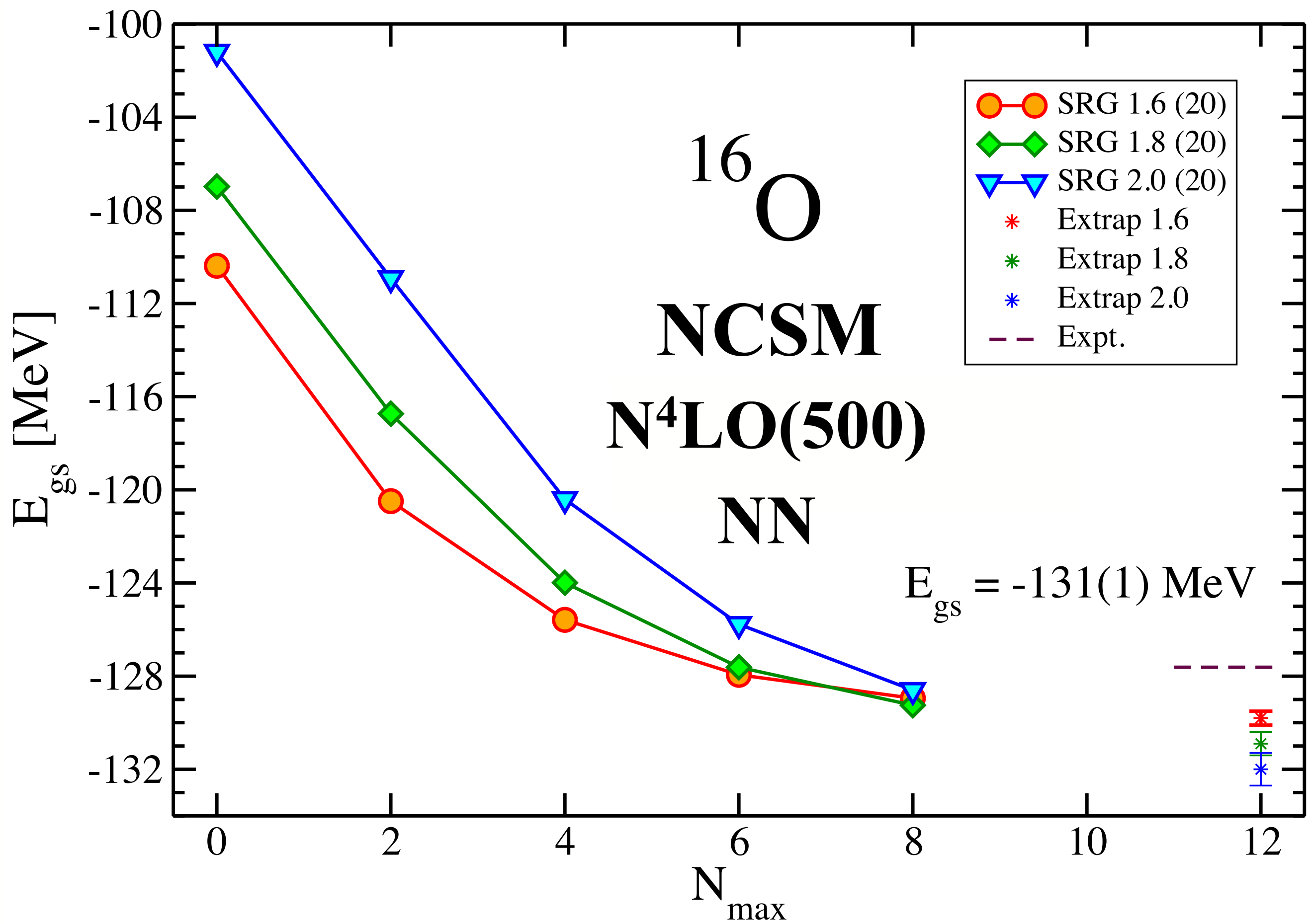
^{16}O: Ground-State Energy

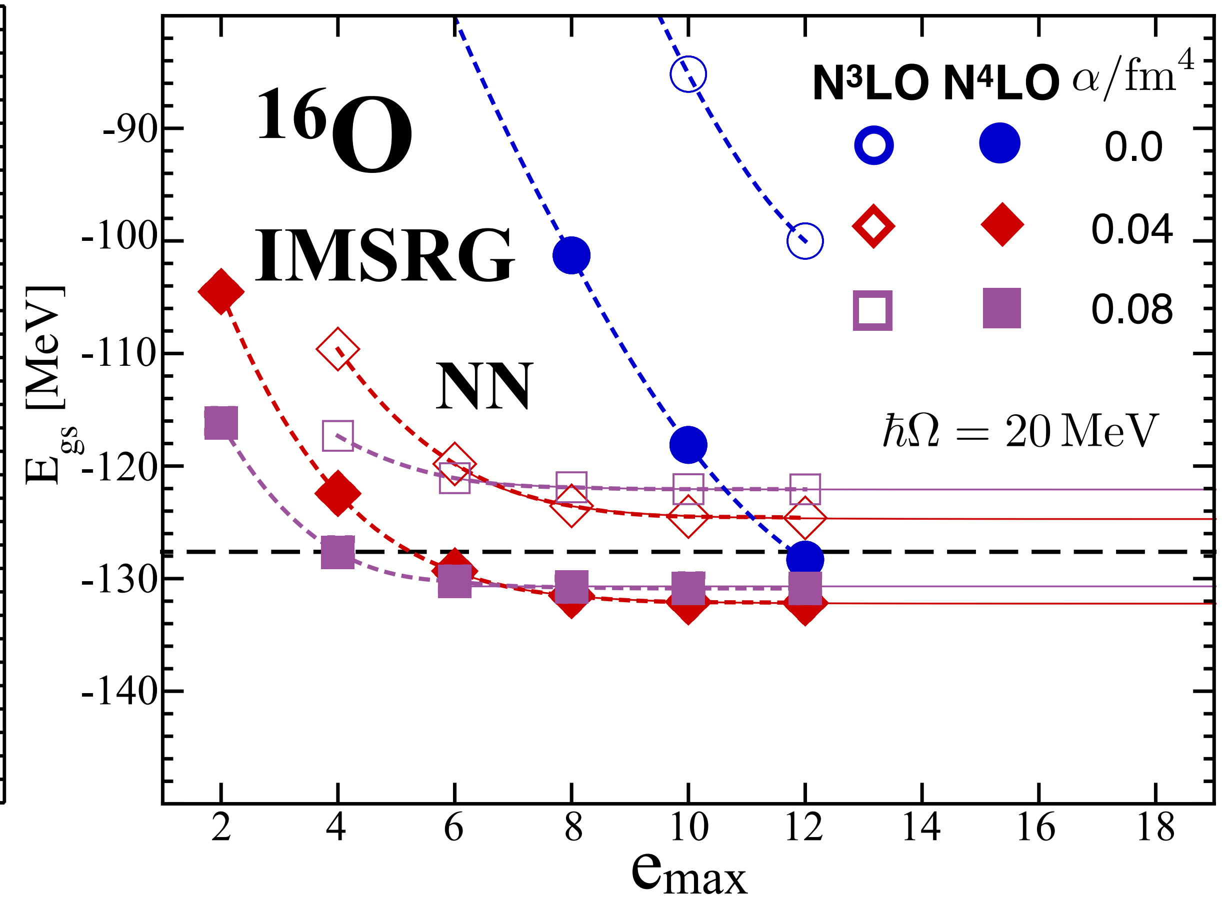




- requires repulsive 3N force
- no significant SRG induced 4N contributions

^{16}O: Ground-State Energy





- requires repulsive 3N force
- no significant SRG induced 4N contributions

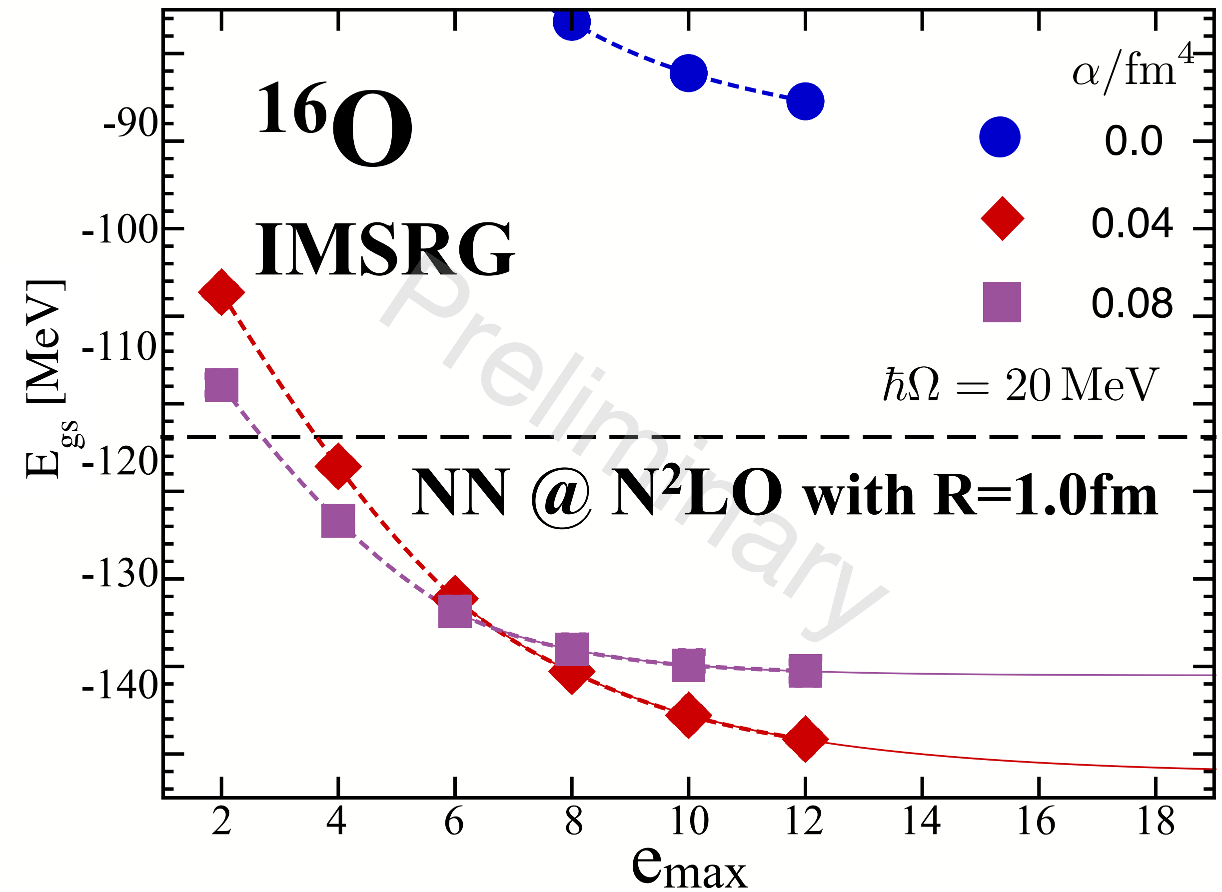
- no surprises in IMSRG calculations
- N^{4}LO(500) is sufficiently soft

^{16}O: Ground-State Energy

counter-example:

- fully-local N^2LO interaction used in Quantum Monte Carlo
  Gezerlis, Tews, Epelbaum et al.
  Phys. Rev. C 90, 054323 (2014)

- difficult to handle in harmonic oscillator basis



interaction for this cutoff is significantly harder

- Normal-Ordering approximation
- induced (IM)SRG many-body contributions

Outlook

- **insufficient knowledge of nuclear force** provides largest uncertainties in ab initio calculations

- **combination of NCSMC with MR-NO** allows to include continuum effects at strongly reduced cost
  - enables heavier targets and **complexer projectiles**
  - splitting of $P_{3/2}$ - $P_{1/2}$ phase shifts in ^{5}He can be used to **constrain 3N** parameters

- novel LENPIC and N^4LO(500) NN interactions have promising properties
  - 3N needs to be added

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- **insufficient knowledge of nuclear force** provides largest uncertainties in ab initio calculations

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  - 3N needs to be added

fit c_D from ^{3}H β-decay
poster by Peter Gysbers

Thank you! Merci!

- **thanks to my collaborators**

  - P. Navrátil, R. Stroberg, J. Holt, R. Kanungo, G. Hackman, A. Kumar, A. Lennarz
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    TU Darmstadt, Germany
  - J. Vary, P. Maris
    Iowa State University, USA
  - J. Dohet-Eraly
    Istituto Nazionale di Fisica Nucleare, Pisa, Italy

LENPIC

NRC·CNRC

NSERC CRSNG

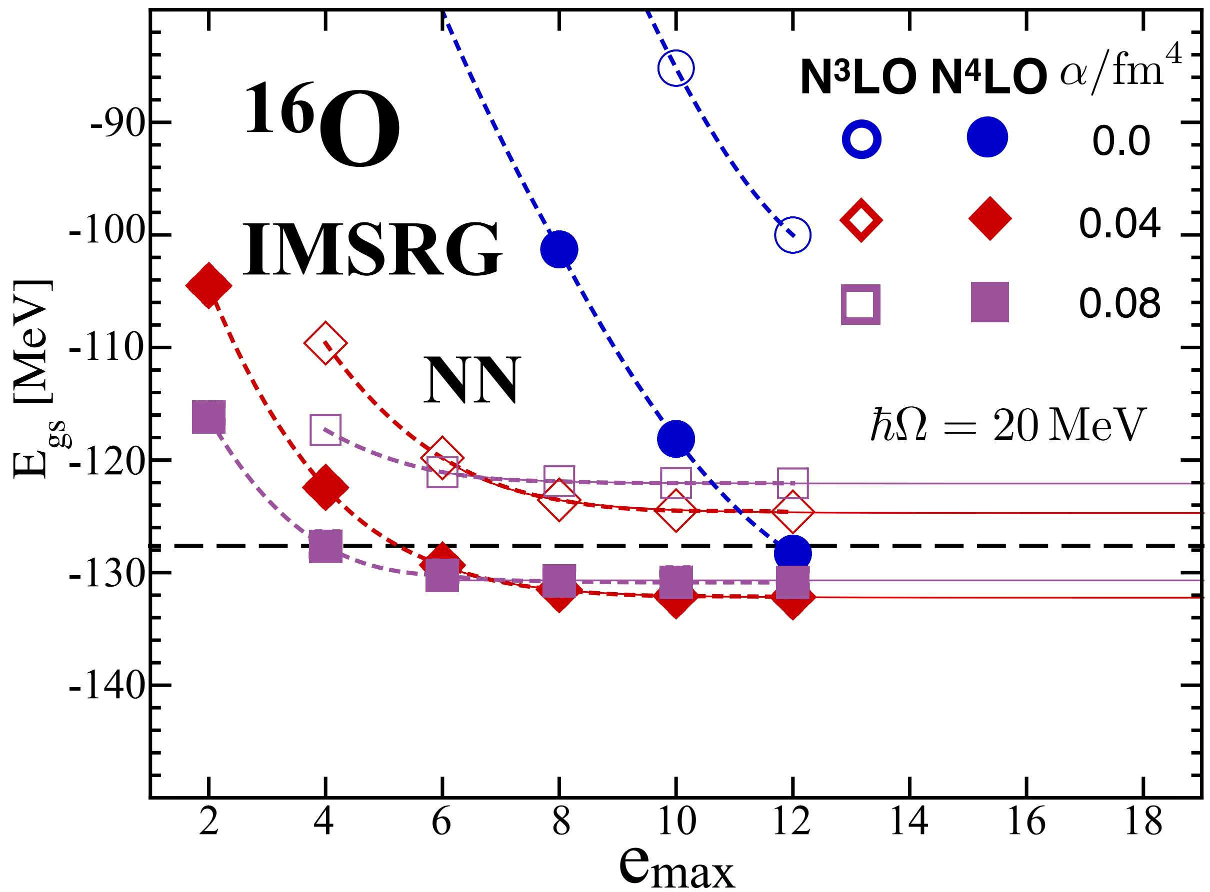
- S. Quaglioni, C. Romero-Redondo
  LLNL Livermore, USA
- G. Hupin
  Université Paris-Sud, France
- H. Hergert, S. Bogner
  MSU, USA

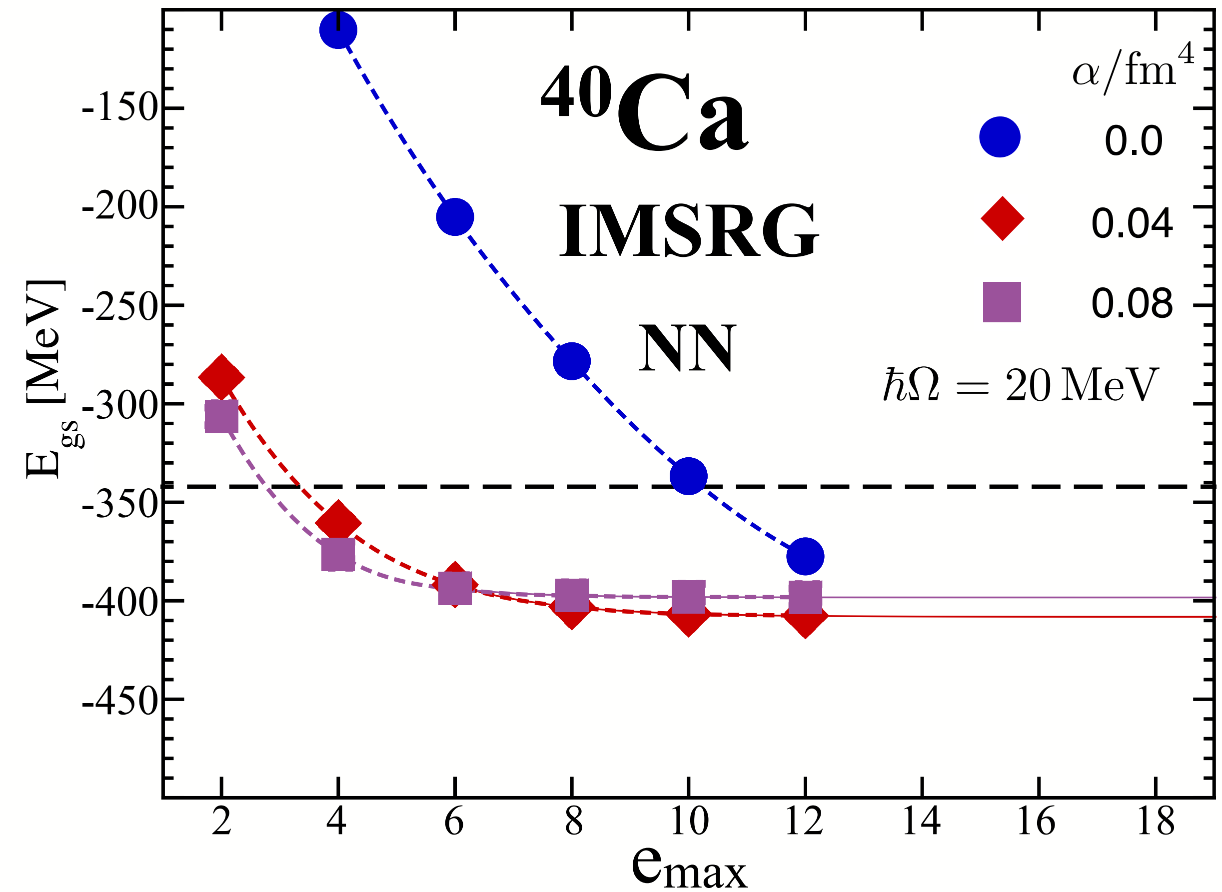
LLNL — MIC | JUROPA — JÜLICH FORSCHUNGSZENTRUM | LOEWE-CSC — CSC Center for Scientific Computing Frankfurt | HOPPER — NERSC | OLCF — Oak Ridge National Laboratory, Oak Ridge Leadership Computing Facility

COMPUTING TIME

Supplements

^{16}O & ^{40}Ca : Ground-State





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