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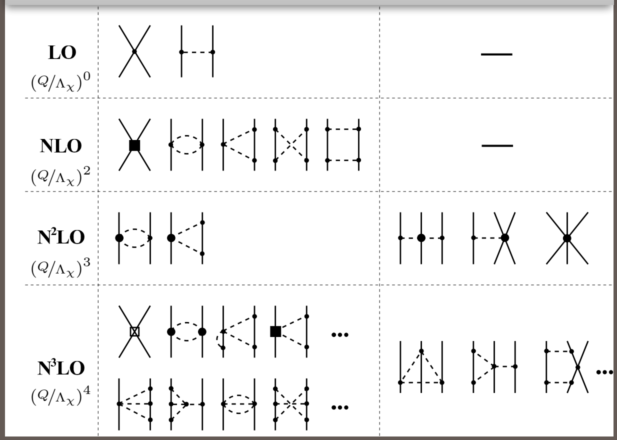
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

Predictive Power of Chiral Interactions for Nuclear Structure and Reaction Calculations in the p-Shell

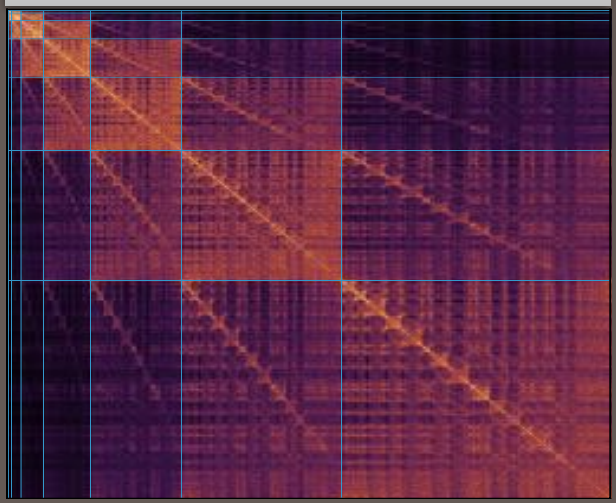
INT Program INT-17-1a
March 27 2017, Seattle

Angelo Calci | TRIUMF

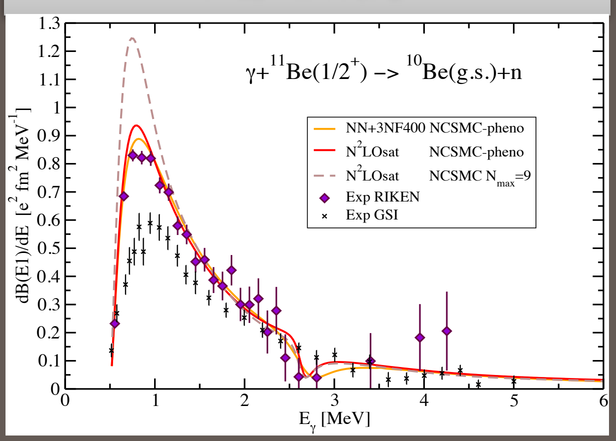
Chiral EFT



SRG



Ab initio



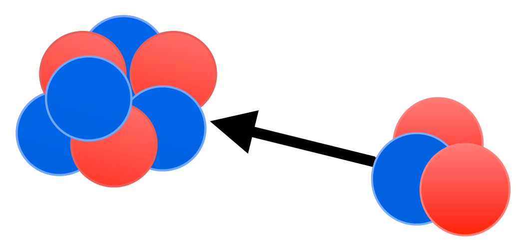
Outline

ab initio description of nuclei

QCD-based interaction

realistic NN+3N interactions

bound states & spectroscopy



resonances & scattering states

(Importance Truncated) NCSM

ab initio description of nuclear clusters

Resonating Group Method (RGM)

describing relative motion of clusters

NCSM with Continuum

continuum effects in spectroscopy

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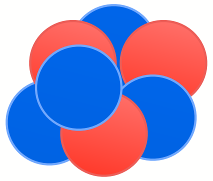


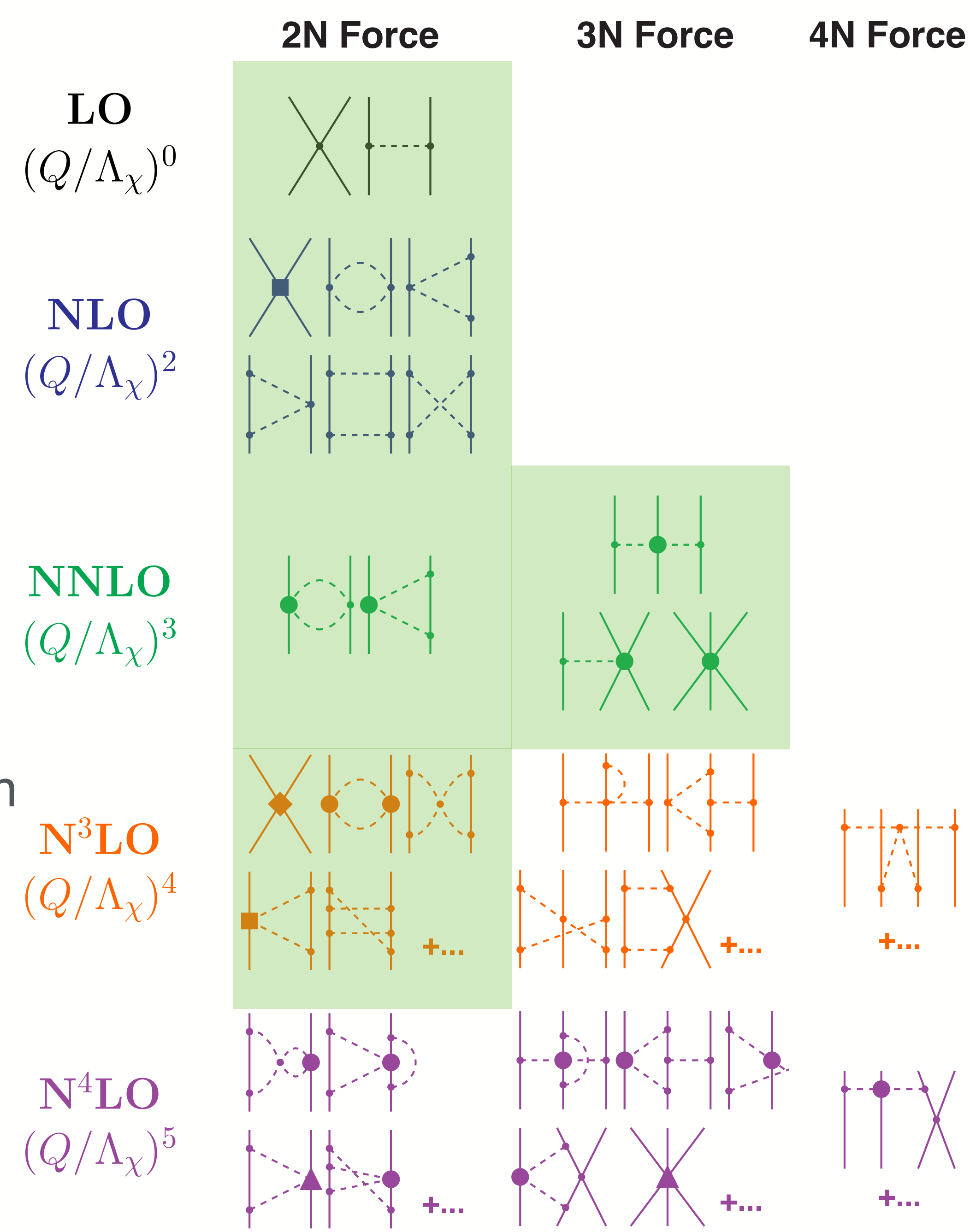
Chiral NN+3N Interactions

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

- **standard interaction:**
  - NN @ N^{3}LO: Entem & Machleidt, 500MeV cutoff
  - 3N @ N^{2}LO: Navrátil, local, 500MeV cutoffs & modifications of the 3N force

- **optimized N^{2}LO interaction:**
  - NN: Ekström et al., 500MeV cutoff, LECs fitted with POUNDerS
  - 3N: Navrátil, local, 500MeV cutoff, fit to ^{4}He & Triton

- **EGM N^{2}LO interaction:**
  - NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal



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- **standard interaction:**
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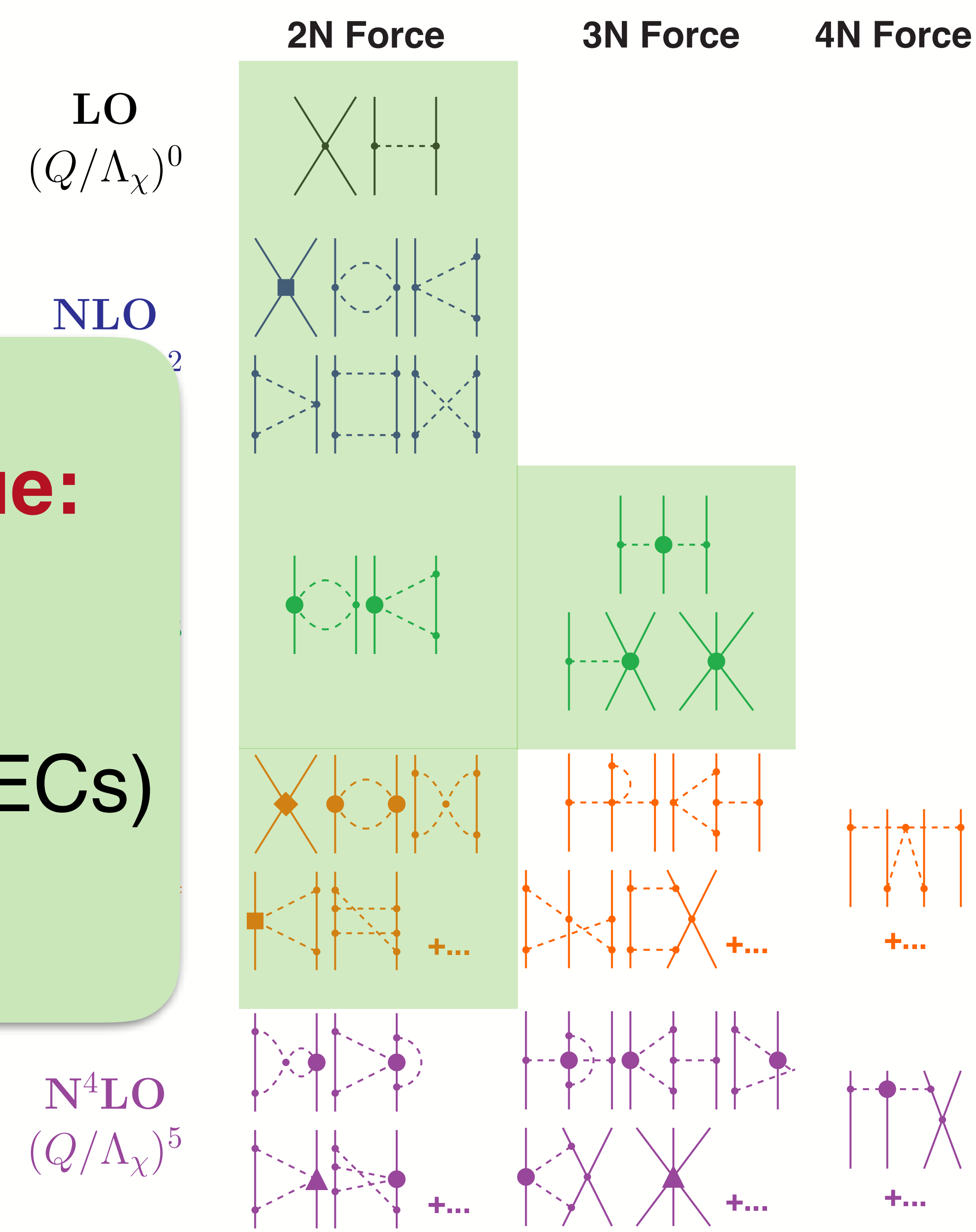
  - 3N @ N²LO: Navrátil, local, 500MeV cutoffs & modifications of the 3N force

chiral interactions are not unique:

- chiral order
- regularization
- fit of low-energy constants (LECs)
- (power counting)

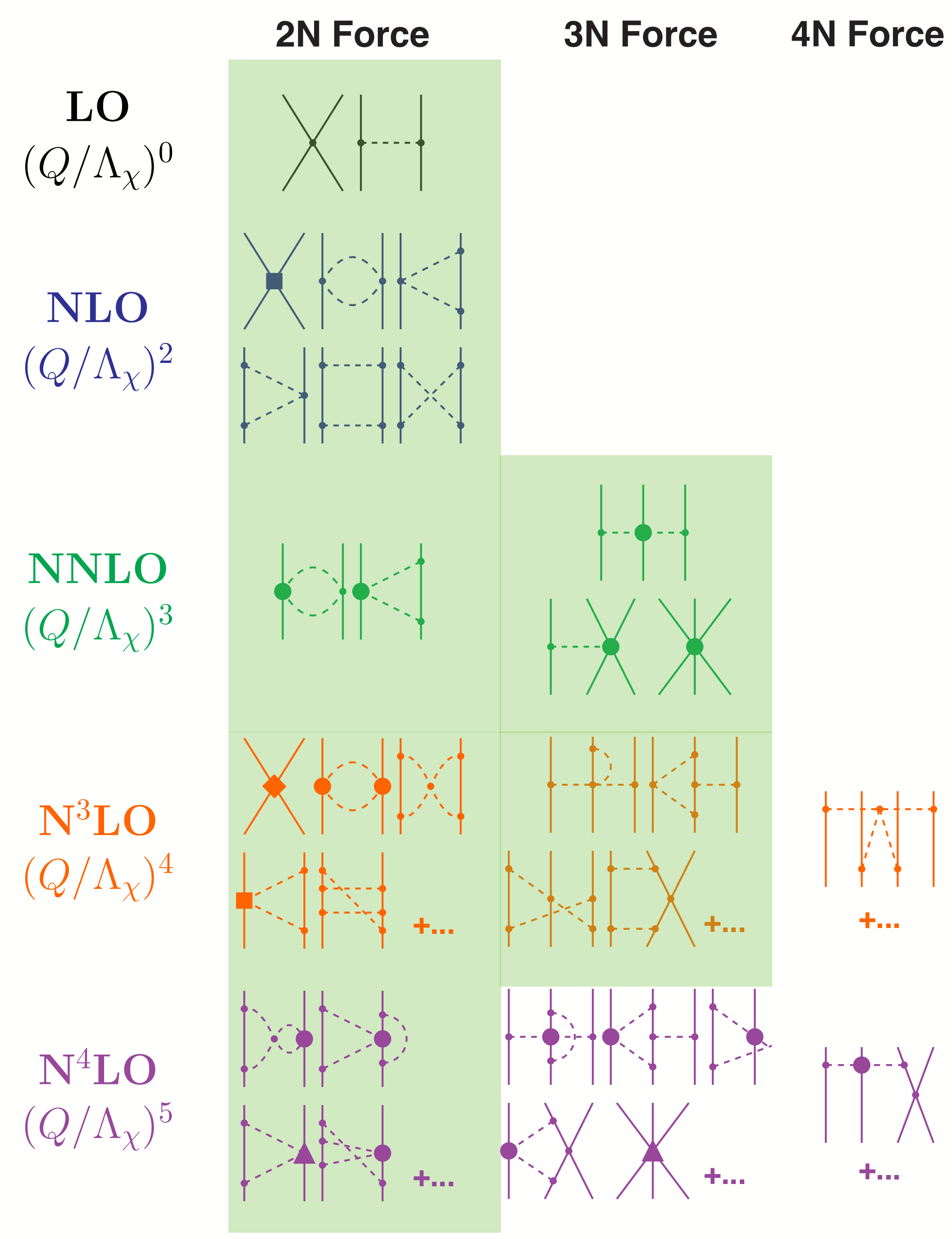
- NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
- 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal



Next Generation Interactions

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

- **standard interaction:**
  - NN @ N³LO: Entem & Machleidt, 500MeV cutoff
  - 3N @ N²LO: Navrátil, local cutoffs
- **N²LO$_{\text{SAT}}$ interaction:**
  - NN+3N: Ekström et al., nonlocal 450MeV cutoff, simultaneous fit to NN data and selected many-body observables
- **LENPIC interaction:**
  - NN up to N⁴LO: Epelbaum et al., semi-local cutoff
  - 3N up to N³LO: under construction
- **N⁴LO(500):**
  - NN @ N⁴LO: Machleidt et al., 500MeV cutoff



Similarity Renormalization Group (SRG)

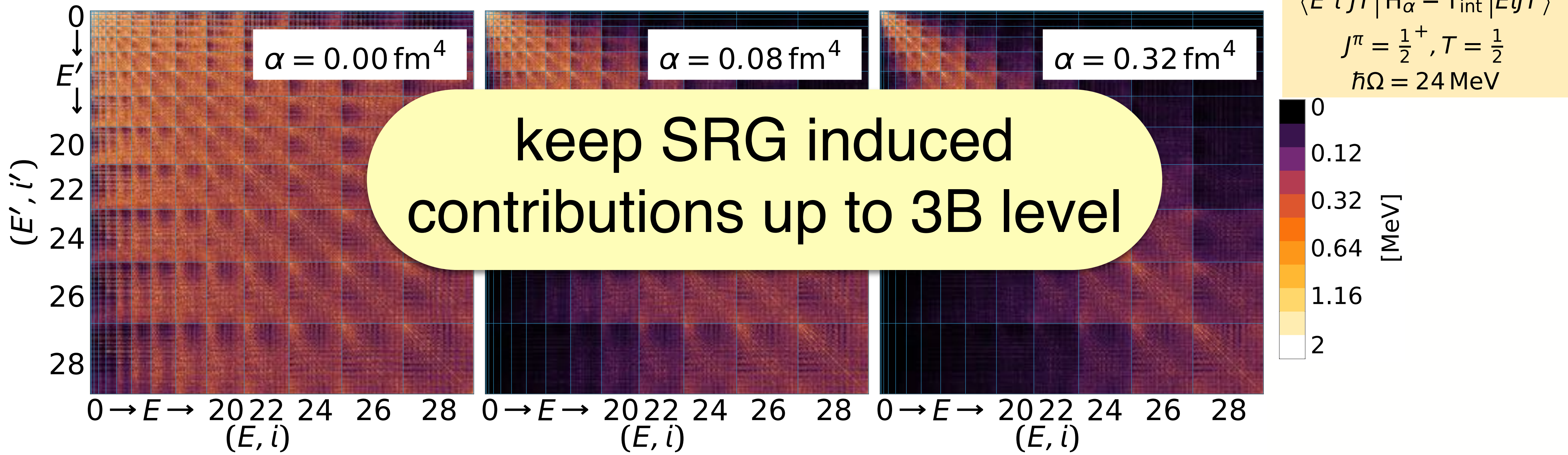
accelerate convergence by **pre-diagonalizing** the Hamiltonian with respect to the many-body basis

- **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



keep SRG induced contributions up to 3B level

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(Importance Truncated) NCSM

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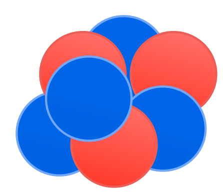
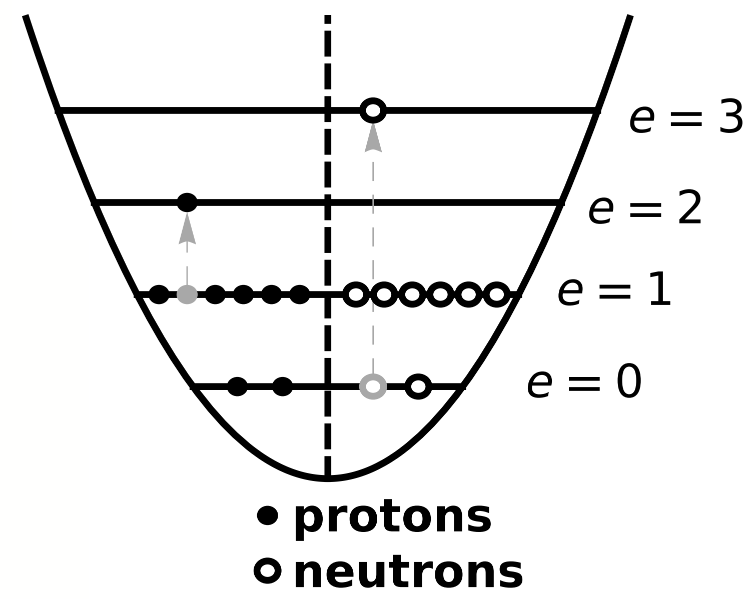


No-Core Shell Model (NCSM)

- solving the eigenvalue problem:

$$\mathrm{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$

- **model space:**
  spanned by Slater determinants with unperturbed excitation energy up to $N_{max}\hbar\Omega$



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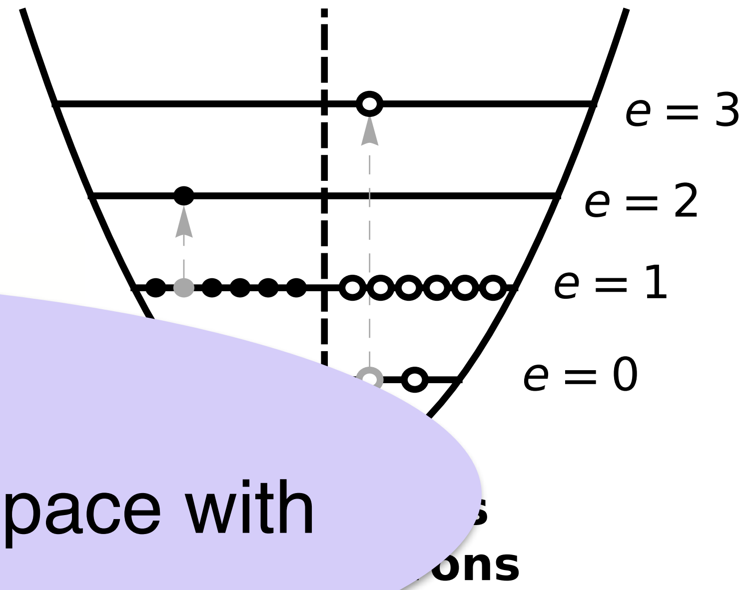

problem of NCSM

enormous increase of model space with particle number A

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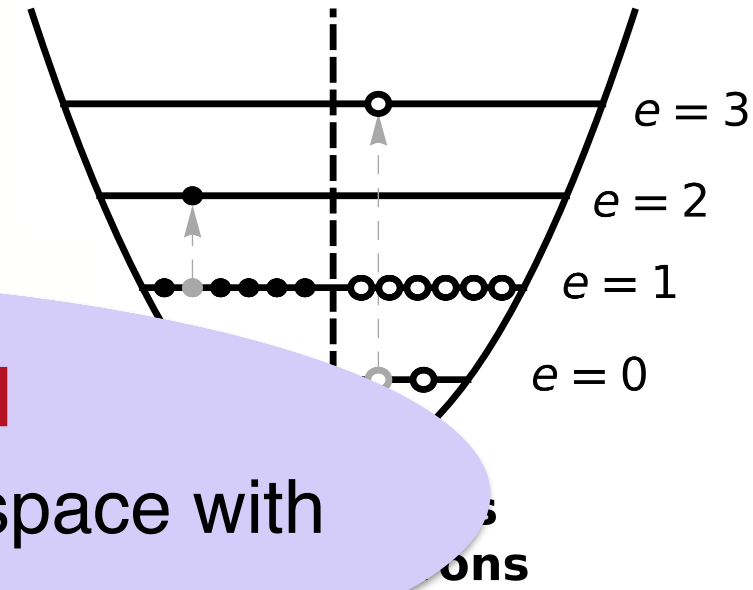

- **model space:**

  spanned b

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  up to $N_{max}\hbar\Omega$

problem of NCSM

enormous increase of model space with particle number A

Importance Truncated NCSM

- a priori determination of relevant basis states via first-order perturbation theory

$$\kappa_\nu = -\frac{\left\langle\Phi_\nu\right|\mathrm{H}_{\mathrm{int}}\left|\Psi_{\mathrm{ref}}\right\rangle}{\epsilon_\nu - \epsilon_{\mathrm{ref}}}$$

- **importance truncated space** spanned by basis states with $|\kappa_\nu| \geq \kappa_{\mathrm{min}}$

No-Core Shell Model (NCSM)

- solving the eigenvalue problem:

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  spanned b…
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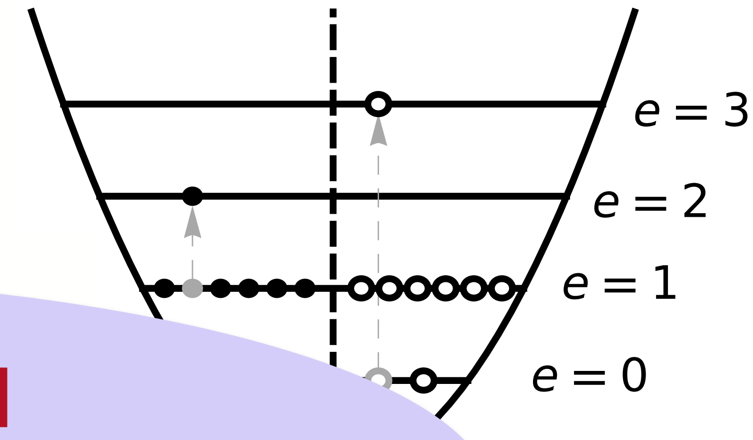

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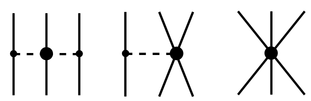
Importanc…

- a…
  p…
- **importance truncated space** spanned by basis states with $|\kappa_\nu| \geq \kappa_{min}$

- **extrapolation** of $\kappa_{min} \rightarrow 0$ recovers effect of omitted contributions
- IT-NCSM provides **same results** as full NCSM
- **expands** application **range** to larger A

Sensitivity on chiral 3N interactions

- analyze the sensitivity of spectra on **low-energy constants** (c_i, c_D, c_E) and **cutoff** (Λ) of the chiral 3N interaction at N^{2}LO



- why this is interesting:
  - **impact of N^{3}LO contributions**: some N^{3}LO diagrams can be absorbed into the N^{2}LO structure by shifting the c_i constants

$$\bar{c}_1 = c_1 - \frac{g_A^2 M_\pi}{64\pi F_\pi^2}\,, \quad \bar{c}_3 = c_3 + \frac{g_A^4 M_\pi}{16\pi F_\pi^2}\,, \quad \bar{c}_4 = c_4 - \frac{g_A^4 M_\pi}{16\pi F_\pi^2}$$

(Bernard et al., Ishikawa, Robilotta)

  - **uncertainty propagation**: sizable variations of the c_i from different extractions (also affects NN)

$$c_1 = -1.23 \ldots -0.76\,, \quad c_3 = -5.94 \ldots -3.20\,, \quad c_4 = 3.40 \ldots 5.40 \;\; [\text{GeV}^{-1}]$$

  - **cutoff dependence**: does the cutoff choice in the 3N interaction affect nuclear structure observables?

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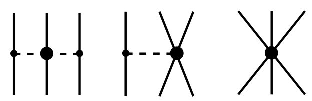

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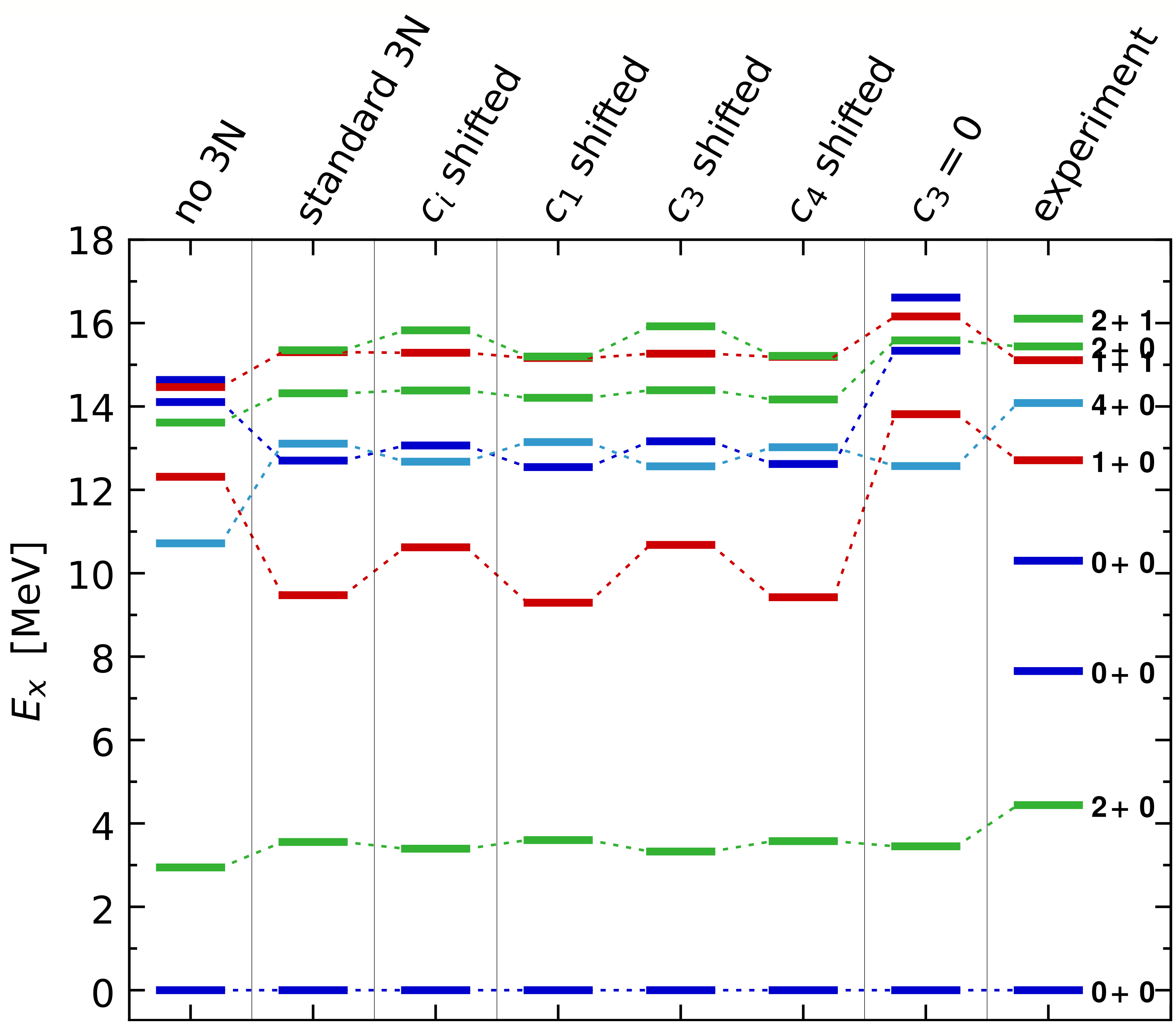
  - **uncertainty propagation**: sizable v... dif-ferent extractions (also affects NN)

$$c_1 = -1.23 \ldots -0.76\,, \quad c_3 = -5.94 \ldots - 3$$

  - **cutoff dependence**: does the cutoff c... eracti-on affect nuclear structure observables?

provide **constraints** for chiral Hamiltonians and **quantify uncertainties**

^{12}C: Sensitivity to c_i

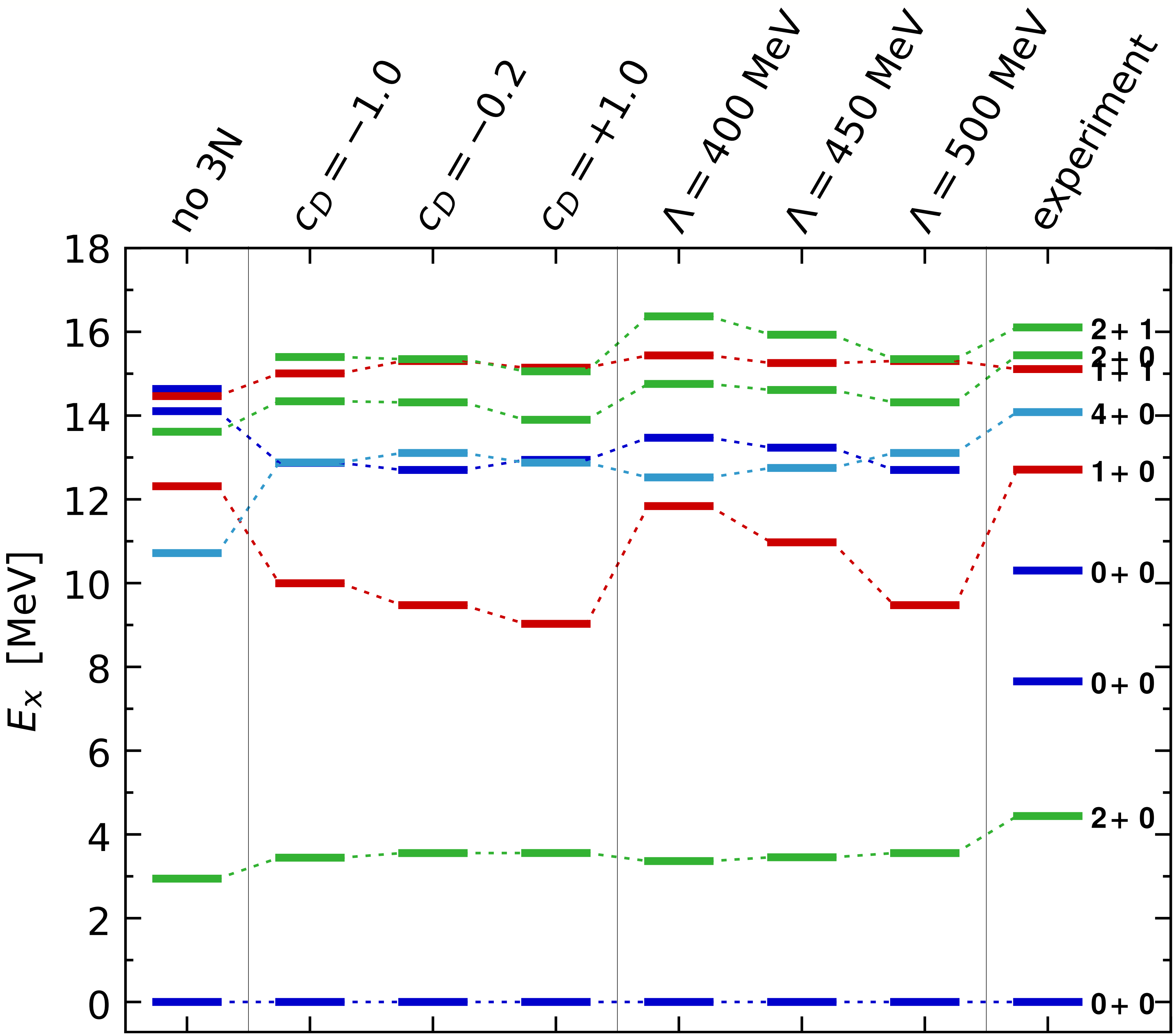


- many states are rather c_i independent
- first 1^+ state shows strong c_3 dependence

IT-NCSM

$\hbar\Omega = 16$ MeV
$N_{\mathrm{max}} = 8$
$\alpha = 0.08\,\mathrm{fm}^4$

^{12}C: Sensitivity to c_D *and cutoff*

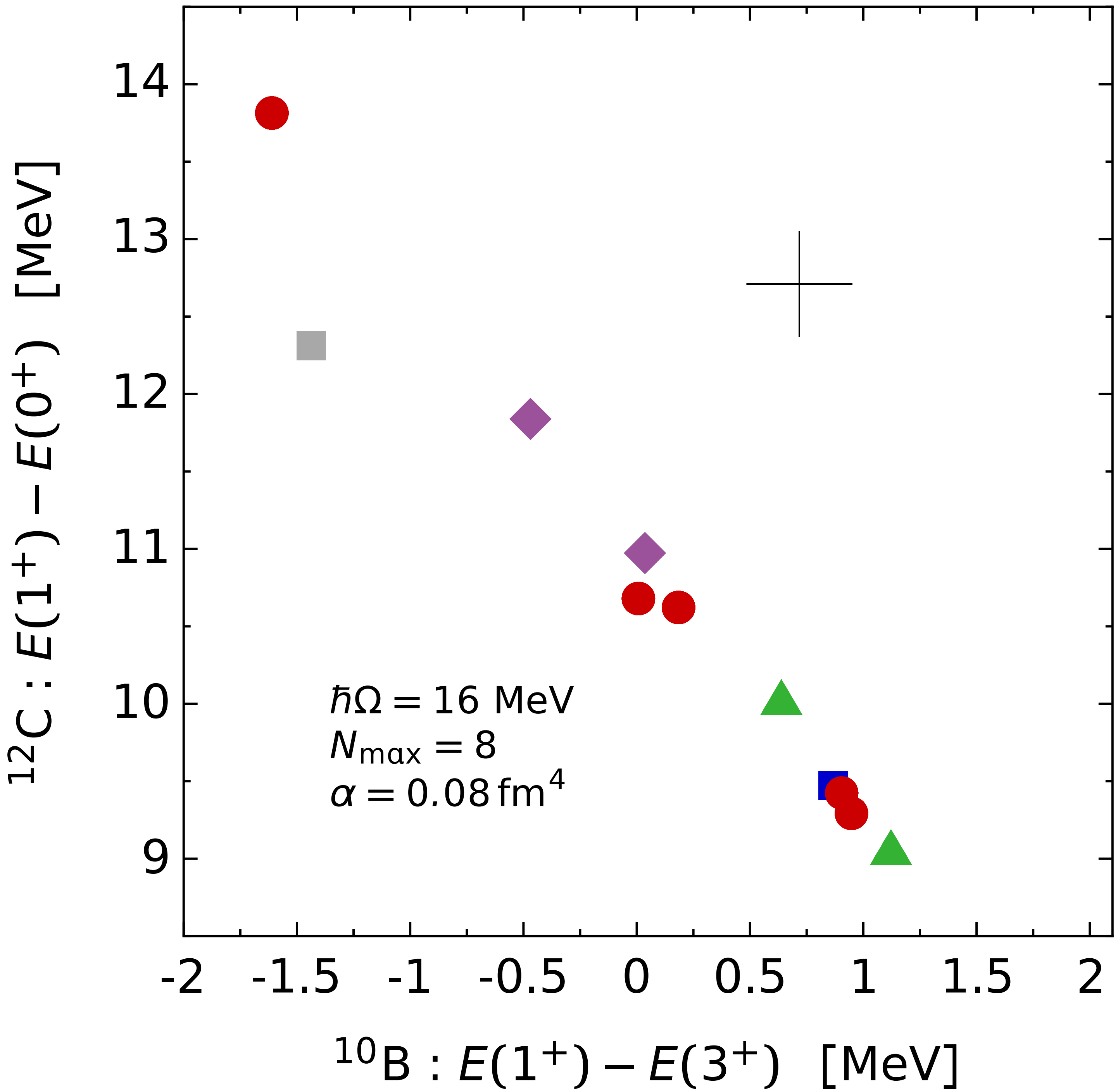


- moderate dependence on c_D, stronger dependence on Λ
- again first 1^+ state is most sensitive

IT-NCSM

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\mathrm{fm}^4$

Correlation Analysis: ^{12}C(1$^+$) vs. ^{10}B(1$^+$)



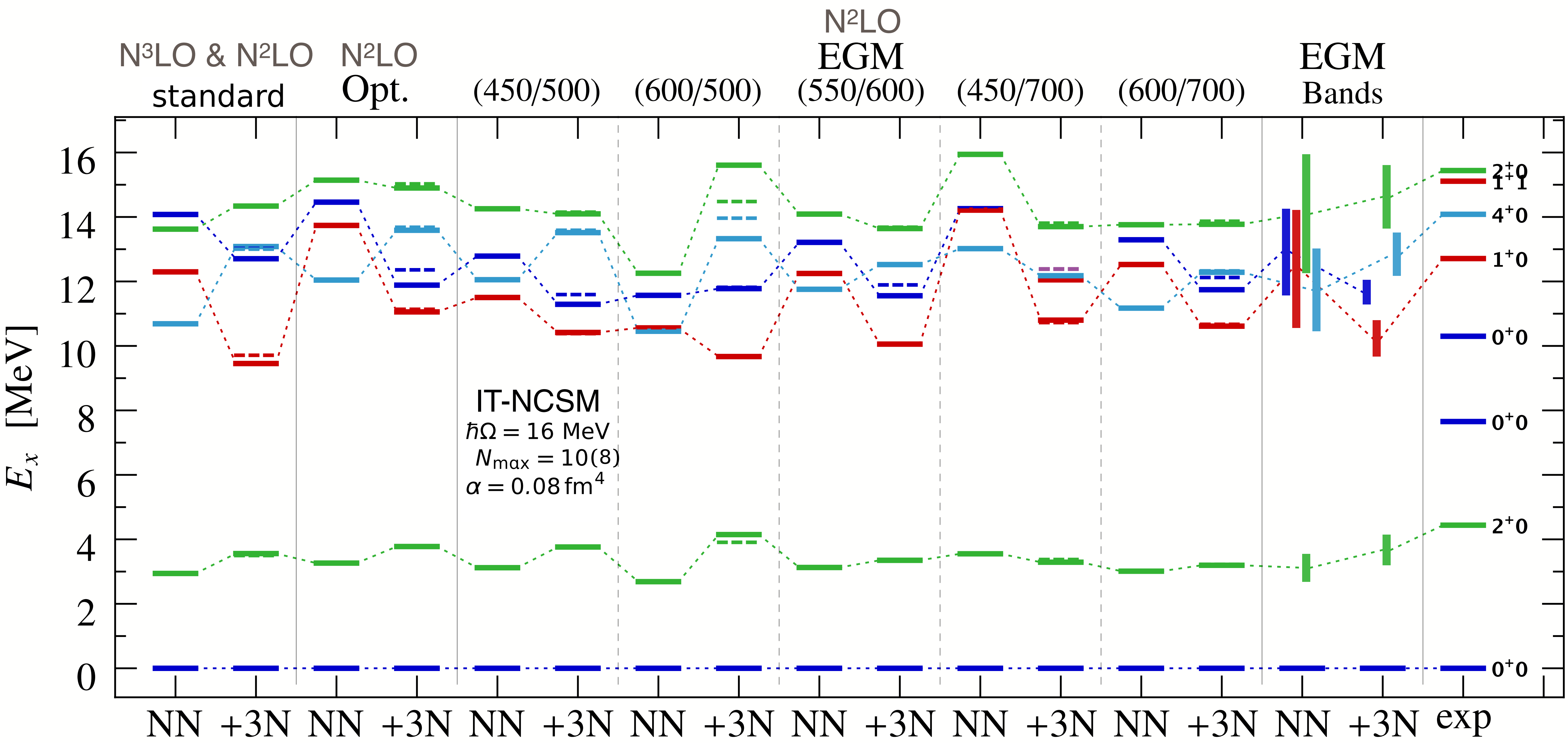
- correlation does not agree with experiment
- hints at problems with E&M NN interaction

standard

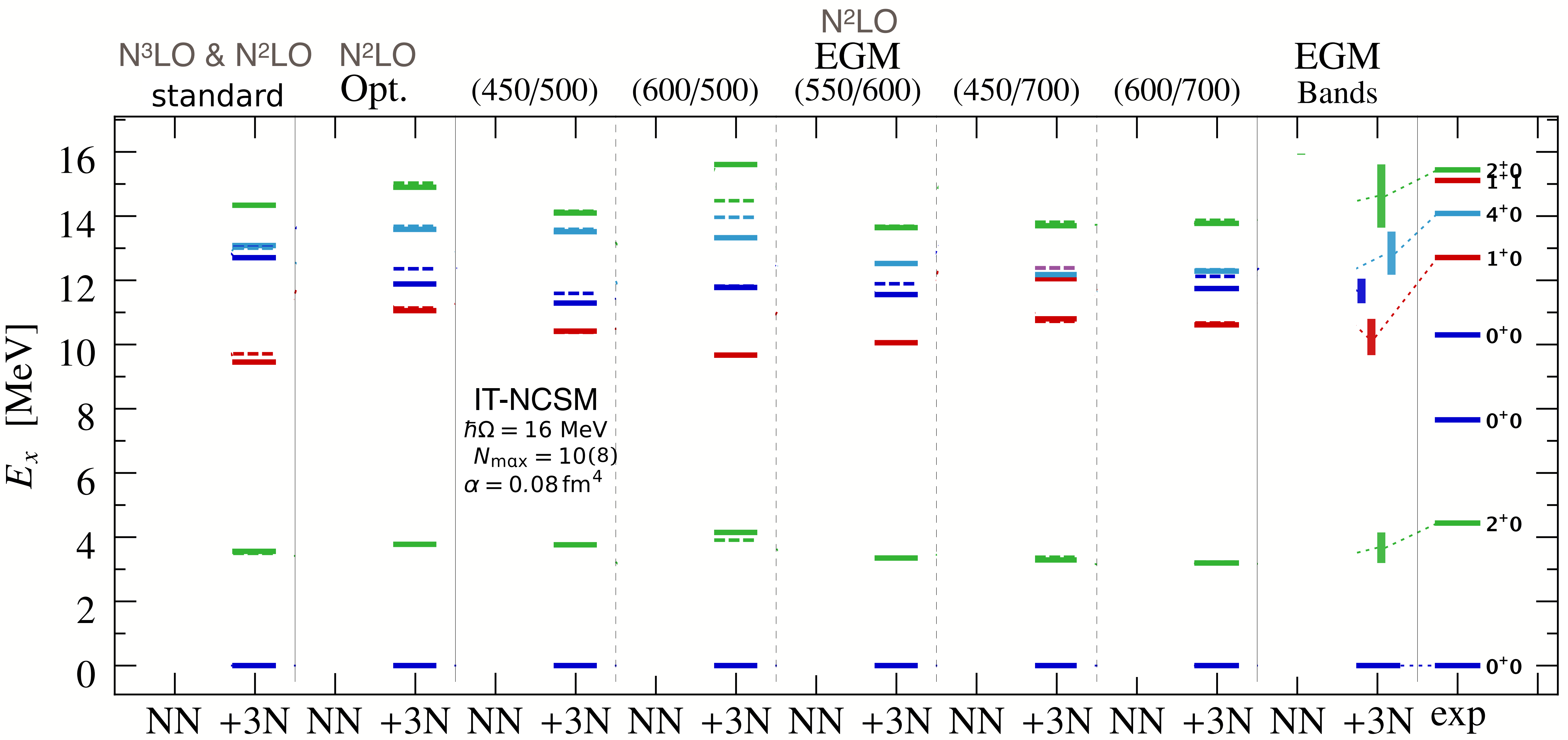
- no 3N
- std 3N
- c_i var
- c_D var
- Λ var

\+ exp

^{12}C: Cutoff Dependence

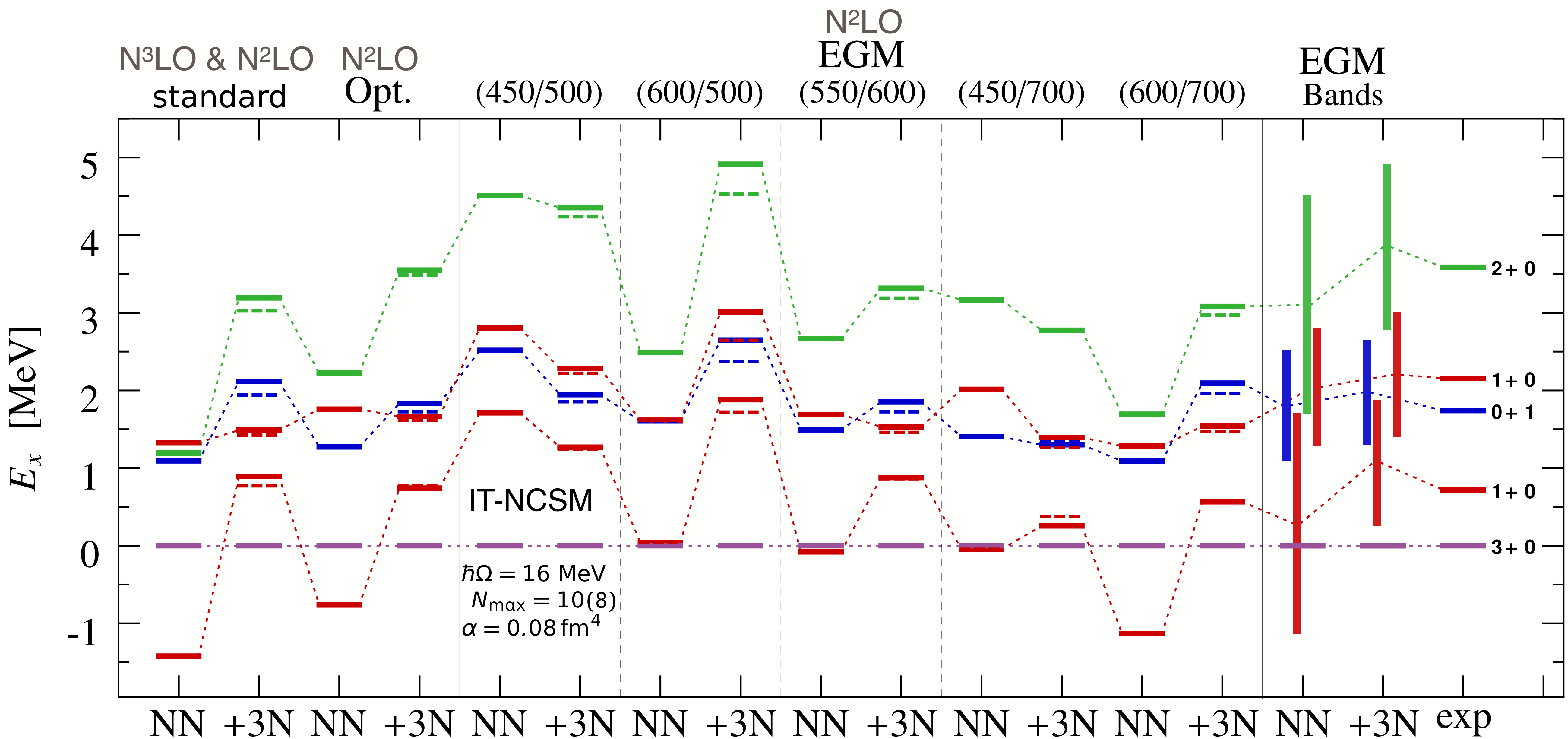


^{12}C: Cutoff Dependence



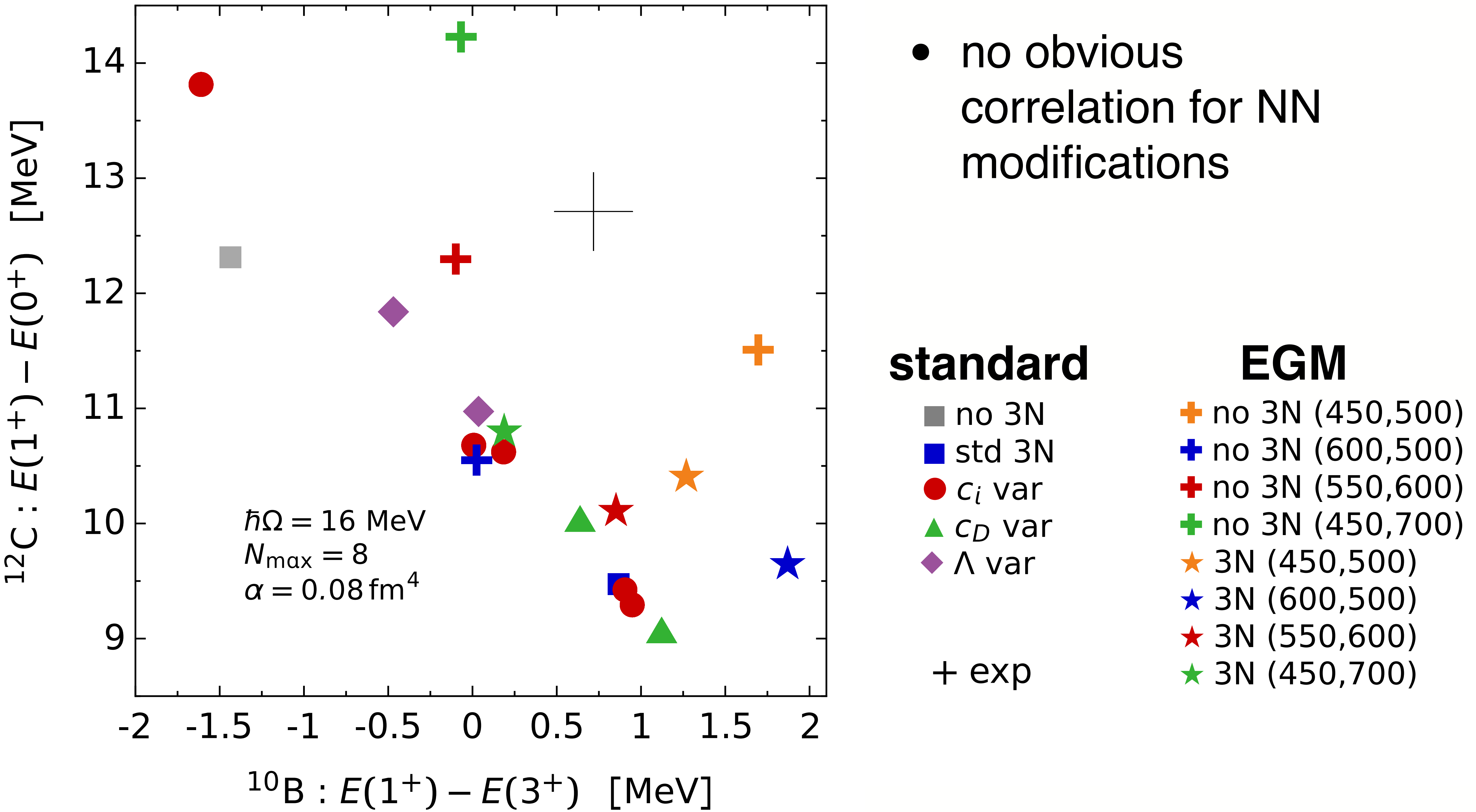
- small cutoff dependence for NN+3N

^{10}B: Cutoff Dependence



- complex system with compressed spectrum
- accurate predictions within large uncertainties

Correlation Analysis: ^{12}C(1^+) vs. ^{10}B(1^+)



- no obvious correlation for NN modifications

Outline

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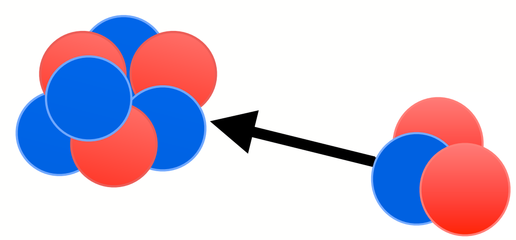

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NCSM with Continuum

continuum effects in spectroscopy

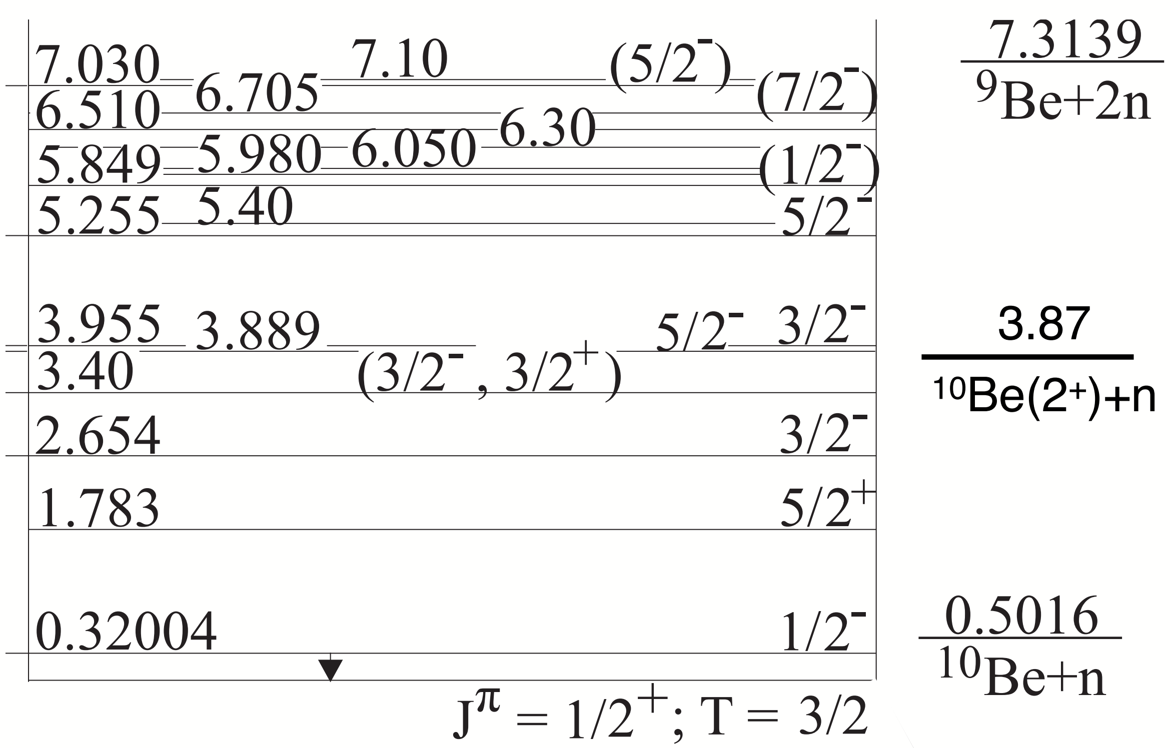
Neutron-rich halo Nucleus ^{11}Be

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

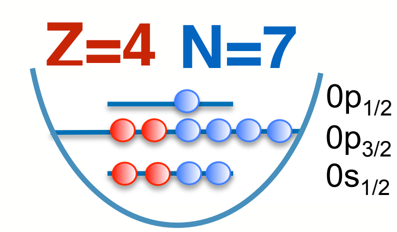
Can *Ab Initio* Theory Explain the Phenomenon of Parity Inversion in ^{11}Be?

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

Neutron-rich halo Nucleus ^{11}Be

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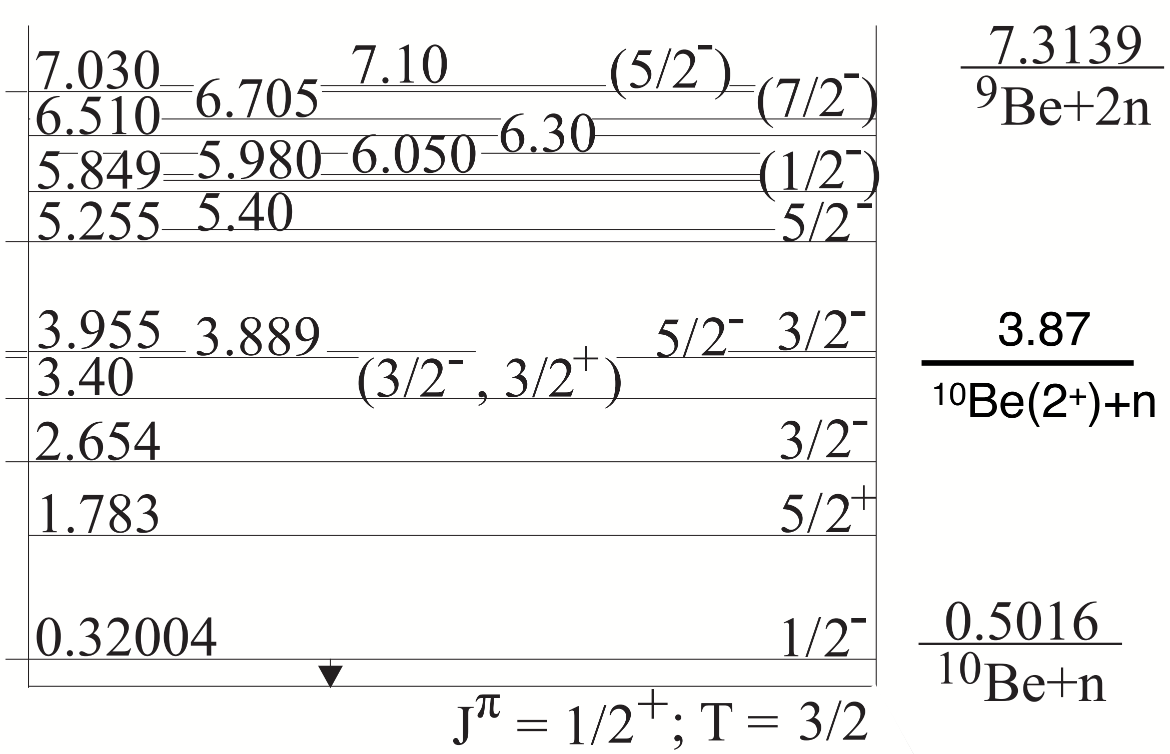
Can **ab initio** theory describe this complicated system?



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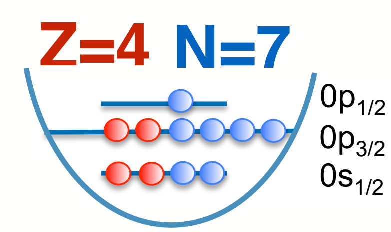

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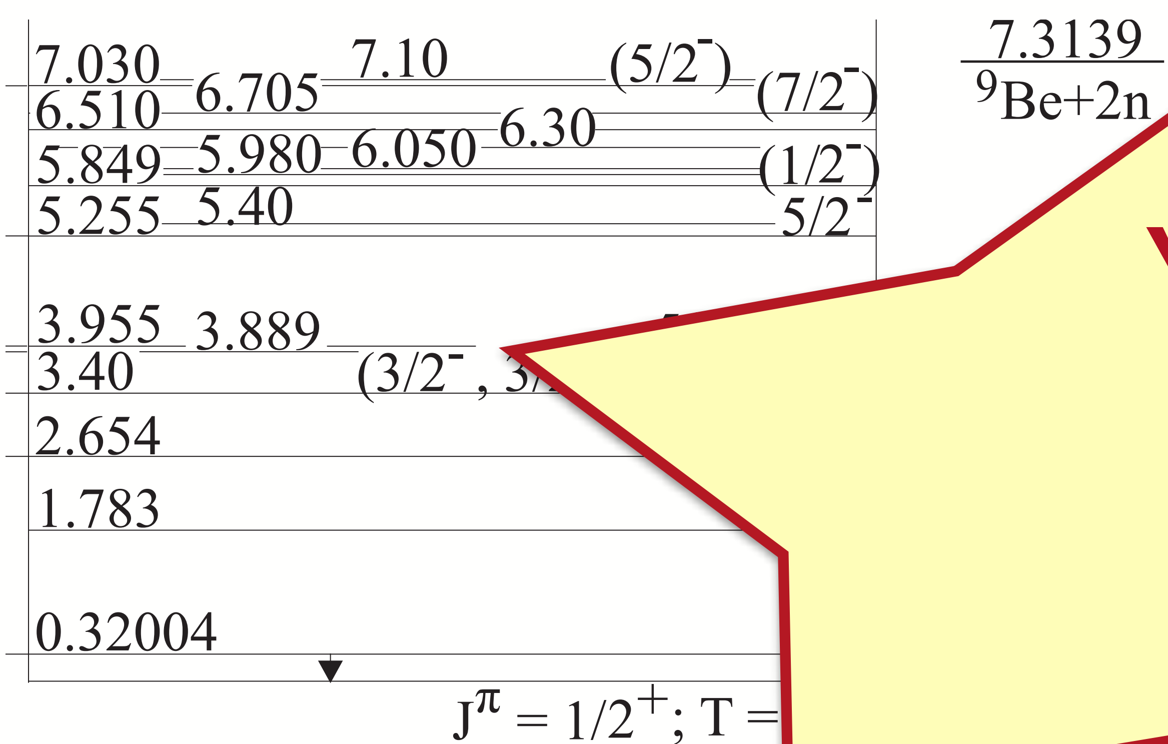

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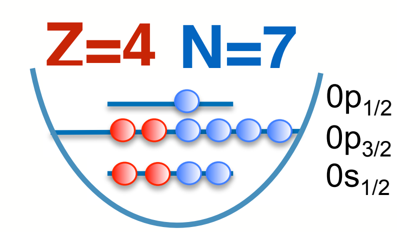

YES

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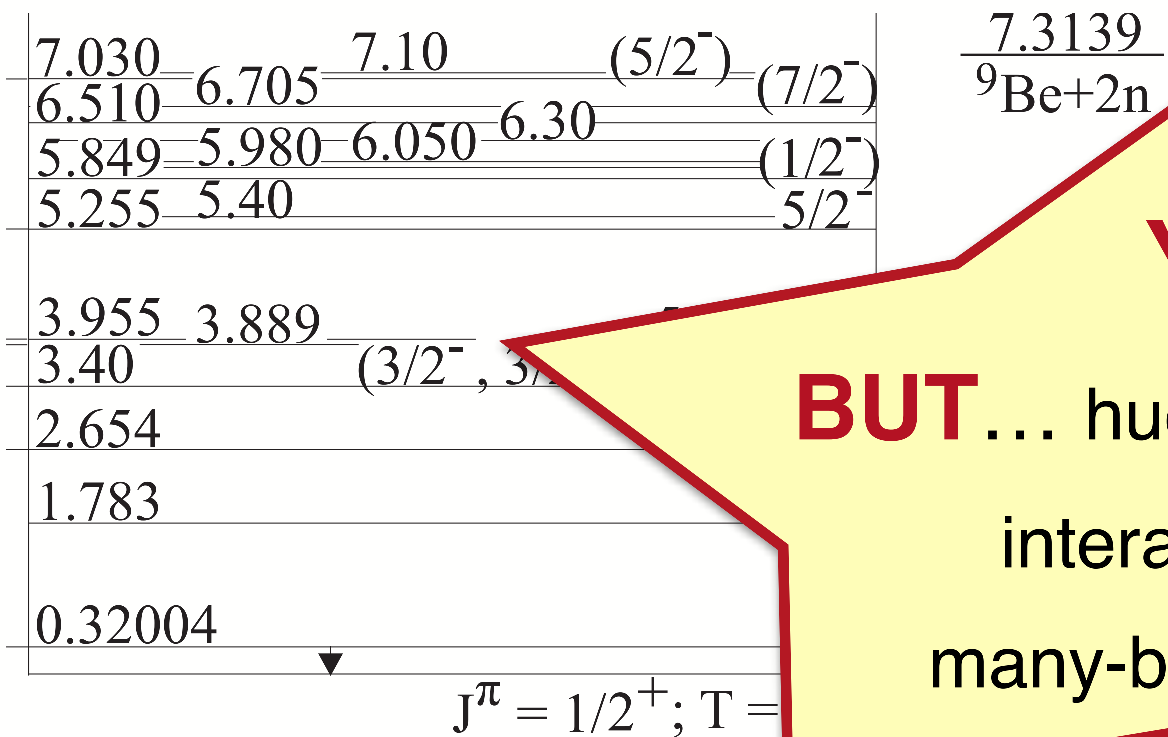

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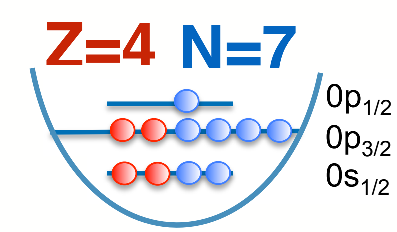


... und J=1/2 states

... n dominated by n-^{10}Be

YES

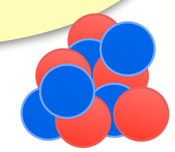
BUT… huge challenge for interaction and many-body method

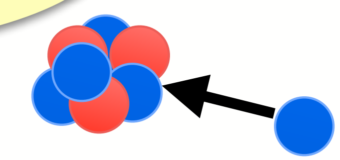
NCSM with Continuum (NCSMC)

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

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

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





expansion in A-body NCSM eigenstates

relative motion of clusters NCSM/RGM expansion

- leads to NCSMC equation

$$\begin{pmatrix} H_{NCSM} & h \\ h & \mathcal{H} \end{pmatrix}\begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = E\begin{pmatrix} \mathbb{1} & g \\ g & \mathbb{1} \end{pmatrix}\begin{pmatrix} c \\ \chi(r)/r \end{pmatrix}$$

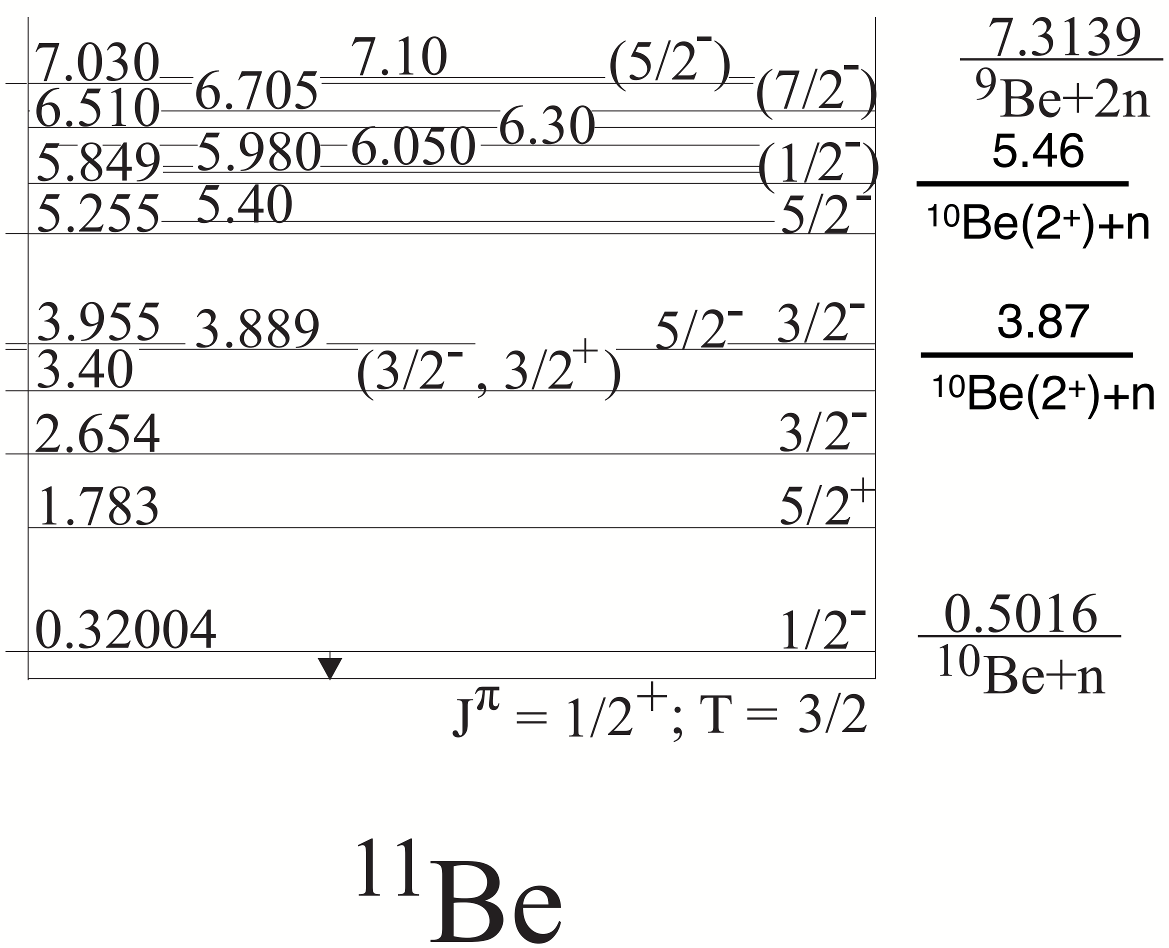
- with 3N contributions in

H_{NCSM}	h	$\mathcal{H}$
covered by NCSM	given by $\left\langle\Psi_A E_{\lambda'} J^\pi T\right|\mathrm{H}\left|\xi^{J\pi T}_{\nu r}\right\rangle$	contains NCSM/RGM Hamiltonian kernel

^{11}Be: Ab initio NCSMC calculations

- **Halo structure**

  spectrum dominated by n-^{10}Be halo structure



NCSM input

- calculations use NCSM vectors and energies as input
- include n-^{10}Be continuum (0^+,2^+,2^+ states of ^{10}Be)
- include ^{11}Be short-range correlations:
  4 negative parity (at least)
  3 positive parity states of ^{11}Be

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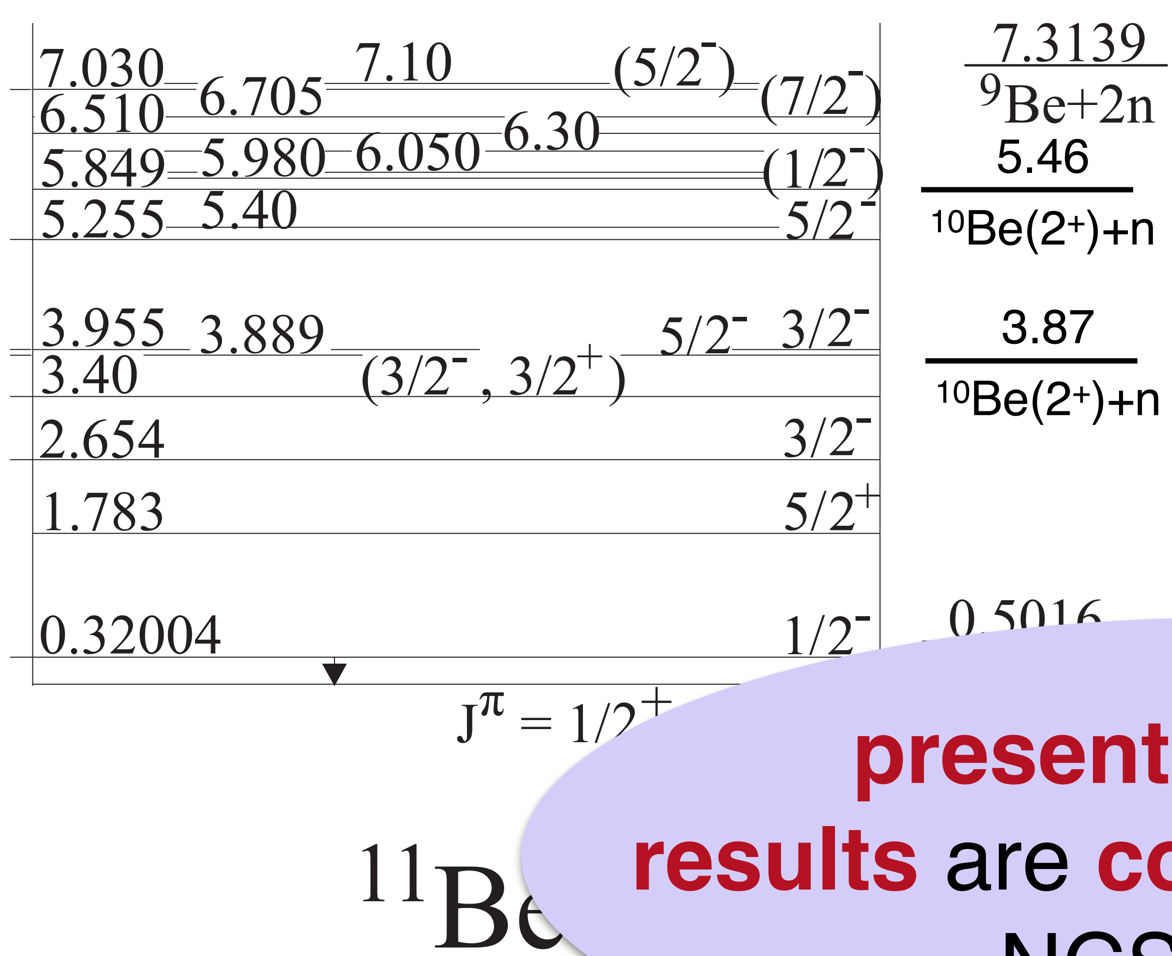

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presented NCSMC results are **converged** w.r.t. to NCSM input

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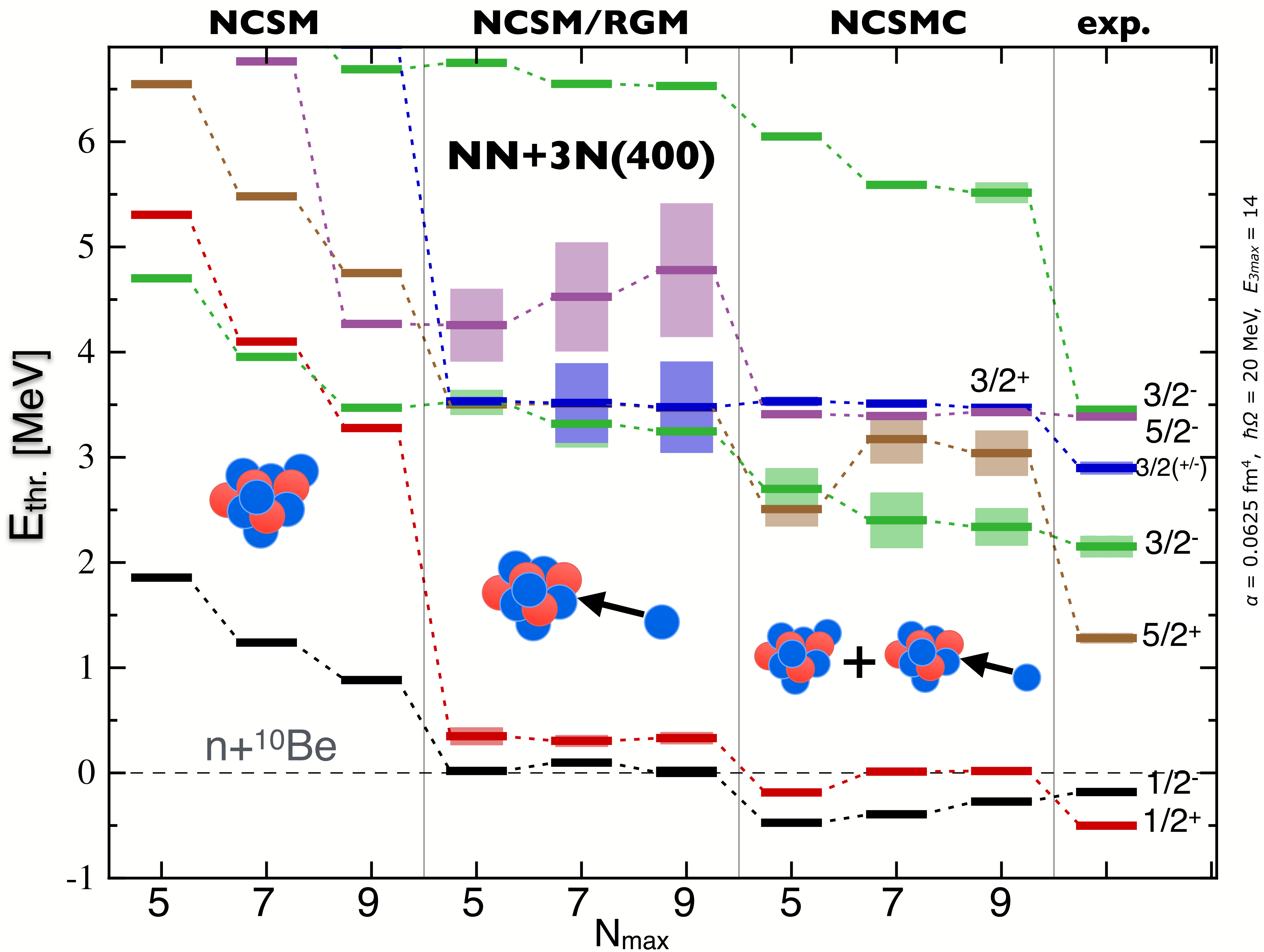
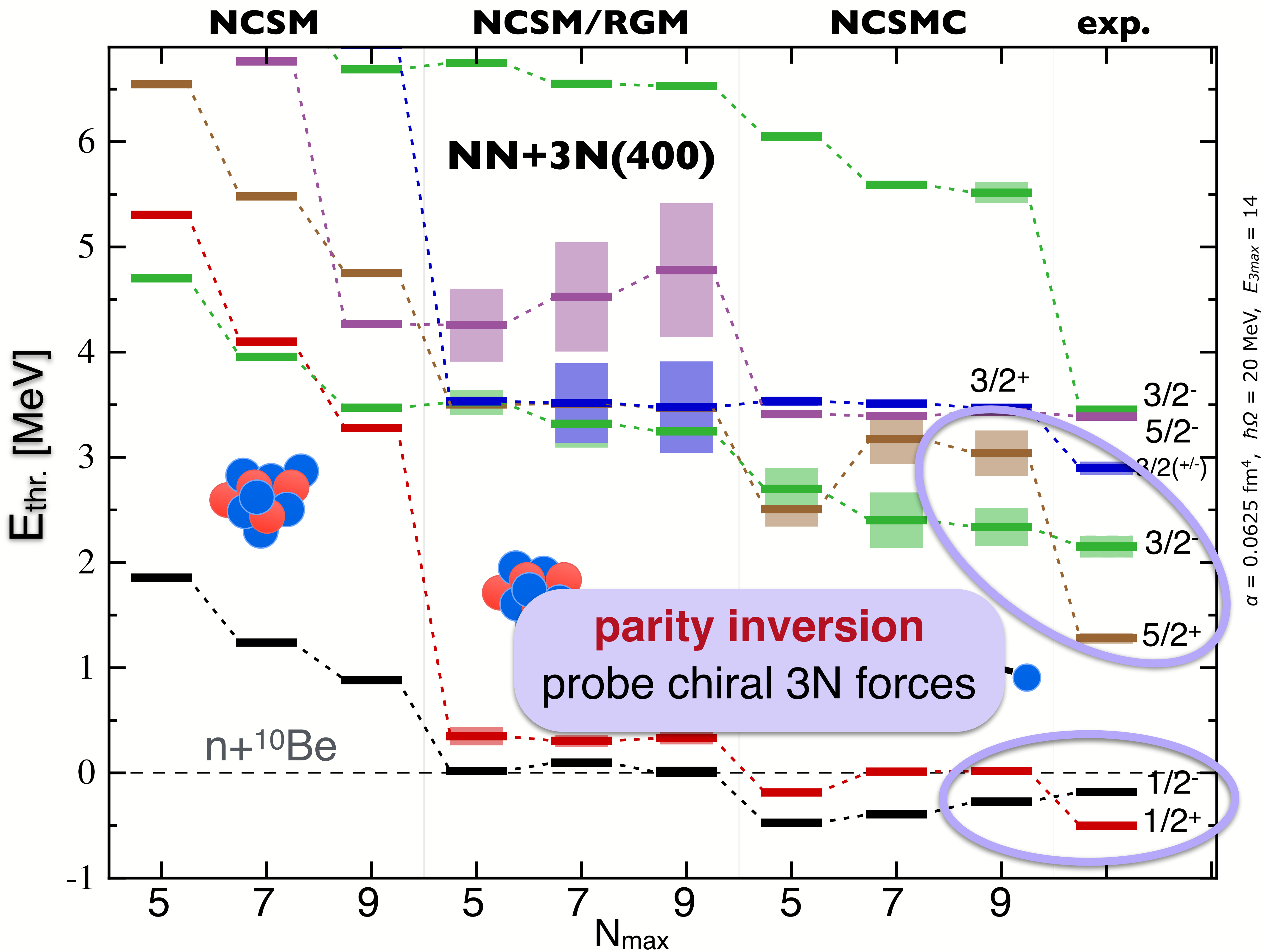
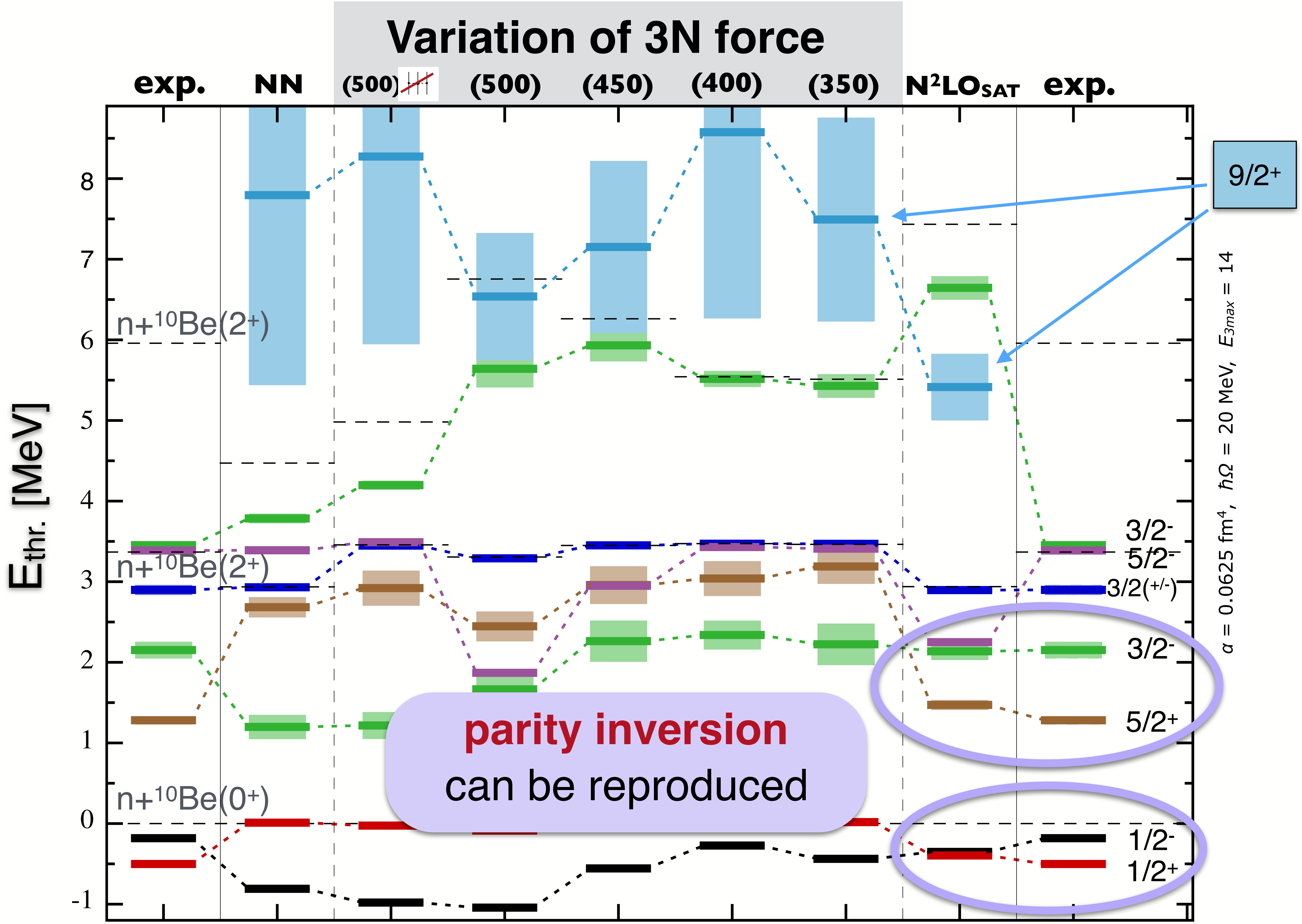
^{11}Be excitation spectrum



^{11}Be excitation spectrum



^{11}Be excitation spectrum

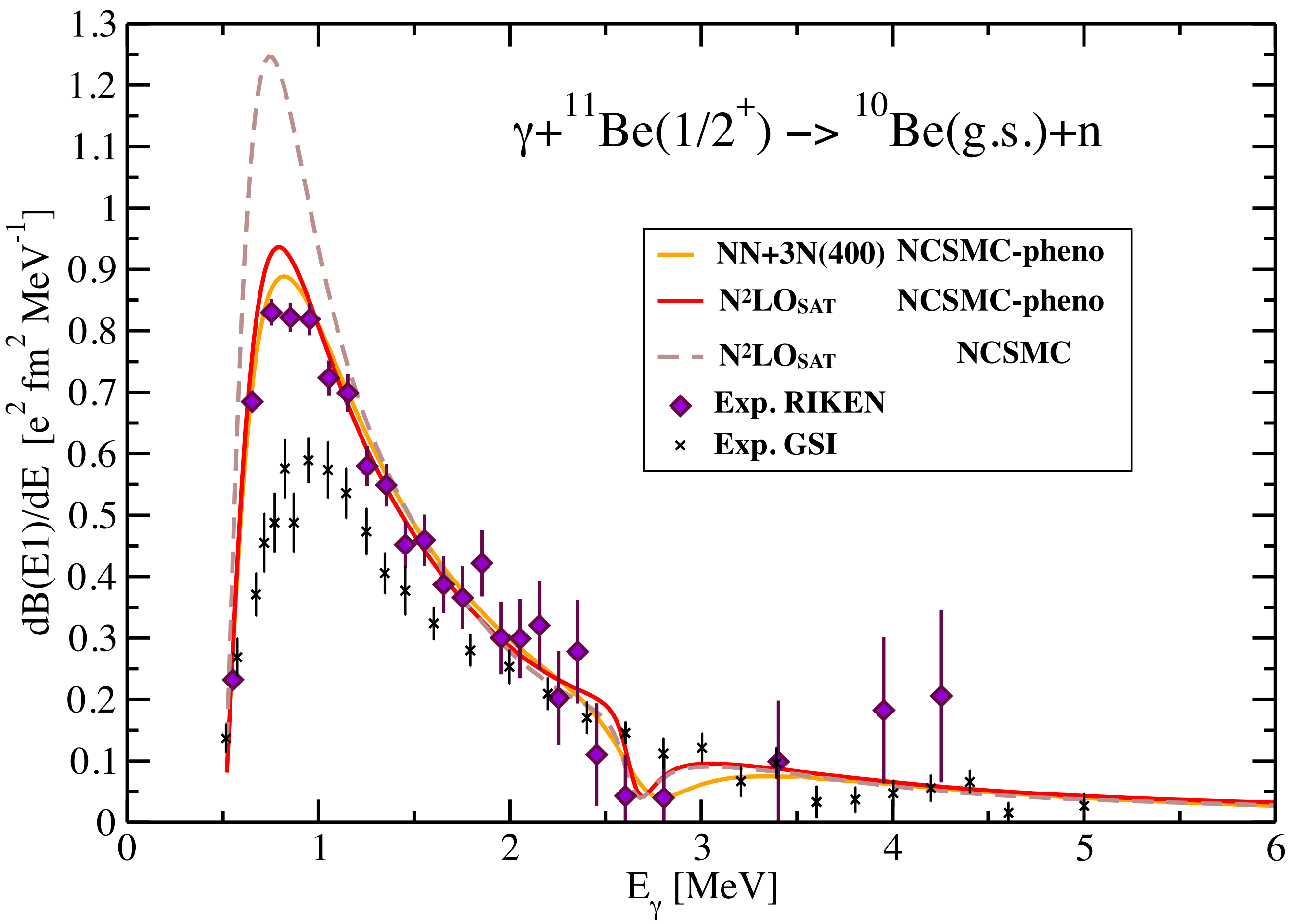


^{11}Be: Photodisintegration process & E1 transition

B(E1:1/2$^-$→1/2$^+$) [e^{2}fm^2]

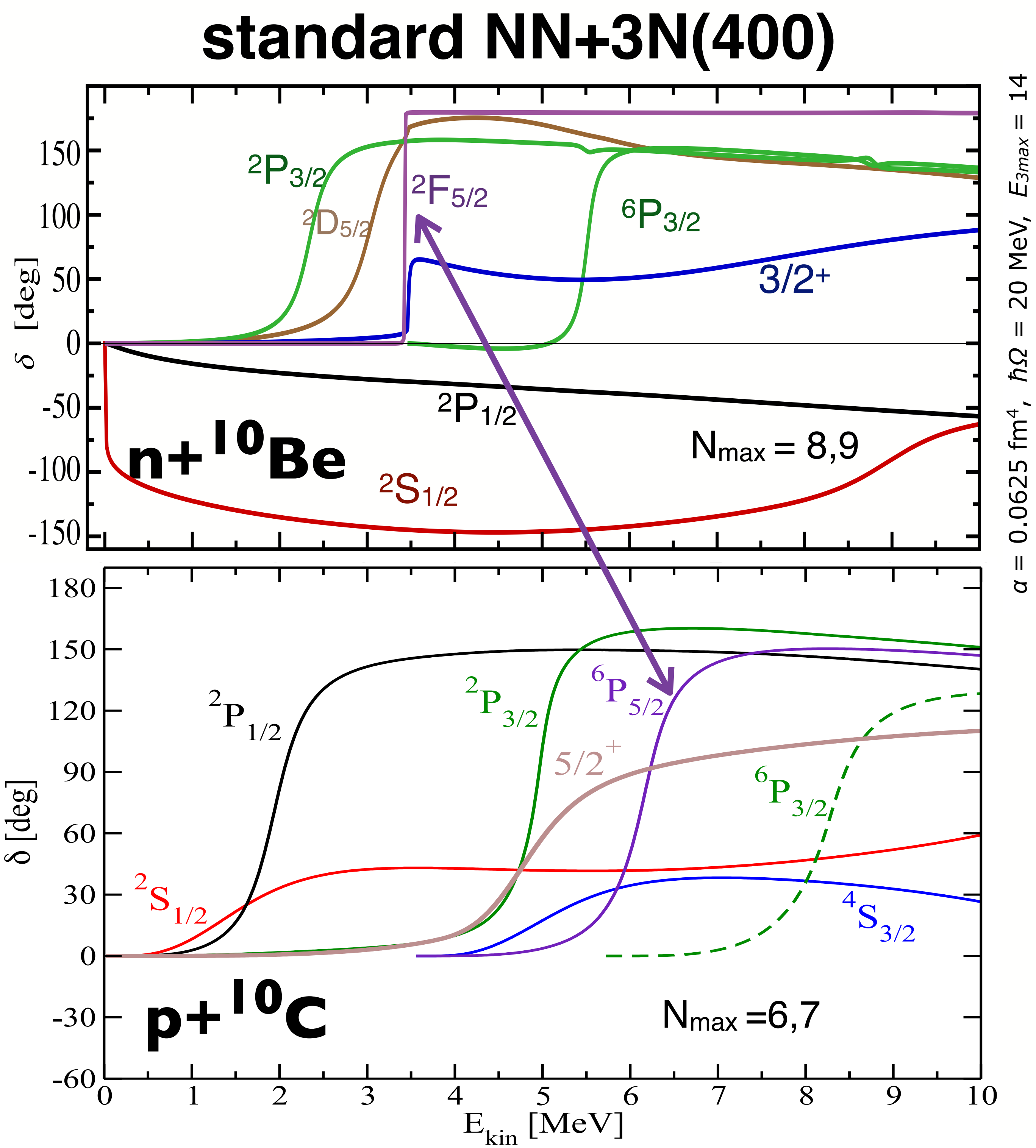
	NCSM	NCSMC	NCSMC-pheno	exp.
NN+3N(400)	0.0005	-	0.146	0.102(2)*
N^{2}LO$_{SAT}$	0.0005	0.127	0.117	

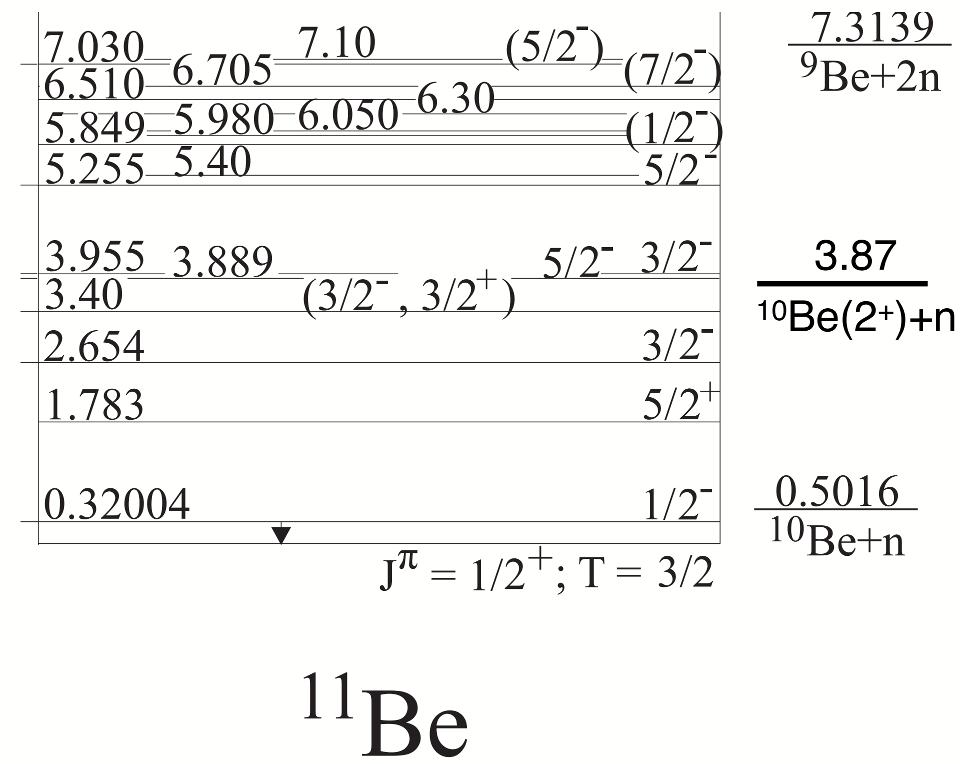
*Kwan et al. Phys. Lett. B 732, 210 (2014)

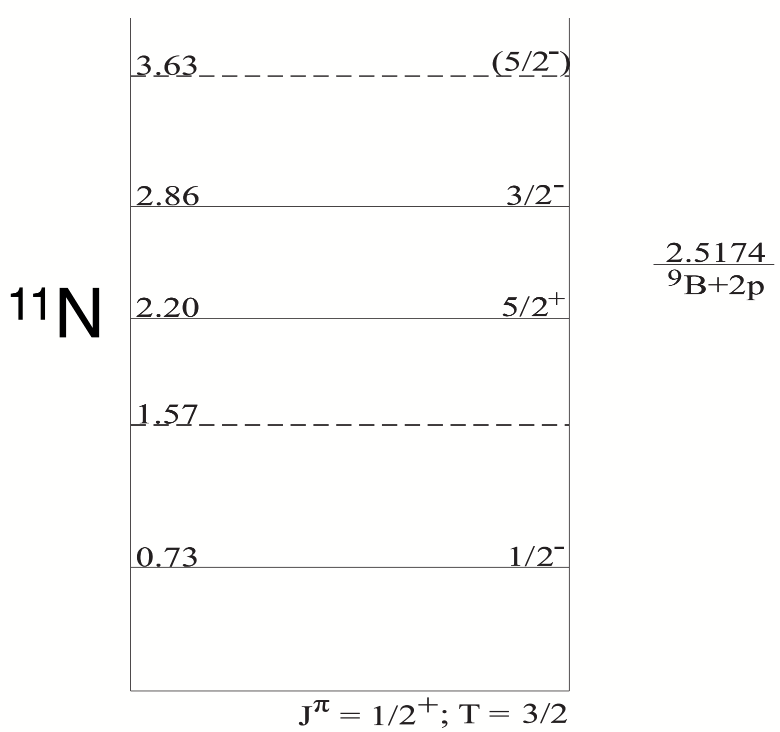


- **strongest known E1** transition between low-lying states (attributed to halo structure)
- reproduced **only** with **continuum effects**
- **conflicting** experimental **measurements**
- ab initio results:
  - **discriminate** between measurements
  - **predict dip** at 3/2$^-$ resonance energy

Mirror nuclei: ^{11}Be and ^{11}N



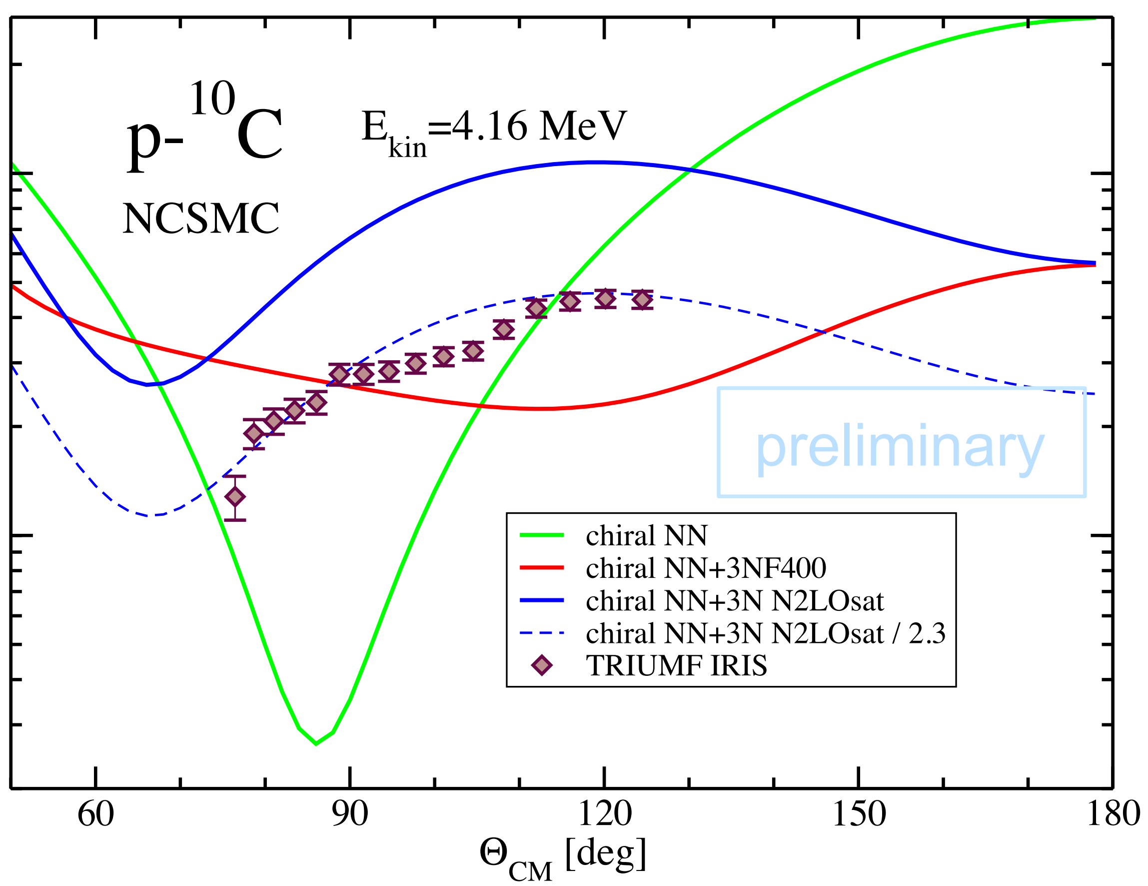


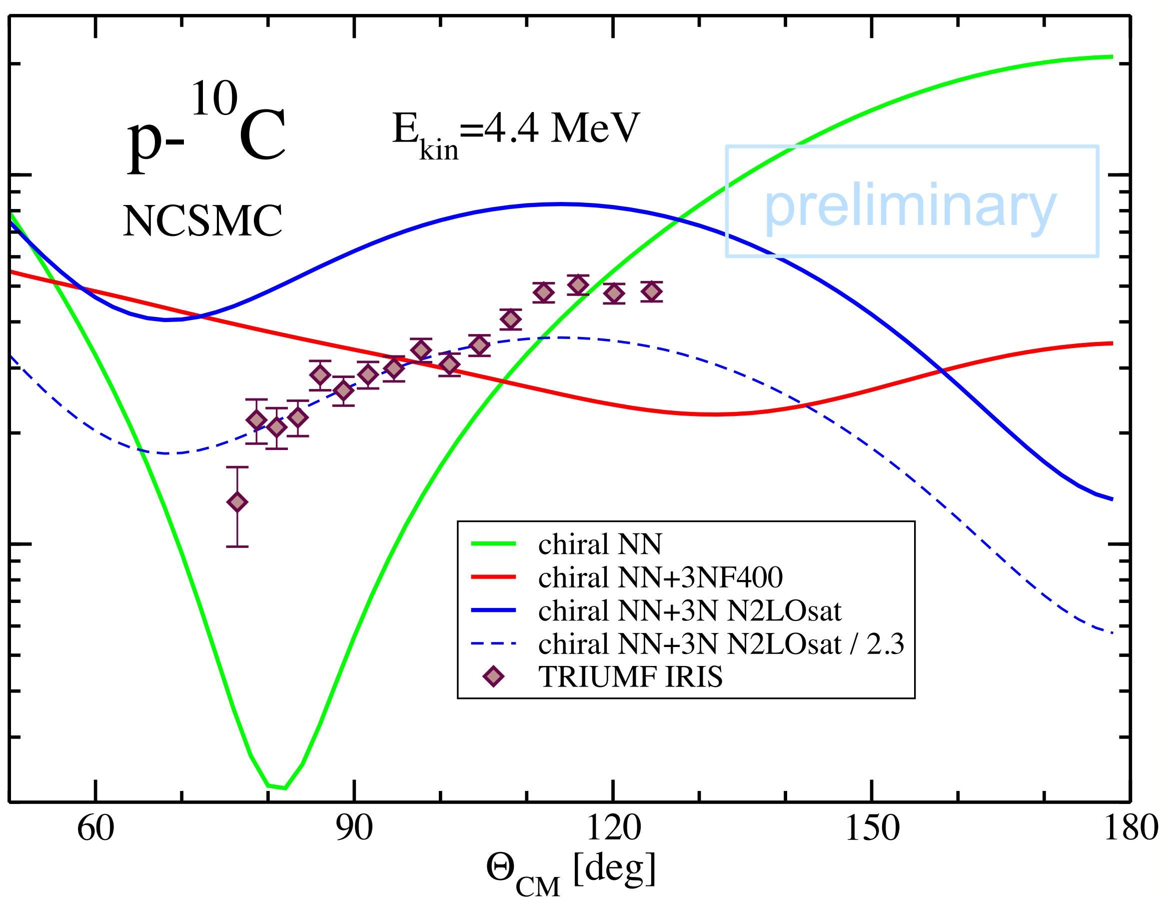


p+^{10}C Scattering: Structure of ^{11}N resonances

Mirror System

elastic scattering allows discrimination among chiral nuclear forces





IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al.* with IRIS collaboration, in preparation

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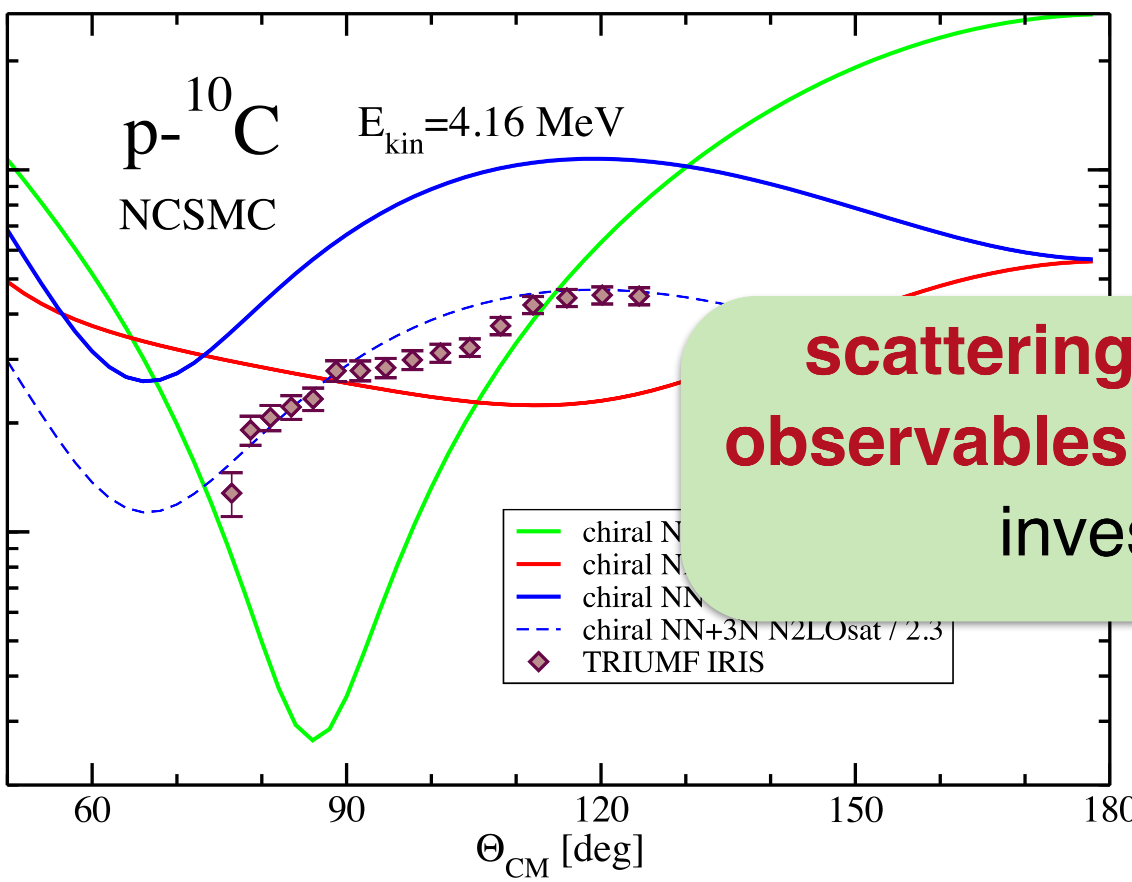

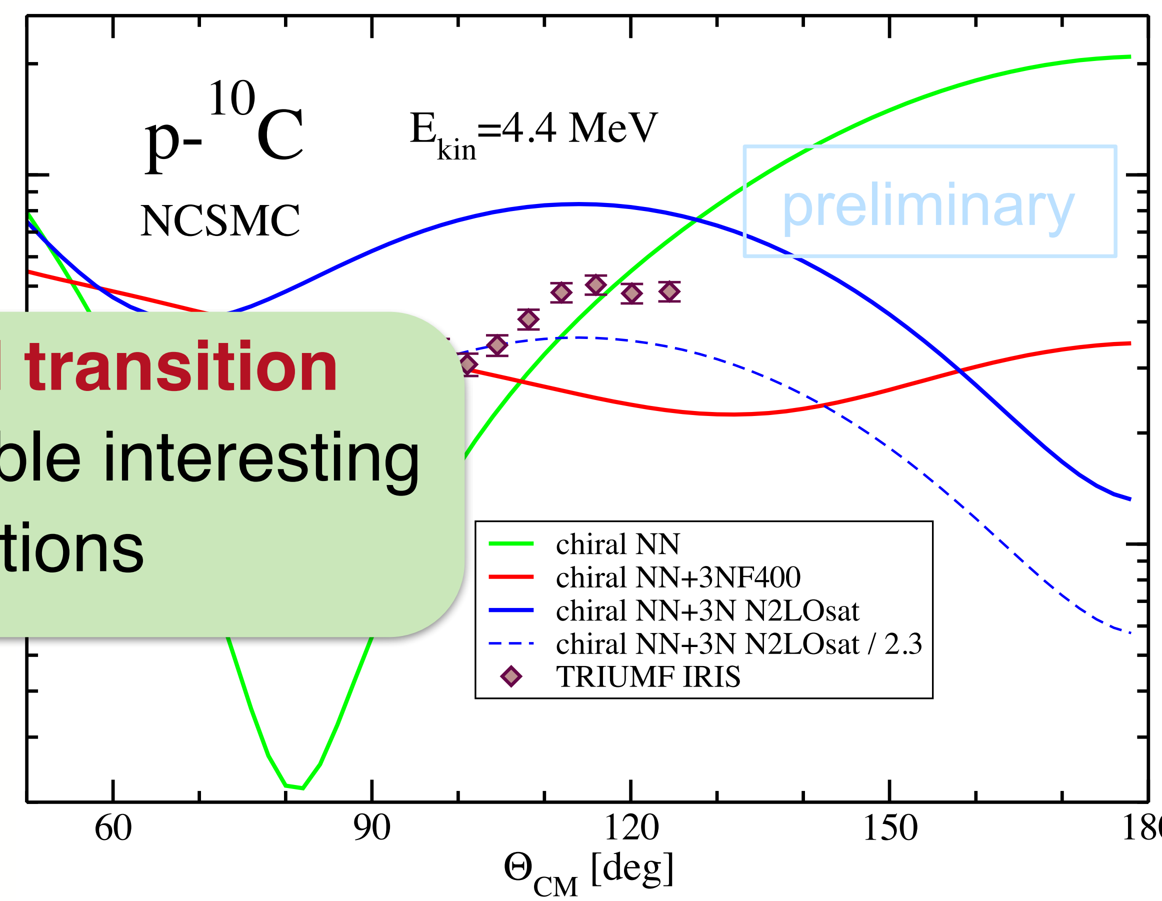

scattering and transition observables enable interesting investigations

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p+^{10}C Scattering: Structure of ^{11}N resonances

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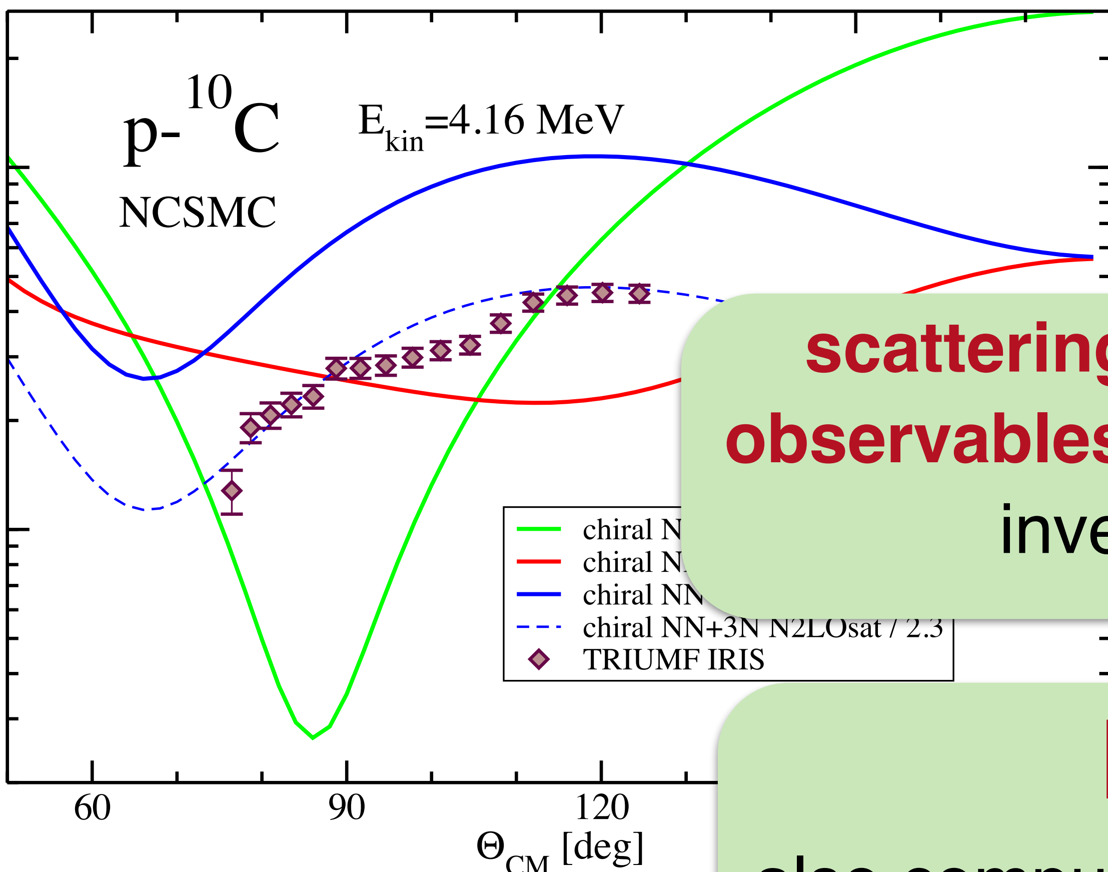

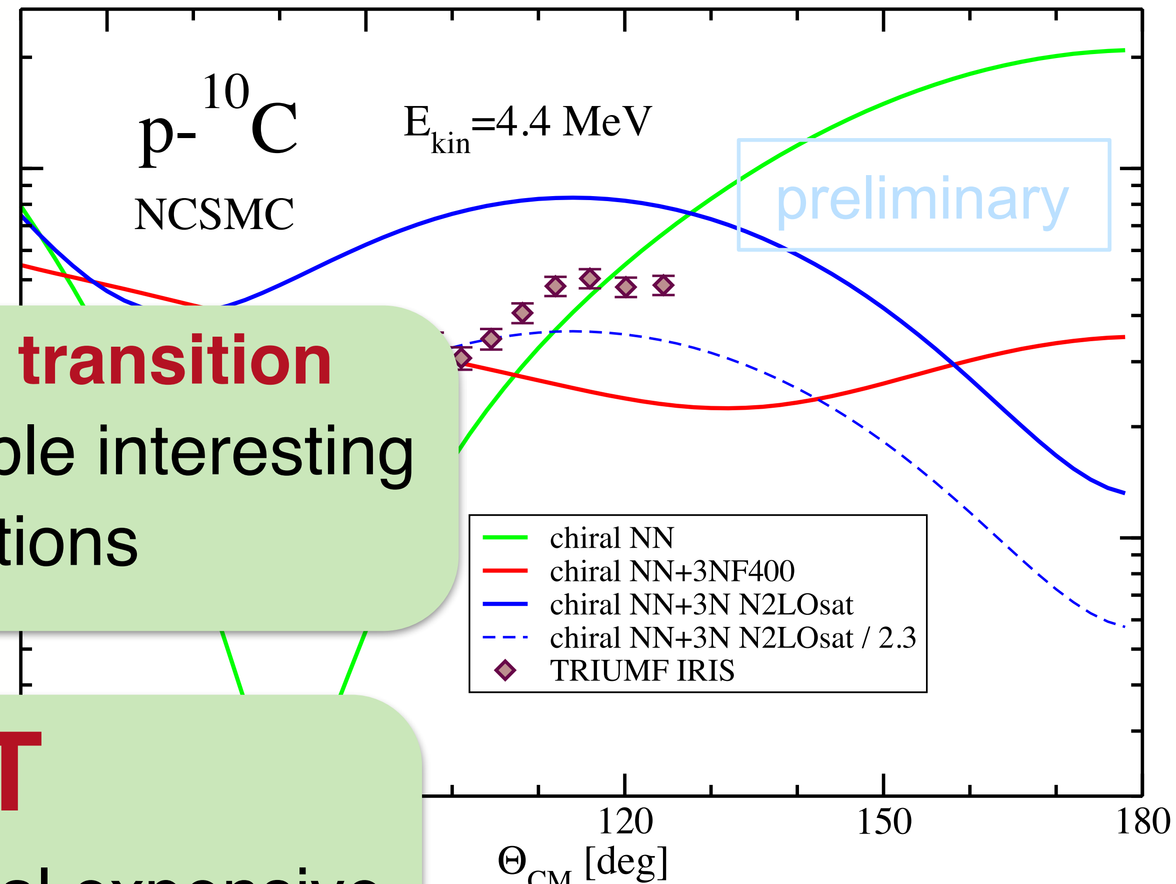

scattering and transition observables enable interesting investigations

BUT
also computational expensive

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A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

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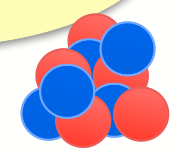
NCSMC with approximated 3N forces

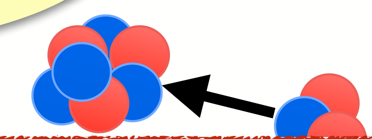
with
P. Navrátil, R. Roth, E. Gebrerufael

NCSM with Continuum (NCSMC)

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

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





expansion in A-body NCSM eigenstates

relative
NCSM

- leads to NCSMC equation

$$\begin{pmatrix} H_{NCSM} & h \\ h & \boxed{\mathcal{H}} \end{pmatrix}\begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = E\begin{pmatrix} \mathbb{1} \\ g \end{pmatrix}$$

bottleneck : inclusion of 3N force

- with 3N contributions in

H_{NCSM}: covered by NCSM

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

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

Normal-ordering (NO) approximation

- standard tool to **reduce particle rank**
- generally NO can be considered as basis transformation

$$V_{3N} \approx \underbrace{\tilde{V}_{0N} + \tilde{V}_{1N} + \tilde{V}_{2N}}_{\text{contain information of reference state and initial 3N force}} + \cancel{\tilde{V}_{3N}}$$

- interested in direct description of **open-shell systems**
  - multi-reference normal ordering (MR-NO)
  - generalization of wicks theorem [Kutzelnigg, Mukherjee]

NCSM/RGM kernels with MR-NO contributions

- reduces computational costs tremendously
- impressively accurate approximation

Derive NCSM/RGM Kernels

0B kernel

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

1B kernel

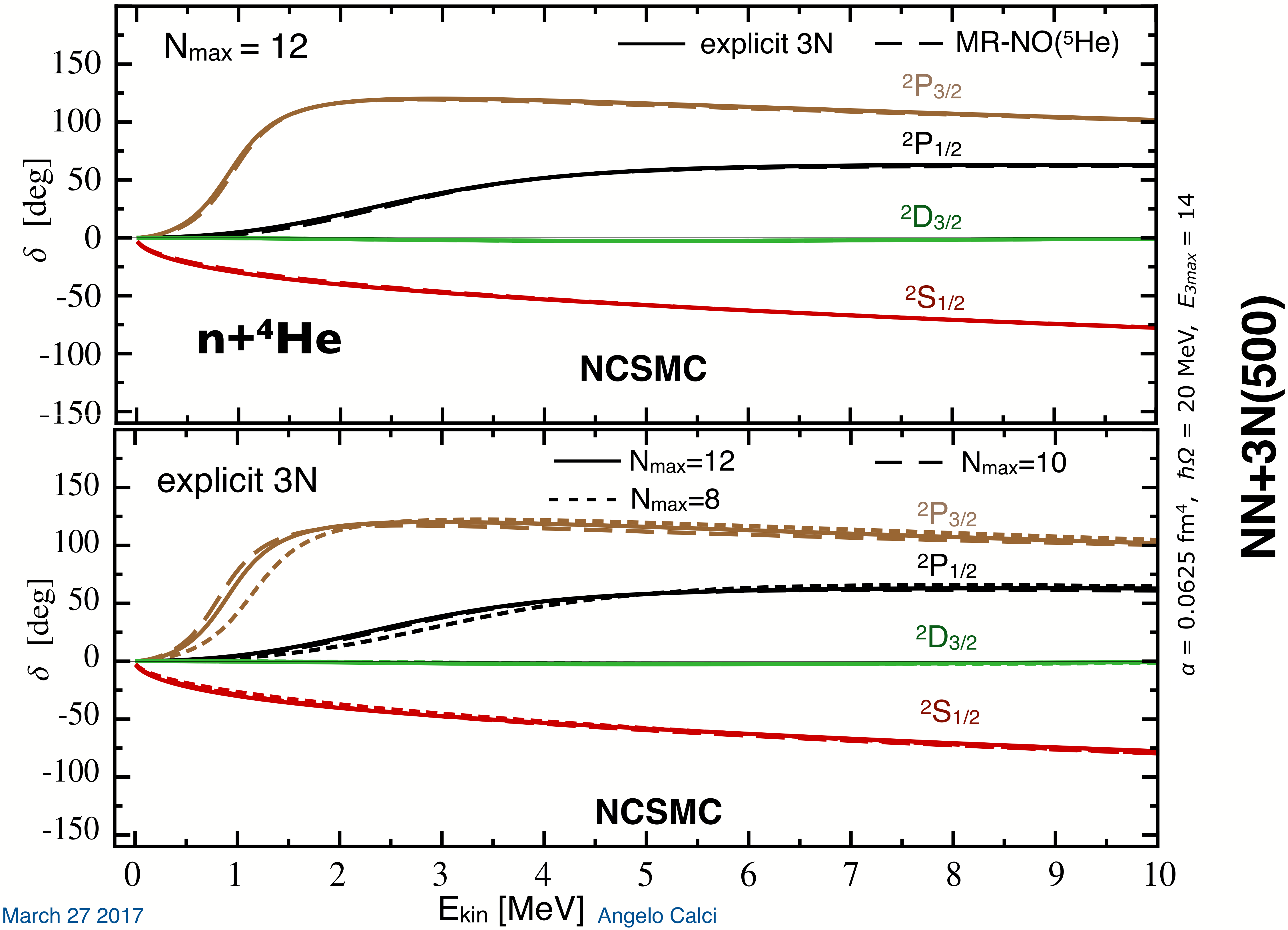
$$
\begin{aligned}
&{}_{SD}< \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_A | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD} \\
&= \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M'_1 m'_j} \sum_{M'_{T_1} m'_t} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I'_1 & j' & \mathcal{J} \\ M'_1 & m'_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T'_1 & \frac{1}{2} & T \\ M'_{T_1} & m'_t & M_T \end{array} \right) \\
&\times \; {}_{SD}< \psi'_{A-1} E'_1 I'^{\pi'_1}_1 M'_1 T'_1 M'_{T_1} | \psi_{A-1} E_1 I_1{}^{\pi_1} M_1 T_1 M_{T_1} >_{SD} \\
&\times \; < n' l' j' m'_j \frac{1}{2} m'_t | V_A | n l j m_j \frac{1}{2} m_t >
\end{aligned}
$$

$$
\begin{aligned}
&-{}_{SD}< \epsilon^{\mathcal{J}\pi T}_{\nu' n'} | \boldsymbol{V}_A \boldsymbol{T}_{A-1,A} | \epsilon^{\mathcal{J}\pi T}_{\nu n} >_{SD} \\
&= -\frac{1}{A-1} \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M'_1 m'_j} \sum_{M'_{T_1} m'_t} \left(\begin{array}{cc|c} I_1 & j & \mathcal{J} \\ M_1 & m_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \left(\begin{array}{cc|c} I'_1 & j' & \mathcal{J} \\ M'_1 & m'_j & \mathcal{M} \end{array} \right) \left(\begin{array}{cc|c} T'_1 & \frac{1}{2} & T \\ M'_{T_1} & m'_t & M_T \end{array} \right) \\
&\times \sum_{\alpha_{A-1}} {}_{SD}< \psi'_{A-1} E'_1 I'^{\pi'_1}_1 M'_1 T'_1 M'_{T_1} | \boldsymbol{a}^\dagger_{nljm_jm_t} \boldsymbol{a}_{\alpha_{A-1}} | \psi_{A-1} E_1 I_1{}^{\pi_1} M_1 T_1 M_{T_1} >_{SD} \\
&\times \; < n' l' j' m'_j \frac{1}{2} m'_t | \boldsymbol{V}_A | \alpha_{A-1} >
\end{aligned}
$$

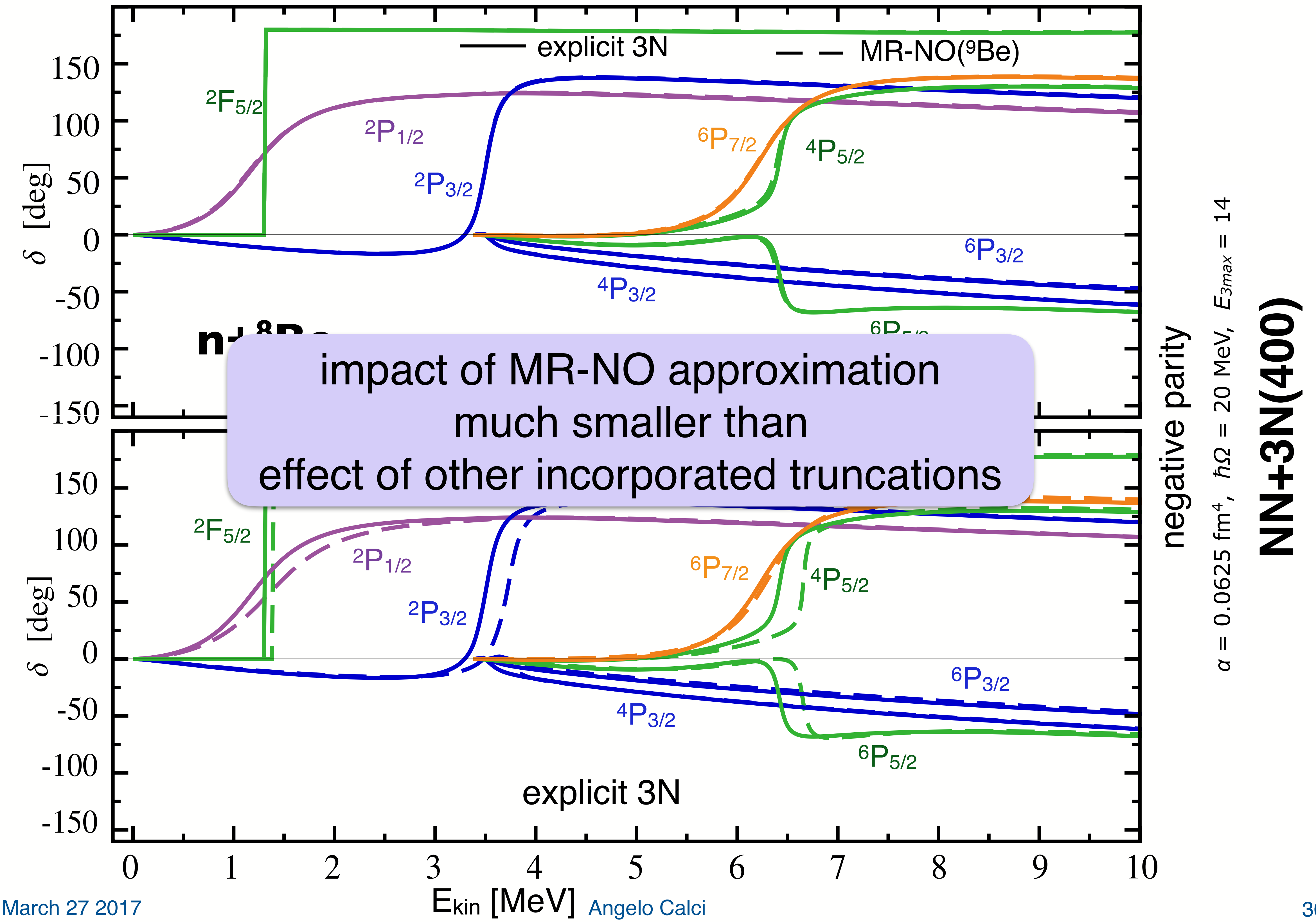
2B kernel

…

NCSMC: Impact of 3N in Kernels



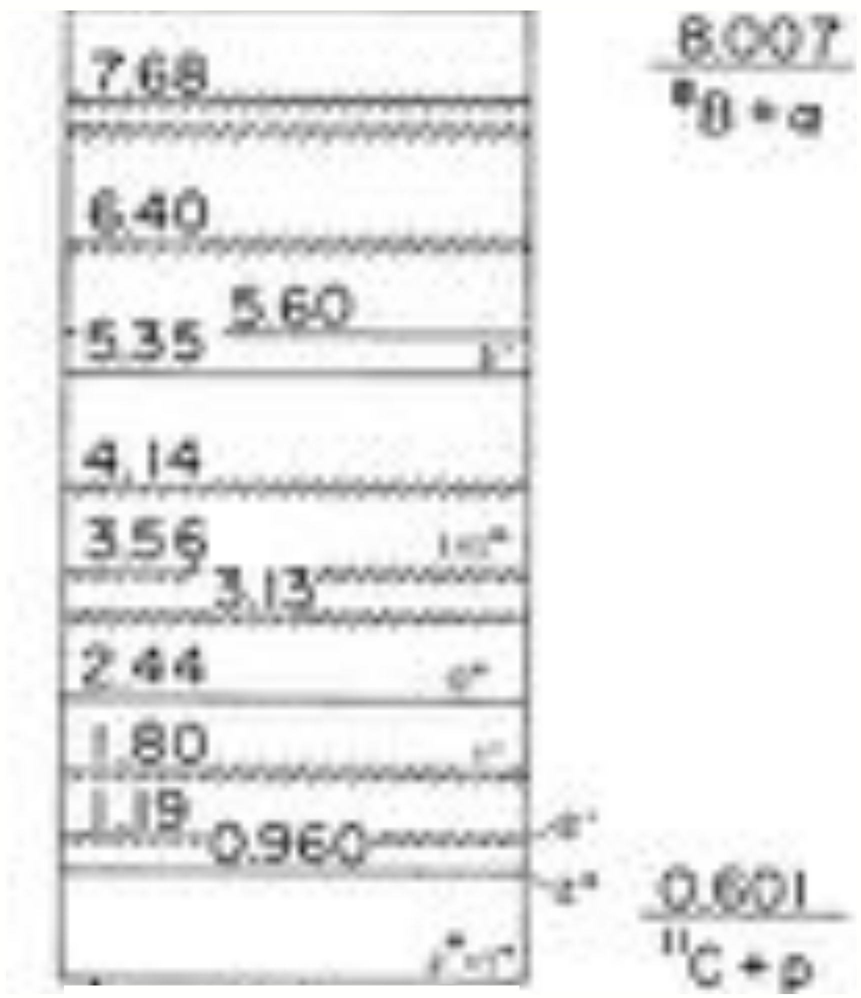
NCSMC: Impact of 3N in Kernels



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



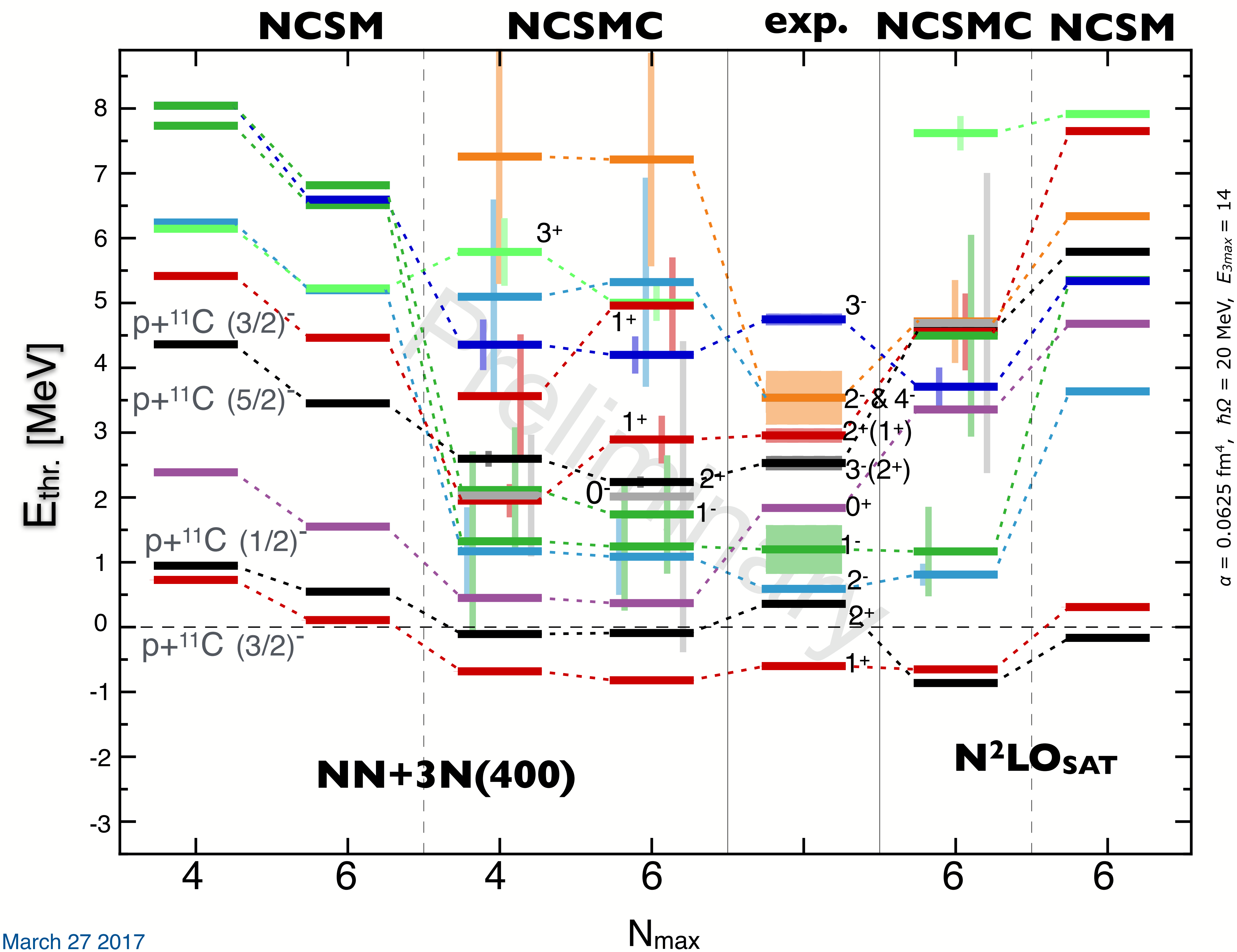
^{12}N

- 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

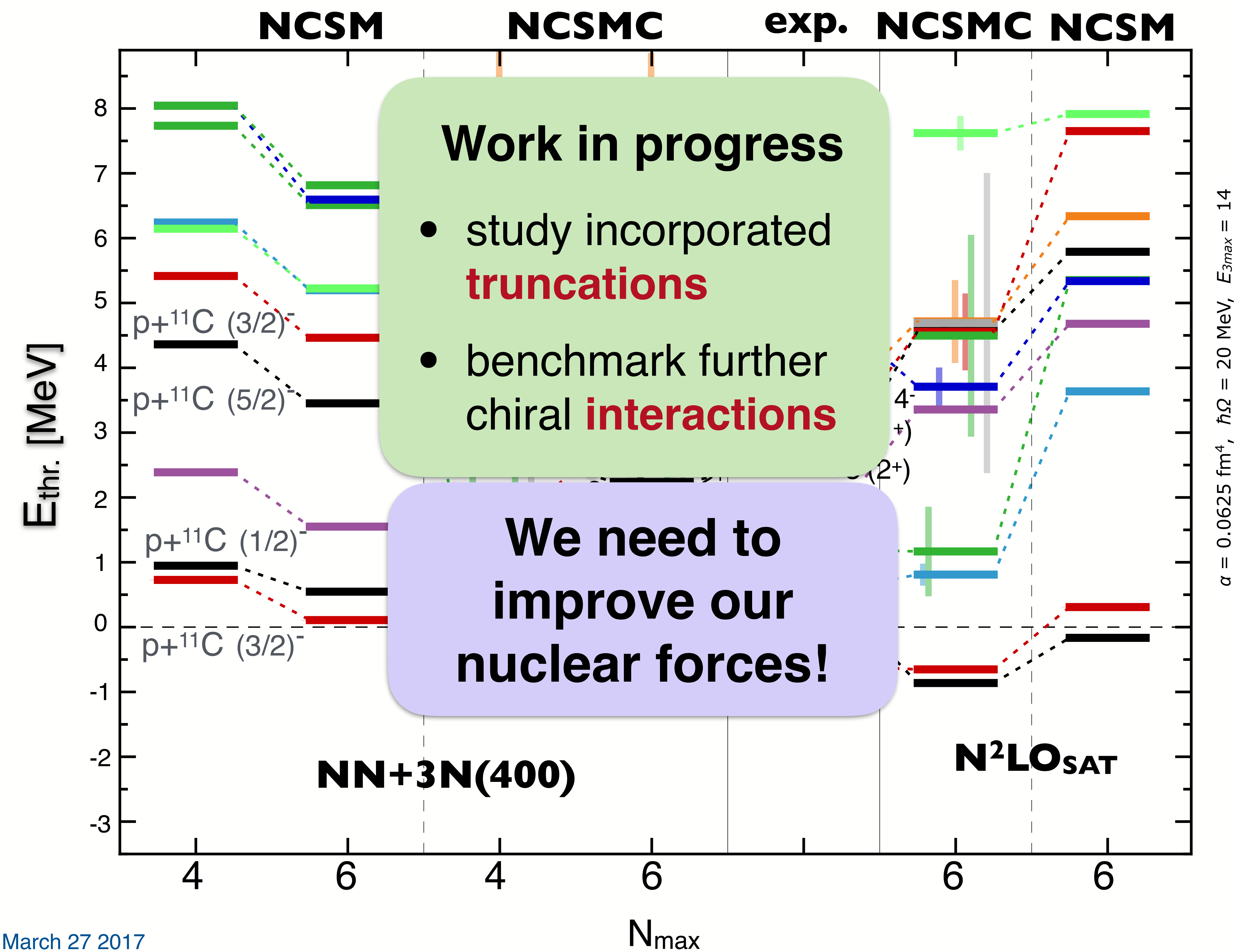
ab initio NCSMC

- 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



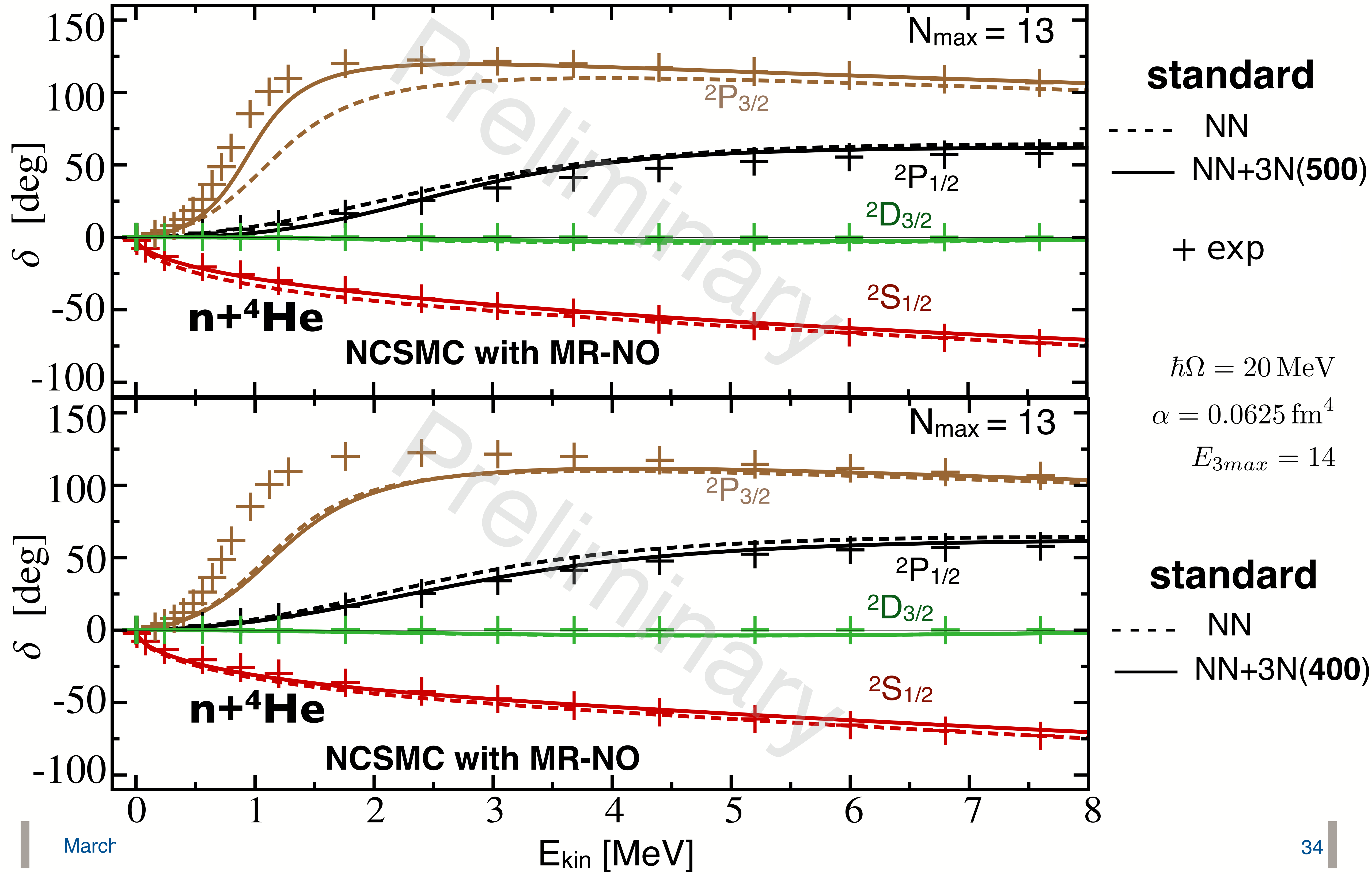
Work in progress

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

We need to improve our nuclear forces!

Probe chiral interaction in light nuclear scattering

n-^{4}He: Standard interaction

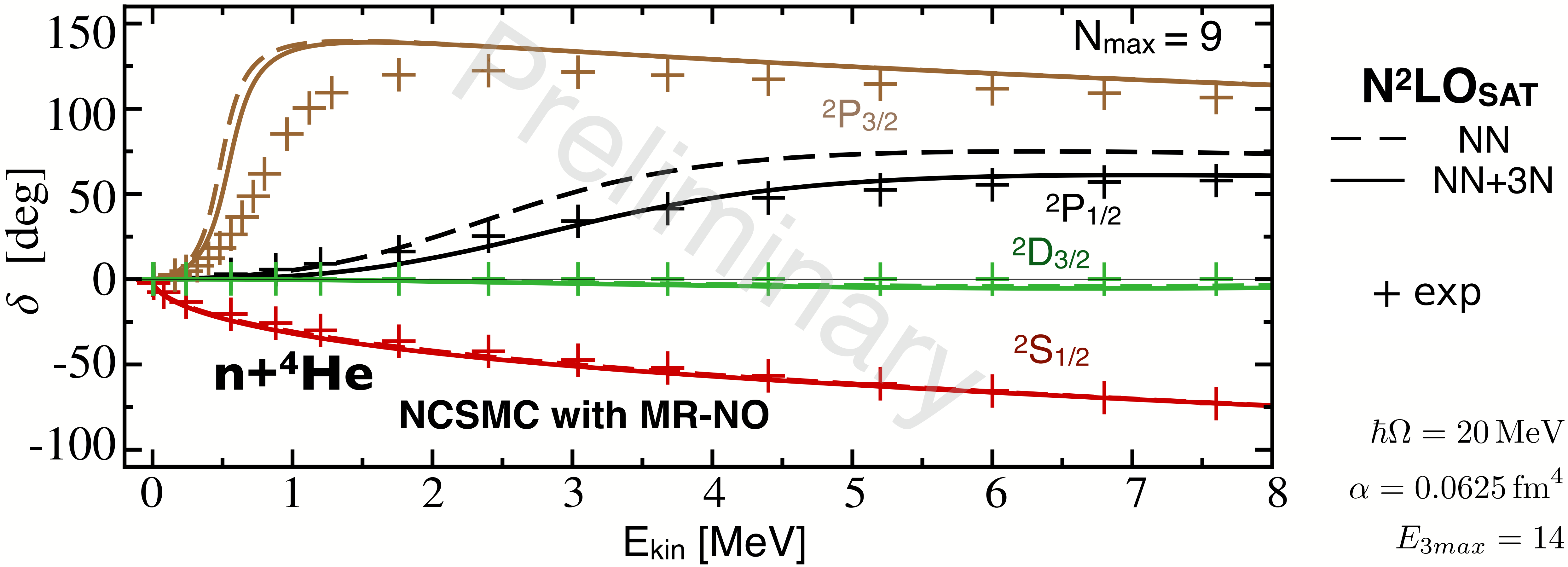


$\hbar\Omega = 20\,\mathrm{MeV}$

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

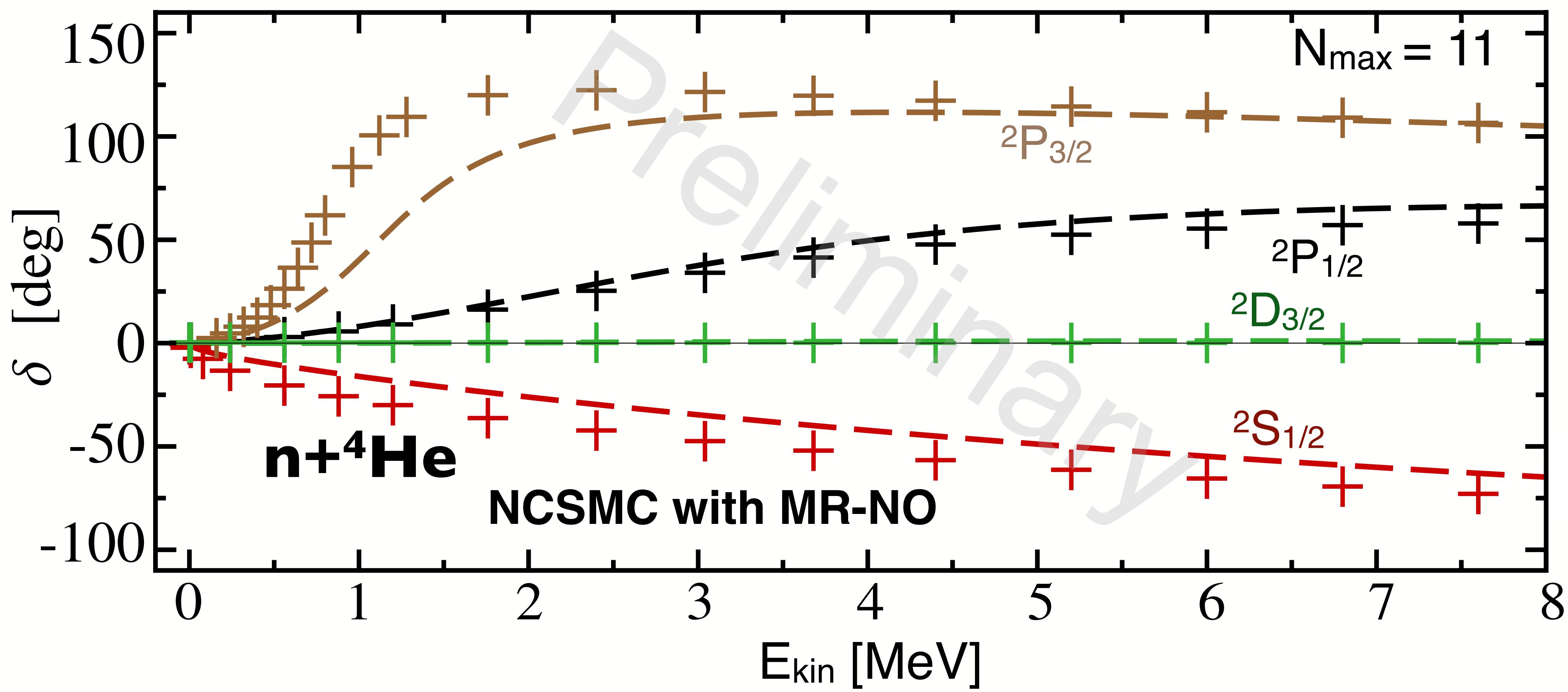
$E_{3max} = 14$

n-^{4}He 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

n-^{4}He with LENPIC interaction



LENPIC interaction

N^{2}LO

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

– – NN

+ exp

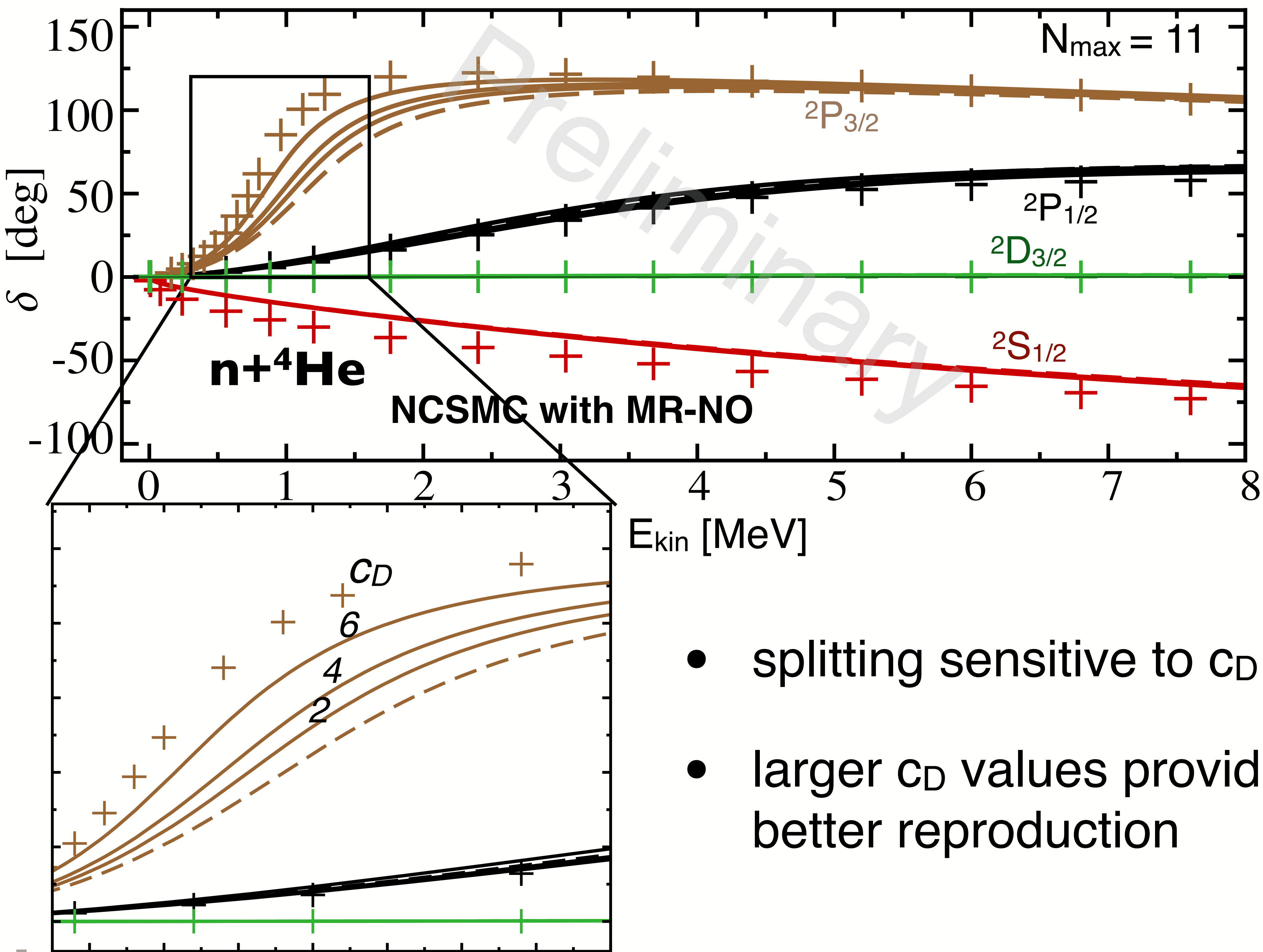
- splitting underestimated without 3N interaction

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

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

$E_{3max} = 14$

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.

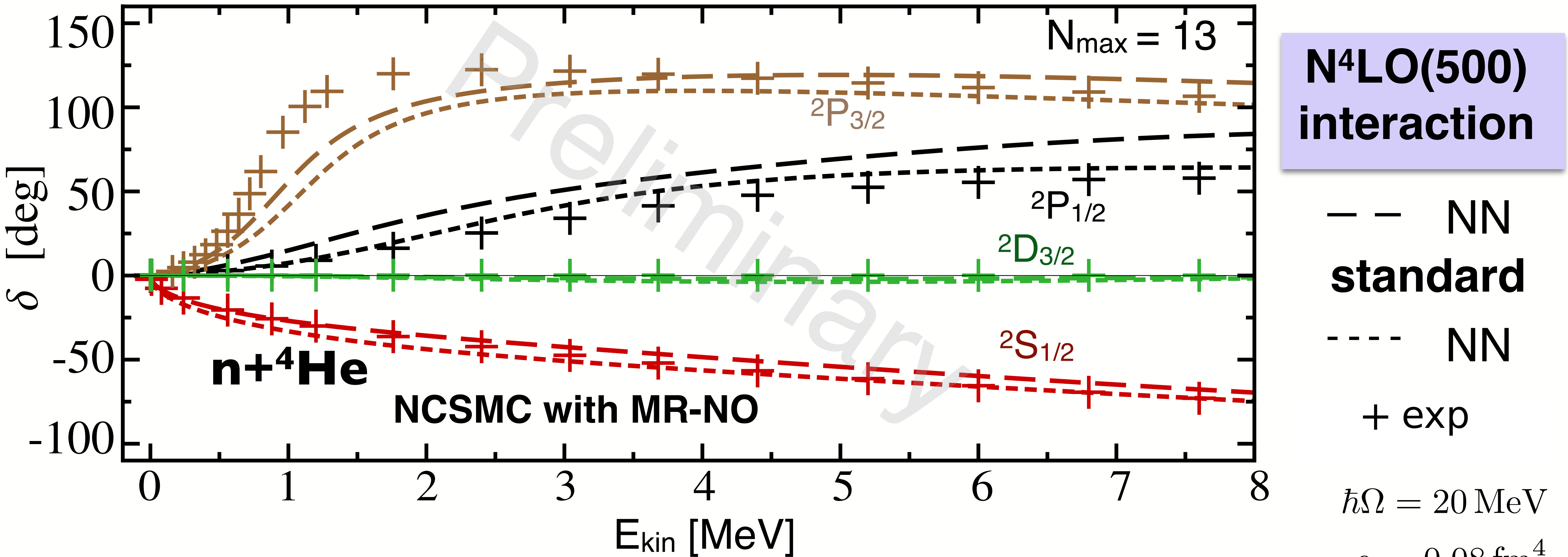
$\hbar\Omega = 24\,\mathrm{MeV}$

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

$E_{3max} = 14$

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

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

Outlook

- **insufficient knowledge of nuclear force** provides largest uncertainties in ab initio calculations
- **p-shell spectra** provide powerful testbed for chiral potential
- **combination of NCSMC with MR-NO** allows to include continuum effects at strongly reduced cost
  - enables heavier targets and **complex projectiles**
  - **probe future interactions** in weakly-bound system
  - splitting of $P_{3/2}$ - $P_{1/2}$ phase shifts in n-^{4}He can be used to **constrain 3N** interaction

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Thank you! Merci!

- **thanks to my collaborators**

LENPIC

- P. Navrátil, R. Stroberg, J. Holt, R. Kanungo, G. Hackman, A. Kumar, A. Lennarz
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