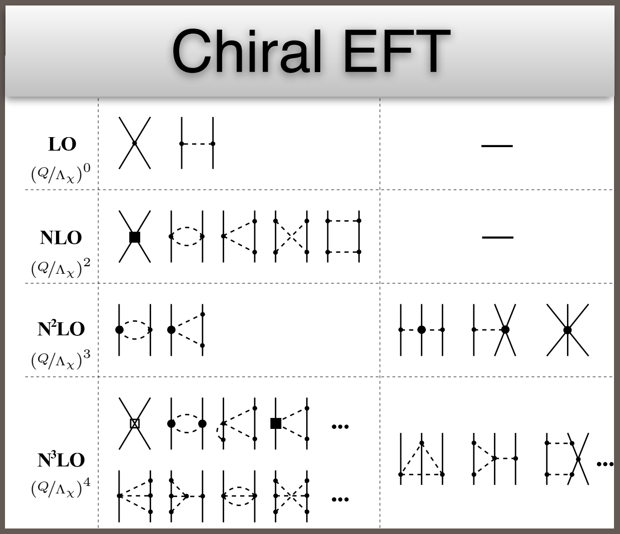
TRIUMF

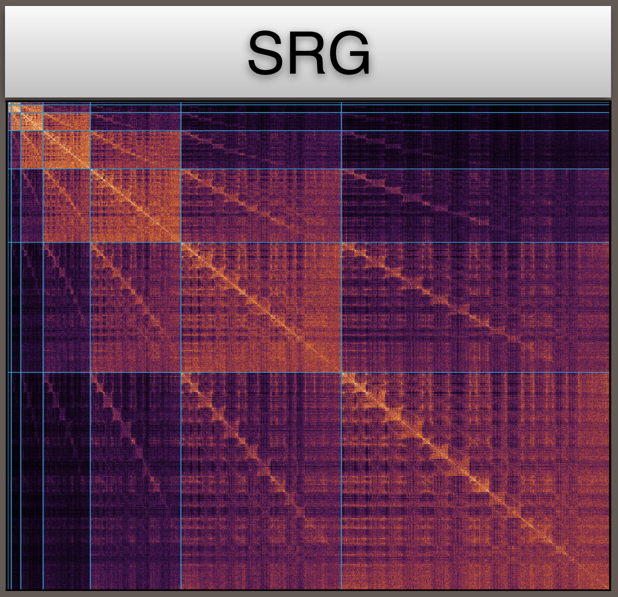
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire
et en physique des particules

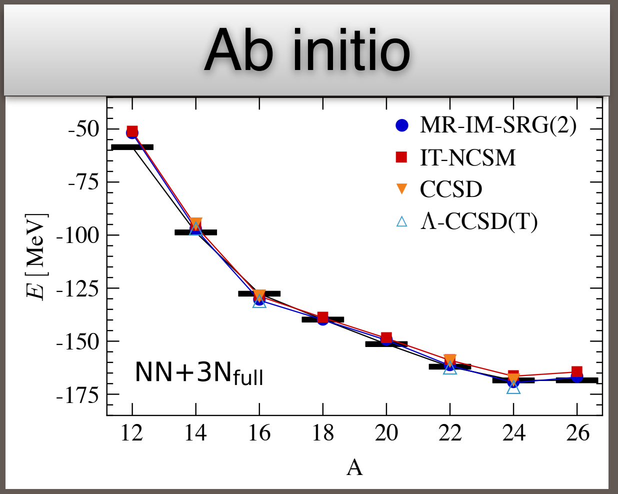
Sensitivities and Correlations from chiral NN+3N Interactions in ab initio Nuclear Structure and Reaction Calculations

INT Program INT-16-1
May 23 2016, Seattle

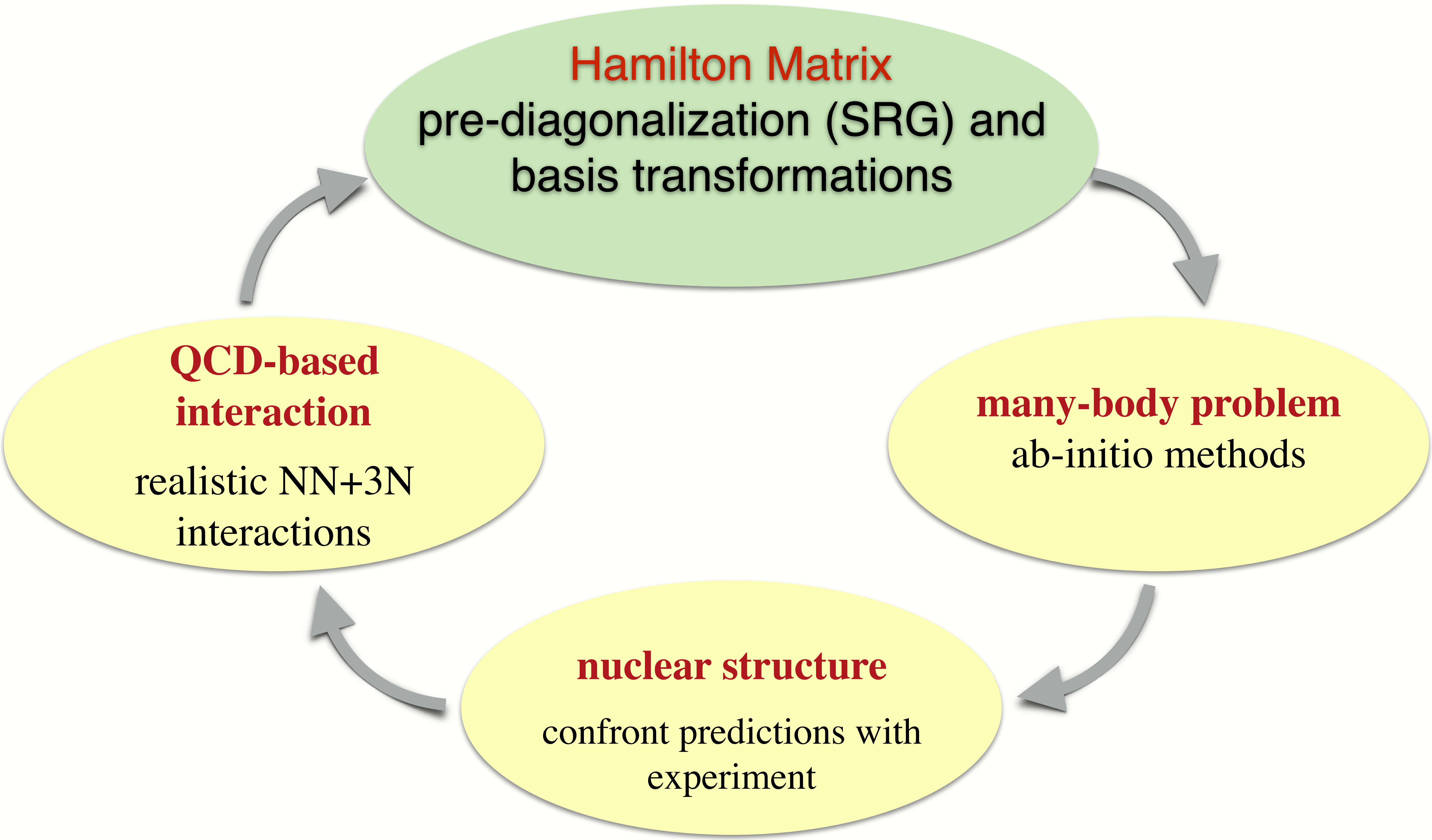
Angelo Calci | TRIUMF







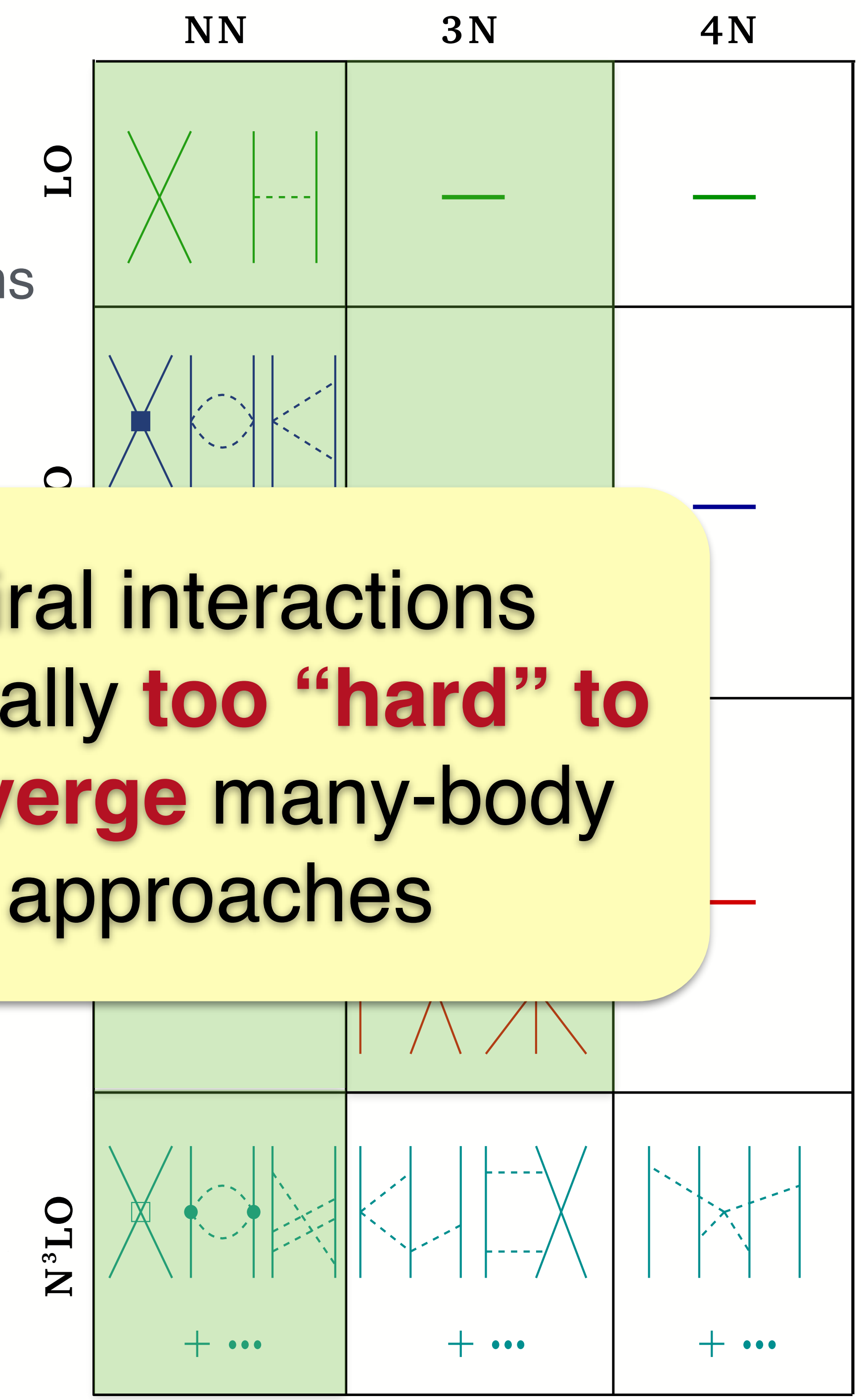
Introduction



Chiral NN+3N Interactions

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

- **standard interaction:**
  - NN @ N^3LO: Entem & Machleidt, 500MeV cutoff
  - 3N @ N^2LO: Navrátil, local, 500MeV cutoffs & modifications
- **optimized N^2LO interaction:**
  - NN: Ekström et al., 500MeV cutoff, LECs fitted v POUNDerS
  - 3N: Navrátil, local, 500MeV cutoff, fit to ^4He & T
- **Epelbaum N^2LO interaction:**
  - NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal
- **N^2LO_{SAT} interaction:**
  - NN+3N: Ekström et al., nonlocal, 450MeV cutoff, simultaneous fit to NN data and many-body observables



chiral interactions generally **too "hard" to converge** many-body approaches

Similarity Renormalization Group

Roth, Langhammer, AC et al.	— Phys. Rev. Lett. 107, 072501 (2011)
Roth, Neff, Feldmeier	— Prog. Part. Nucl. Phys. 65, 50 (2010)
Jurgenson, Navrátil, Furnstahl	— Phys. Rev. Lett. 103, 082501 (2009)
Bogner, Furnstahl, Perry	— Phys. Rev. C 75 061001(R) (2007)

Similarity Renormalization Group (SRG)

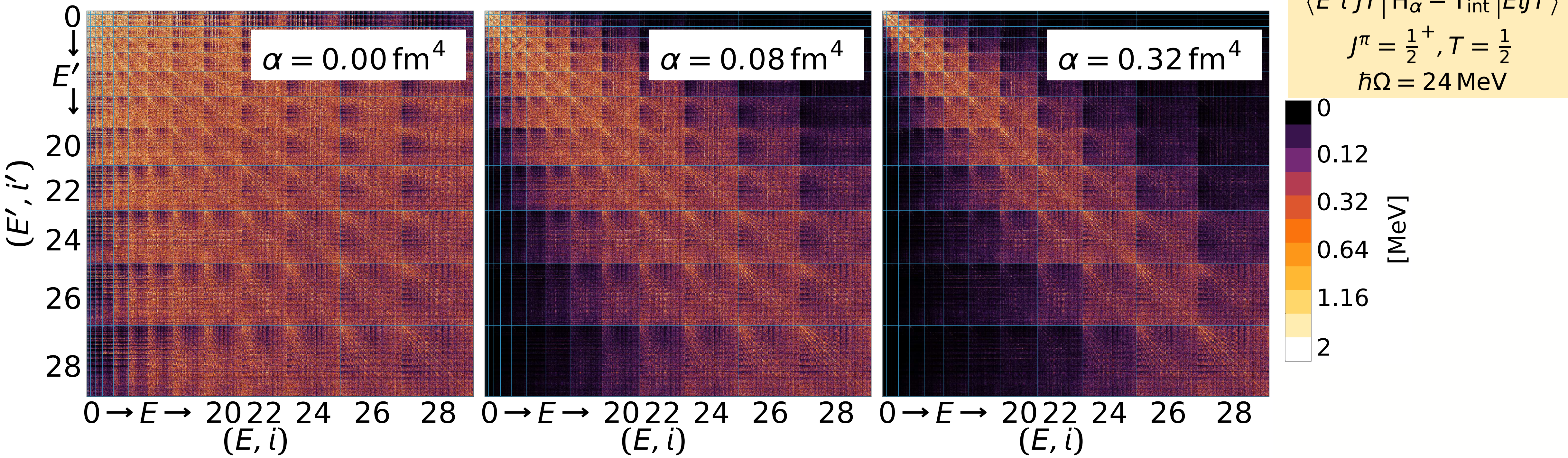
accelerate convergence by **pre-diagonalizing** the Hamiltonian with respect to the many-body basis

- **unitary transformation leads to evolution equation**

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

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

3B-Jacobi HO matrix elements



(Importance Truncated) NCSM

- solving the eigenvalue problem:

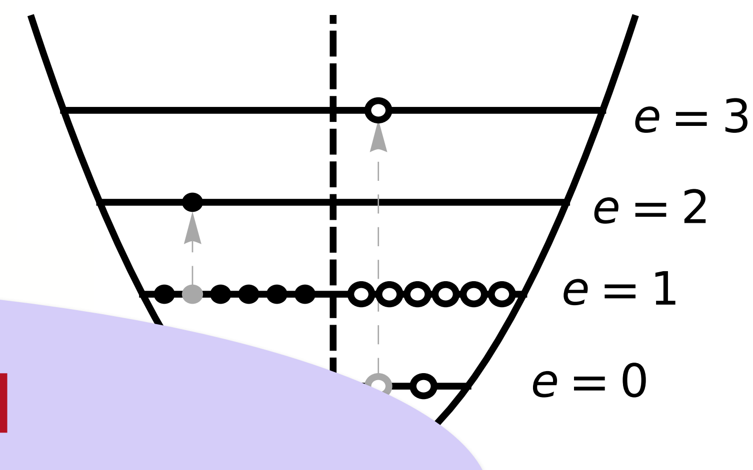
$$H\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$

- **model space:**

  spanned b

  unpertu

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



problem of NCSM

enormous increase of model space with particle number *A*

Importanc

- a

  p

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

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

Uncertainty Quantification of chiral Hamiltonians in Spectroscopy

Uncertainties of Chiral Interactions

in the past

- uncertainties **from many-body approach** included
- observables calculated for **single chiral Hamiltonian** (inconsistent chiral order)
- quality of chiral forces assessed by agreement with experiment

future

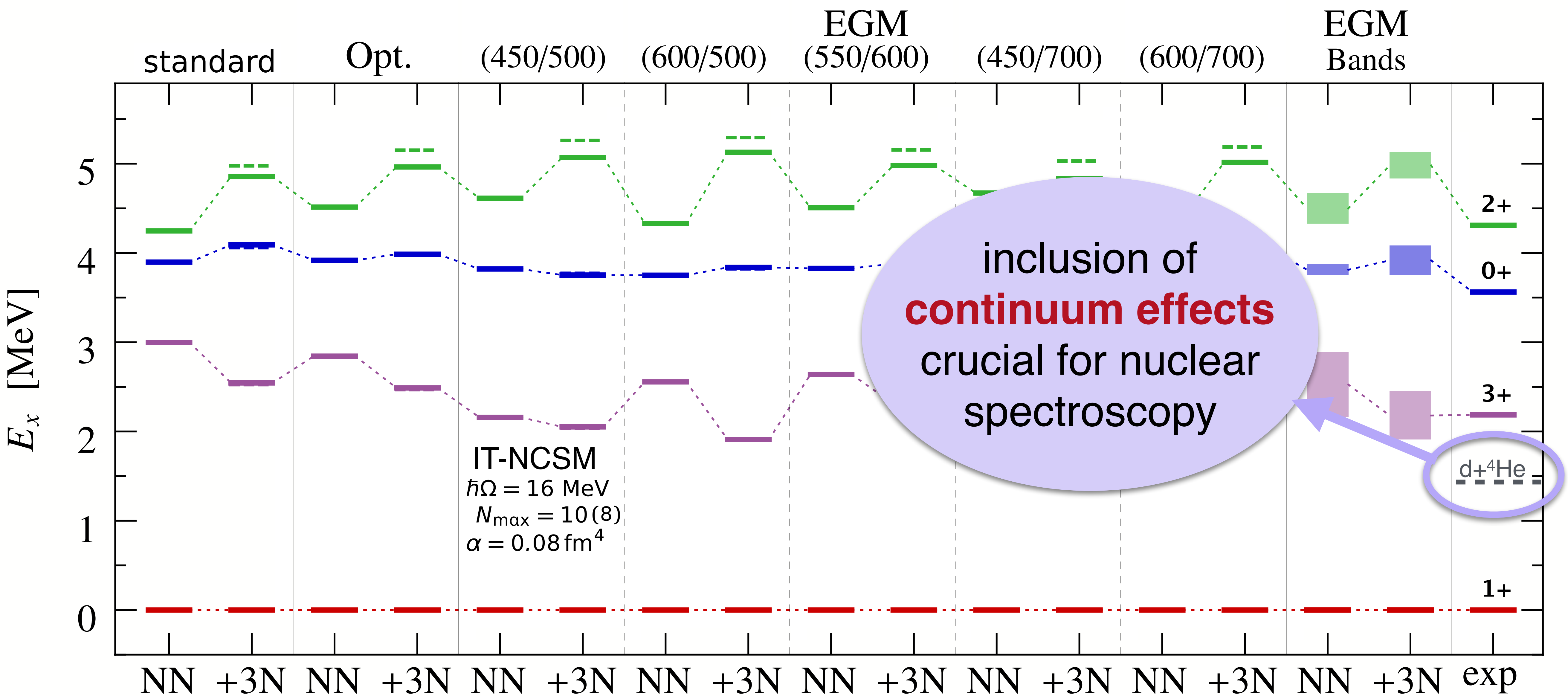
- start with NN+3N force at **consistent** chiral **order**
- use **sequence of cutoffs** and chiral **orders**

➡ estimate **uncertainties** of chiral EFT and many-body approach

nuclear structure physics approaches new era

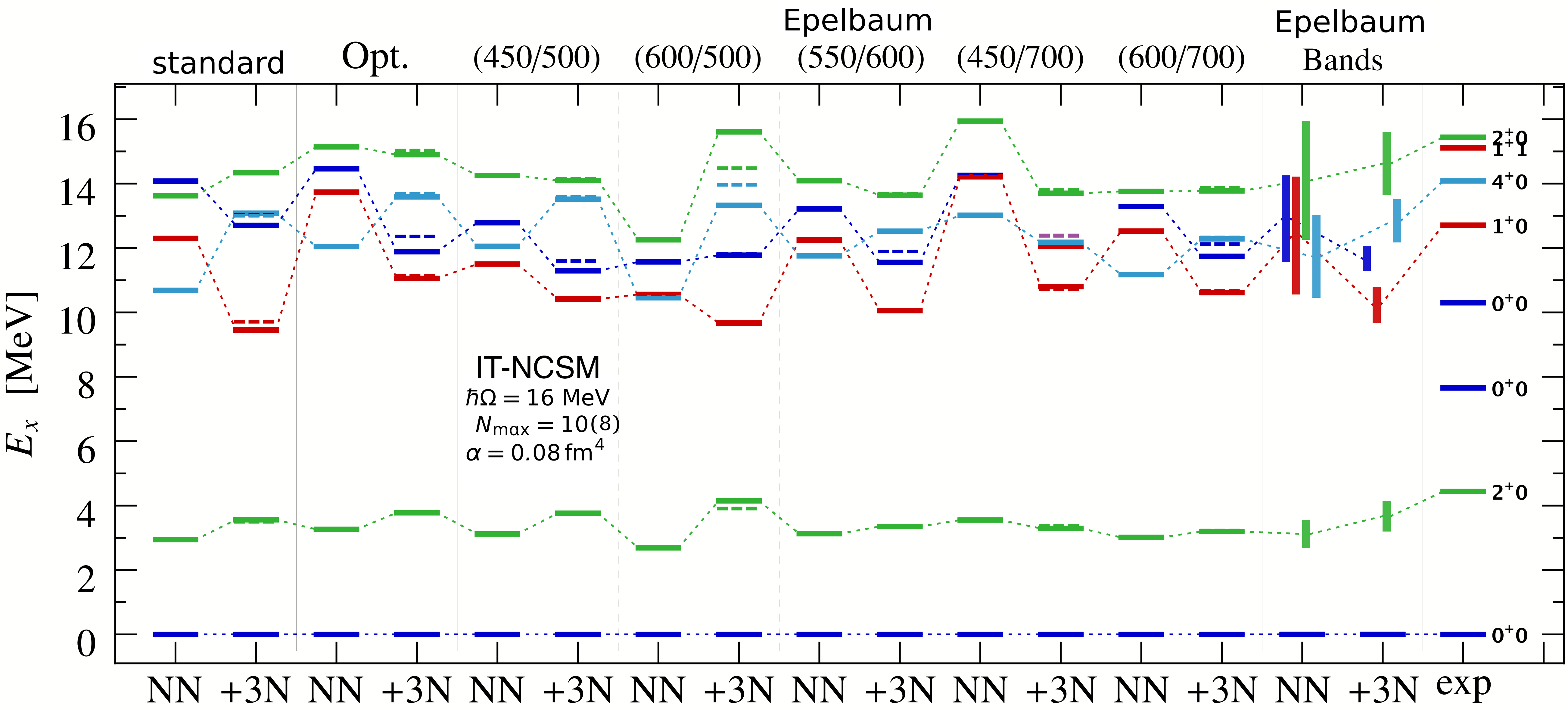
- **ongoing progress** in construction of consistent NN+3N Hamiltonians
- first step towards reliable uncertainty quantification in nuclear spectroscopy

^{6}Li: Cutoff Dependence



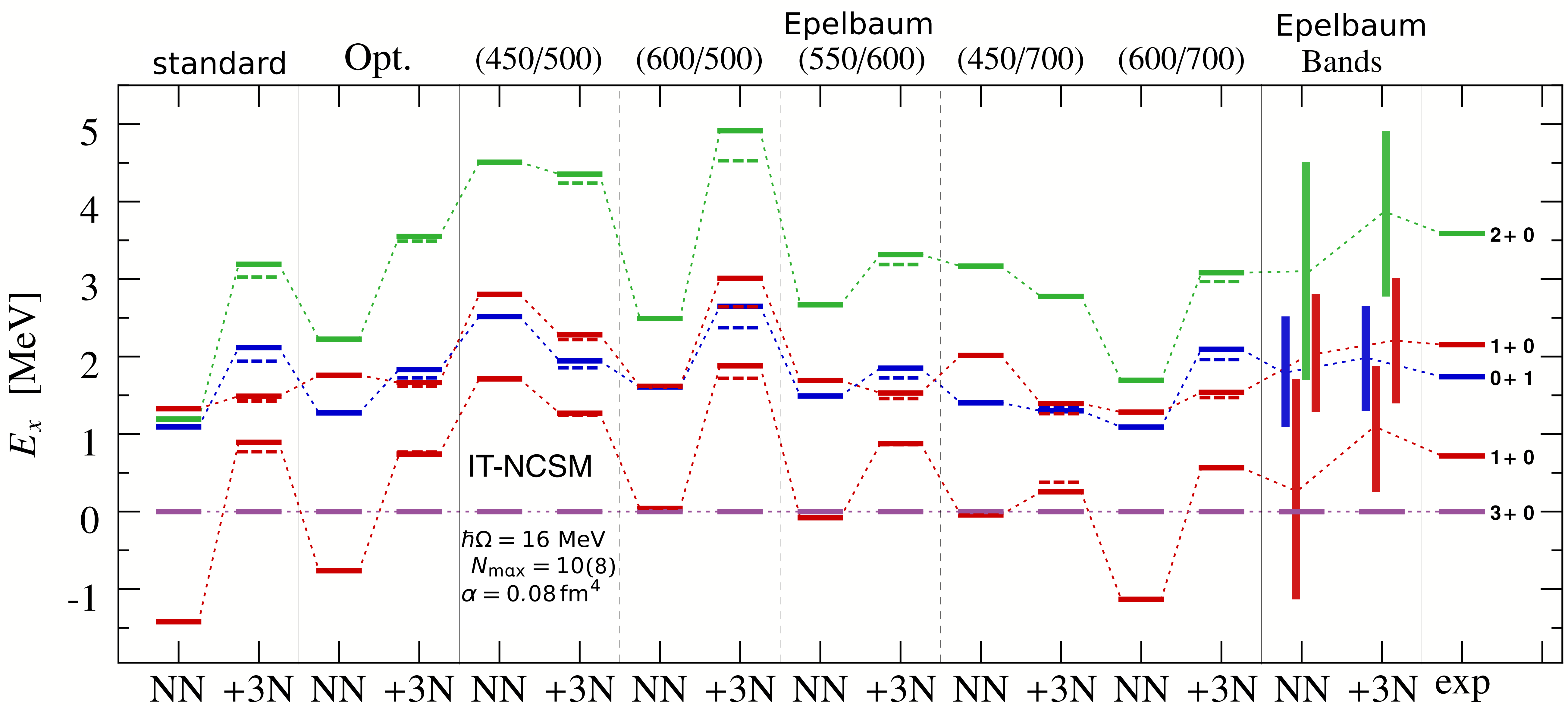
- reasonable predictions
- small cutoff dependence

^{12}C: Cutoff Dependence



- small cutoff dependence for NN+3N

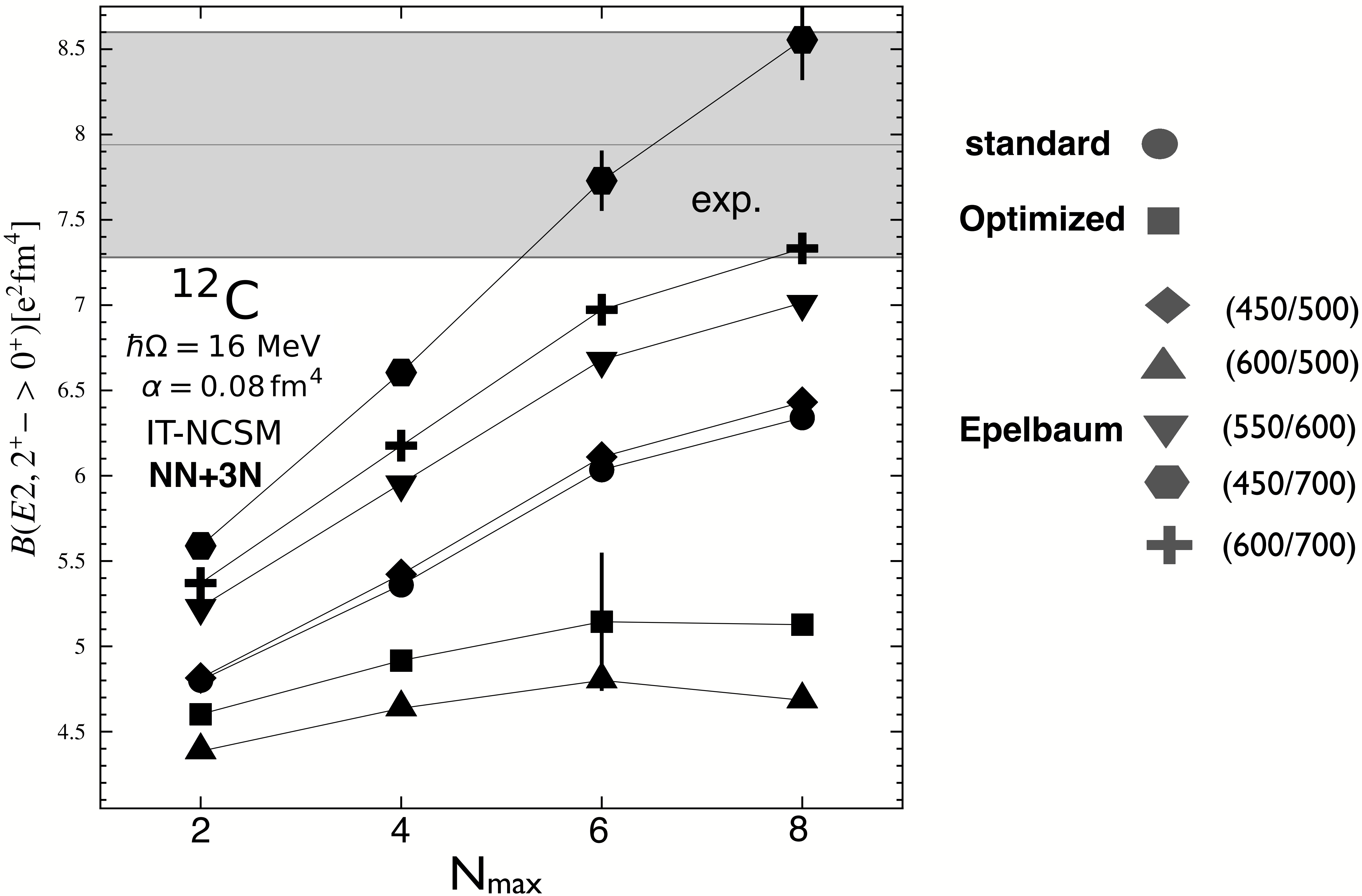
^{10}B: Cutoff Dependence



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

Quadrupole Observables

^{12}C: B(E2) Transition



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B(E2) and Quadrupole moment

challenges in calculating quadrupole observables:

- generally **slow convergence** in HO space
- **chiral uncertainties** impact observables
- **observables** need to be **SRG evolved**

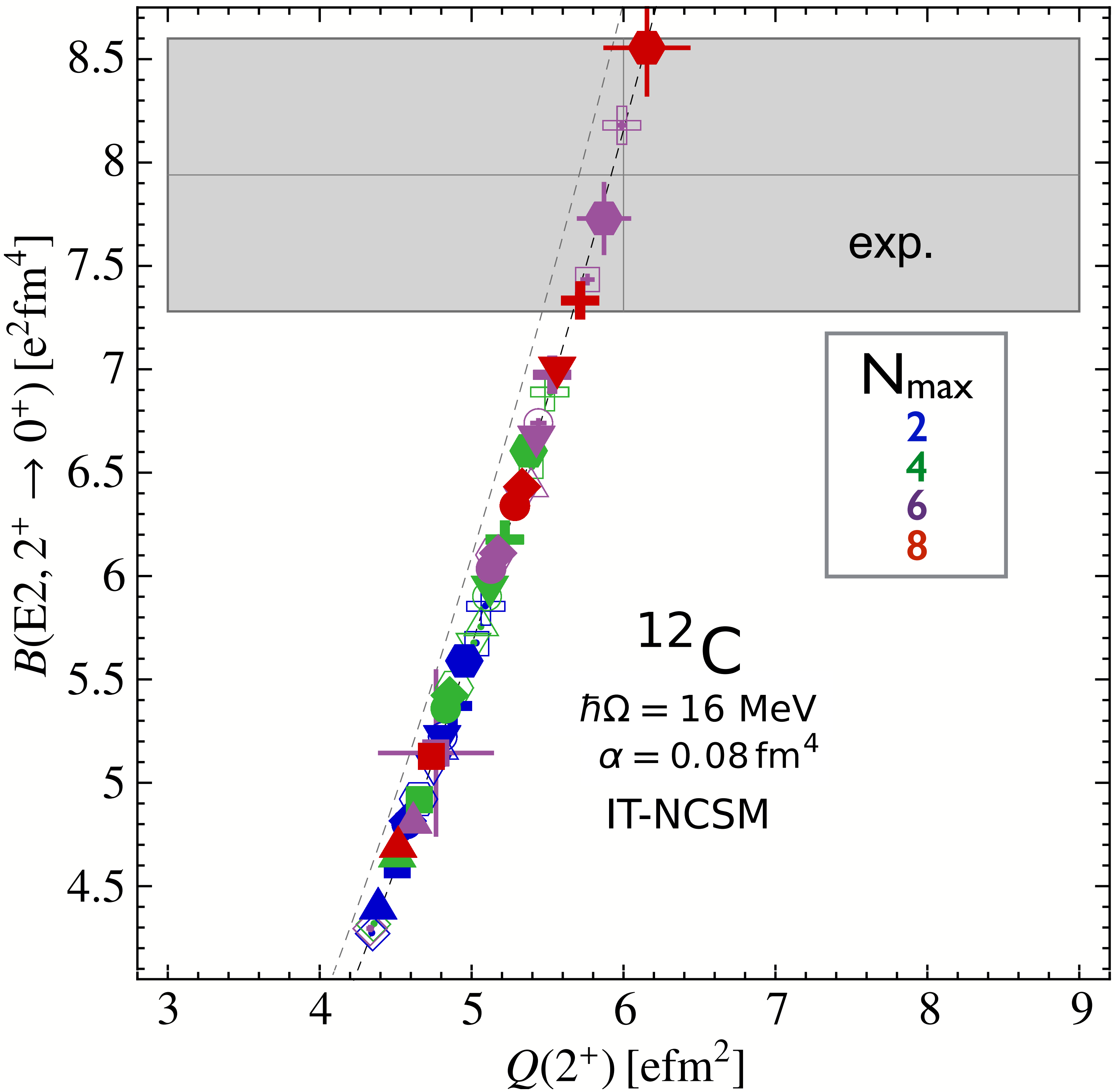
$$\langle \tilde{\Psi}_m | O | \tilde{\Psi}_n \rangle \neq \langle \Psi_m | O | \Psi_n \rangle = \langle \tilde{\Psi}_m | U^\dagger O U | \tilde{\Psi}_n \rangle$$

what we do — what we want — what we need to do

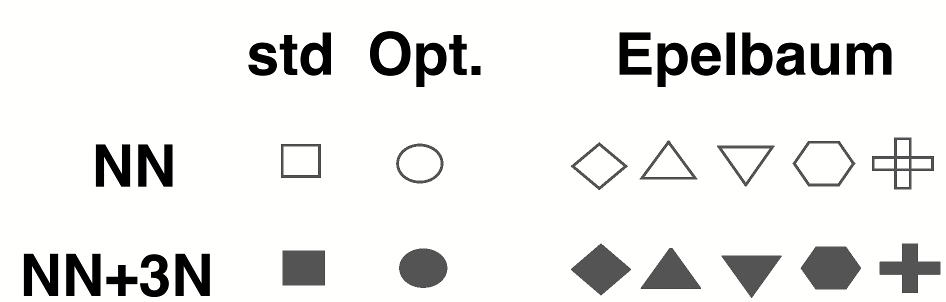
correlations in ab initio calculations

- can provide a solution
- information about underling structure

^{12}C: Quadrupole Correlation



- **robust correlation** between B(E2) and spectroscopic Q value
- independent of:
  - chiral interaction / cutoff
  - model space
  - SRG flow parameter



B(E2) and Quadrupole moment

simple rotational model:

- observables connected via intrinsic quadrupole moment Q_0

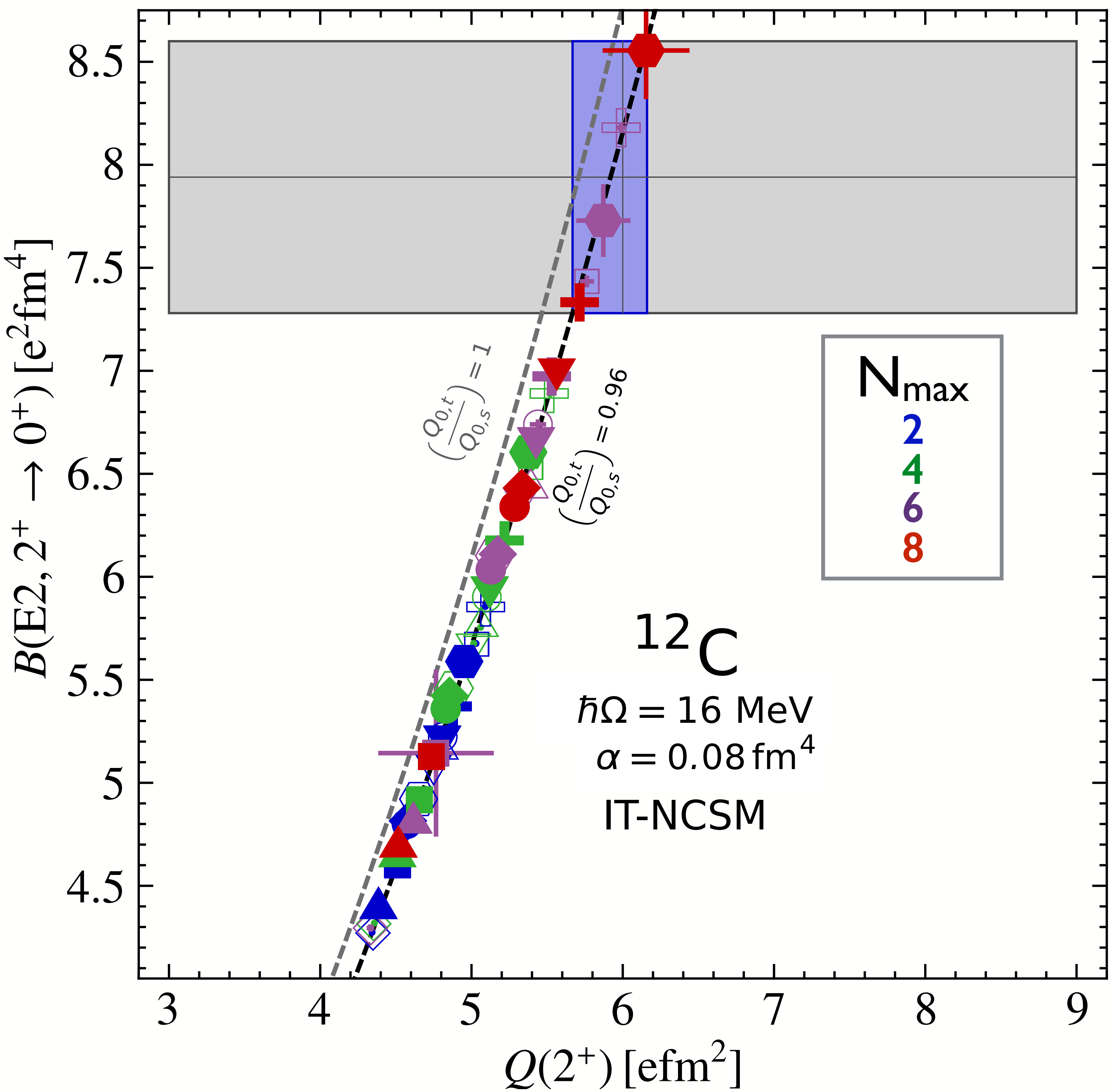
$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_{0,s} \qquad B(E2, J_i \to J_f) = \frac{5}{16\pi} Q_{0,t}^2 \left(\begin{array}{cc|c} J_i & 2 & J_f \\ K & 0 & K \end{array} \right)$$

only parameter

$$B(E2, J_i \to J_f) = \frac{5}{16\pi} \frac{((J+1)(2J+3))^2}{(3K^2 - J(J+1))^2} \left(\begin{array}{cc|c} J_i & 2 & J_f \\ K & 0 & K \end{array} \right) \left(\frac{Q_{0,t}}{Q_{0,s}} \right)^2 Q(J)^2$$

quadratic relation between B(E2) and Quadrupole moment

^{12}C: Quadrupole Correlation

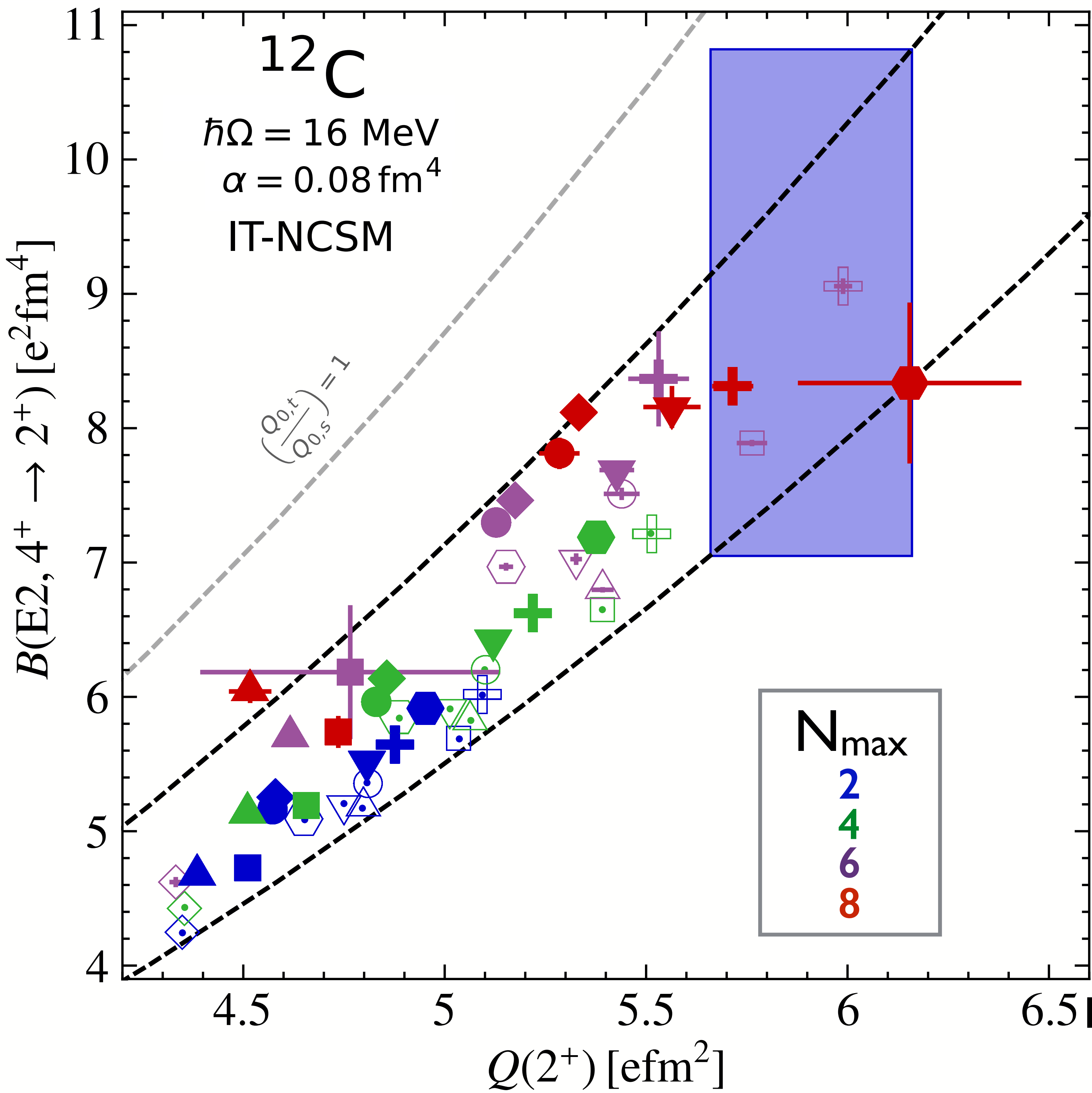


- **robust correlation** between B(E2) and spectroscopic Q value
- independent of:
  - chiral interaction / cutoff
  - model space
  - SRG flow parameter

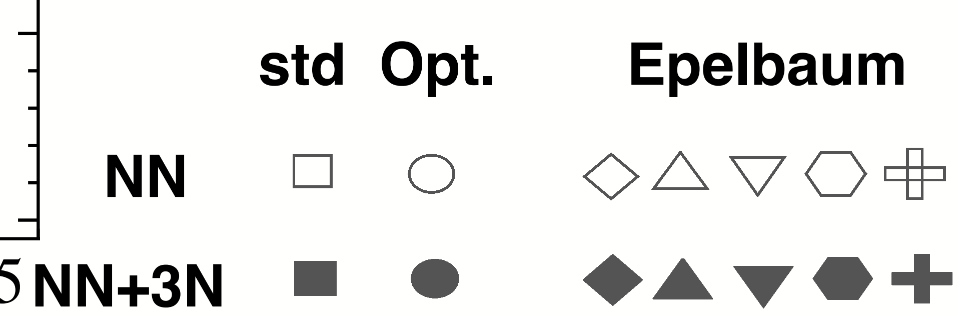
can combine correlation curve with measured B(E2) to **predict Q** precisely

	std	Opt.	Epelbaum
NN	□	○	◇ △ ▽ ⬡ ✚
NN+3N	■	●	◆ ▲ ▼ ⬢ ✚

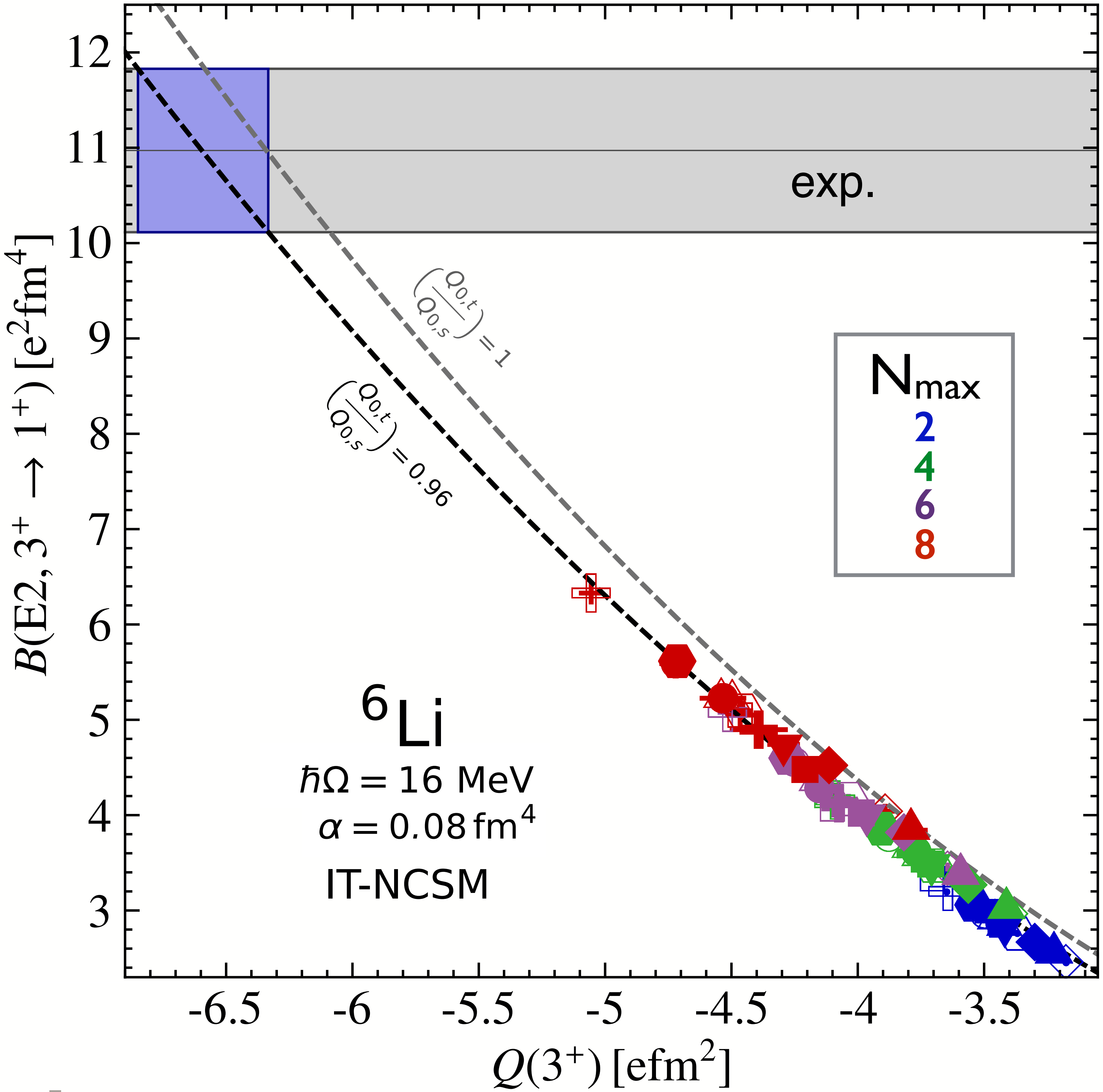
^{12}C: Quadrupole Correlation



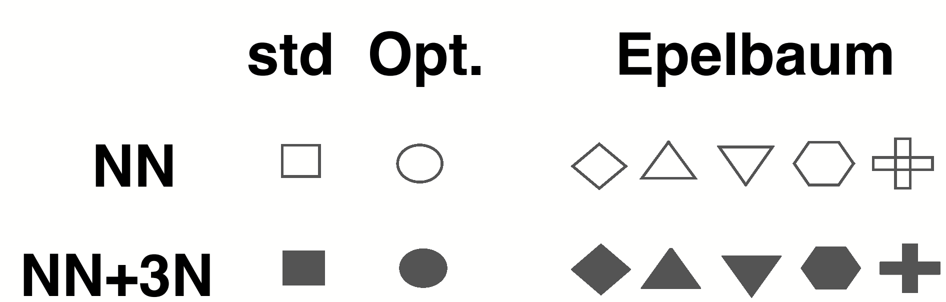
- **less robust correlation** between B(E2) and spectroscopic Q value
- can be used to predict B(E2,4$^+$→2$^+$) rather precise



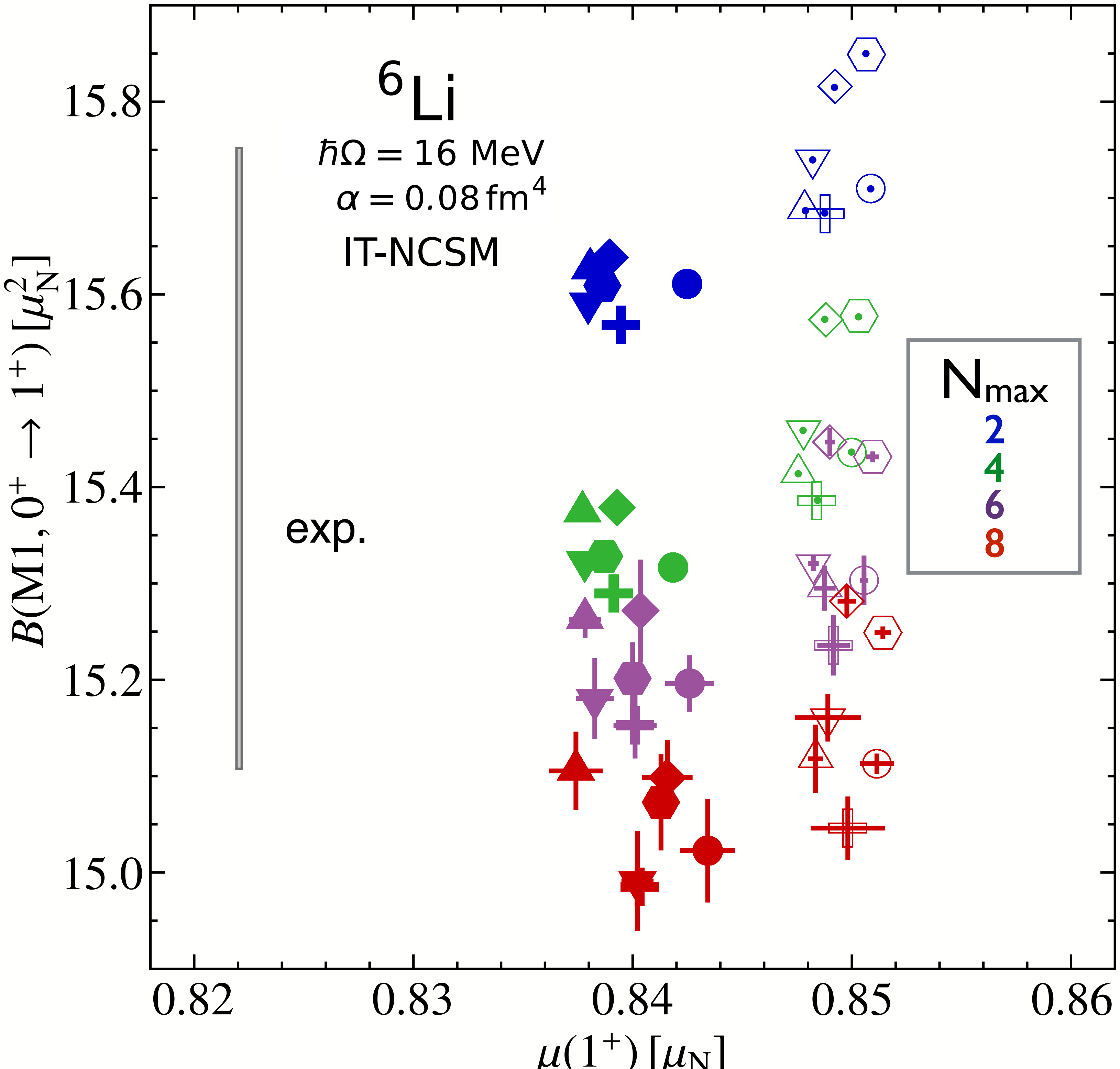
^{6}Li: Quadrupole Correlation



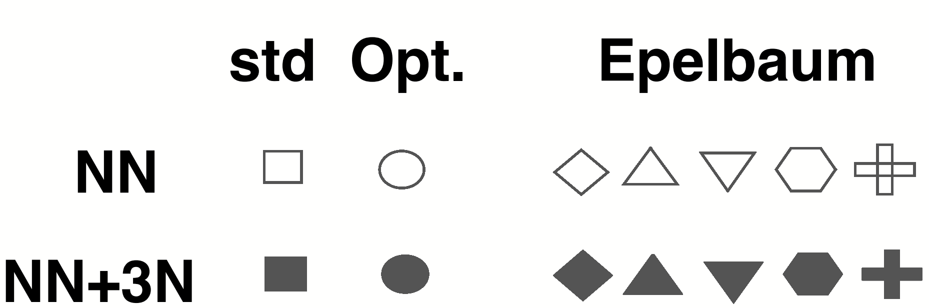
- **robust correlation** between B(E2) and spectroscopic Q value
- independent of:
  - chiral interaction / cutoff
  - model space
  - SRG flow parameter



^{6}Li: Dipol Observables



- magnetic observables almost independent of interaction
- B(M1) not fully converged
- μ converged and **sensitive to 3N**



NCSM with Continuum

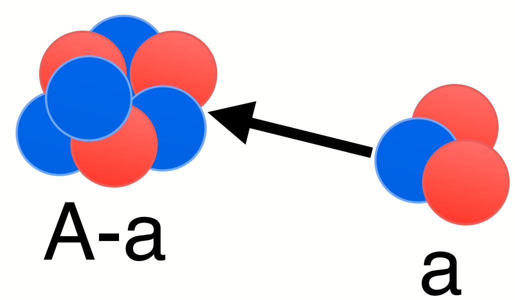
with
P. Navrátil, R. Roth,
J. Langhammer, S. Quaglioni, G. Hupin

NCSM with Continuum

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

ab-initio description of nuclei

bound states & spectroscopy



resonances & scattering states

(IT-)NCSM
ab initio description of nuclear clusters

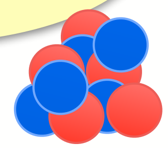
RGM
describing relative motion of clusters

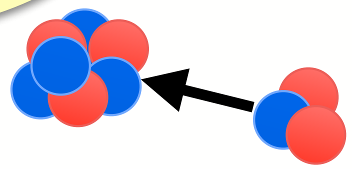
NCSMC
continuum effects in spectroscopy

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**

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





expansion in A-body (IT-)NCSM eigenstates

relative motion of clusters NCSM/RGM expansion

- leads to NCSMC equation

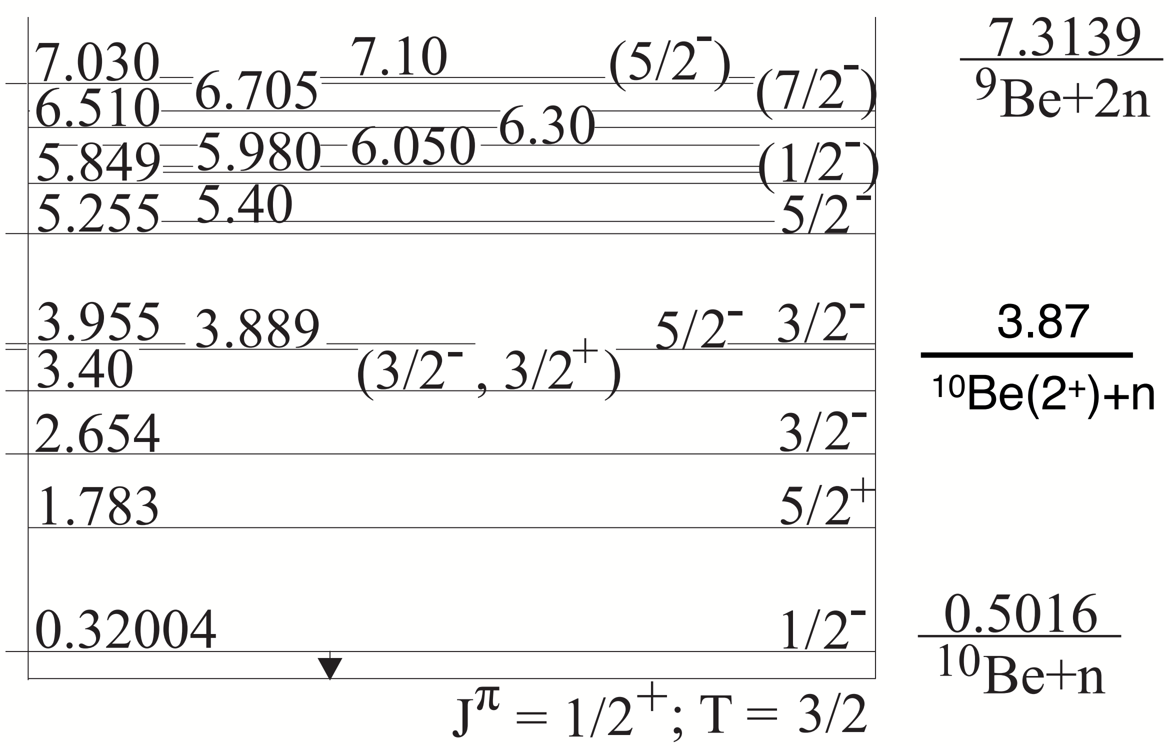
$$\begin{pmatrix} H_{NCSM} & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = E \begin{pmatrix} \mathbb{1} & g \\ g & \mathbb{1} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix}$$

- with 3N contributions in

H_{NCSM}	h	$\mathcal{H}$
covered by (IT-)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

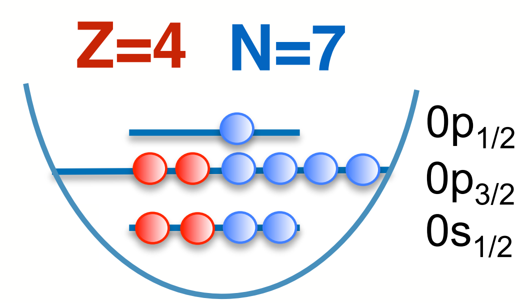
Neutron-rich halo Nucleus ^{11}Be

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



^{11}Be

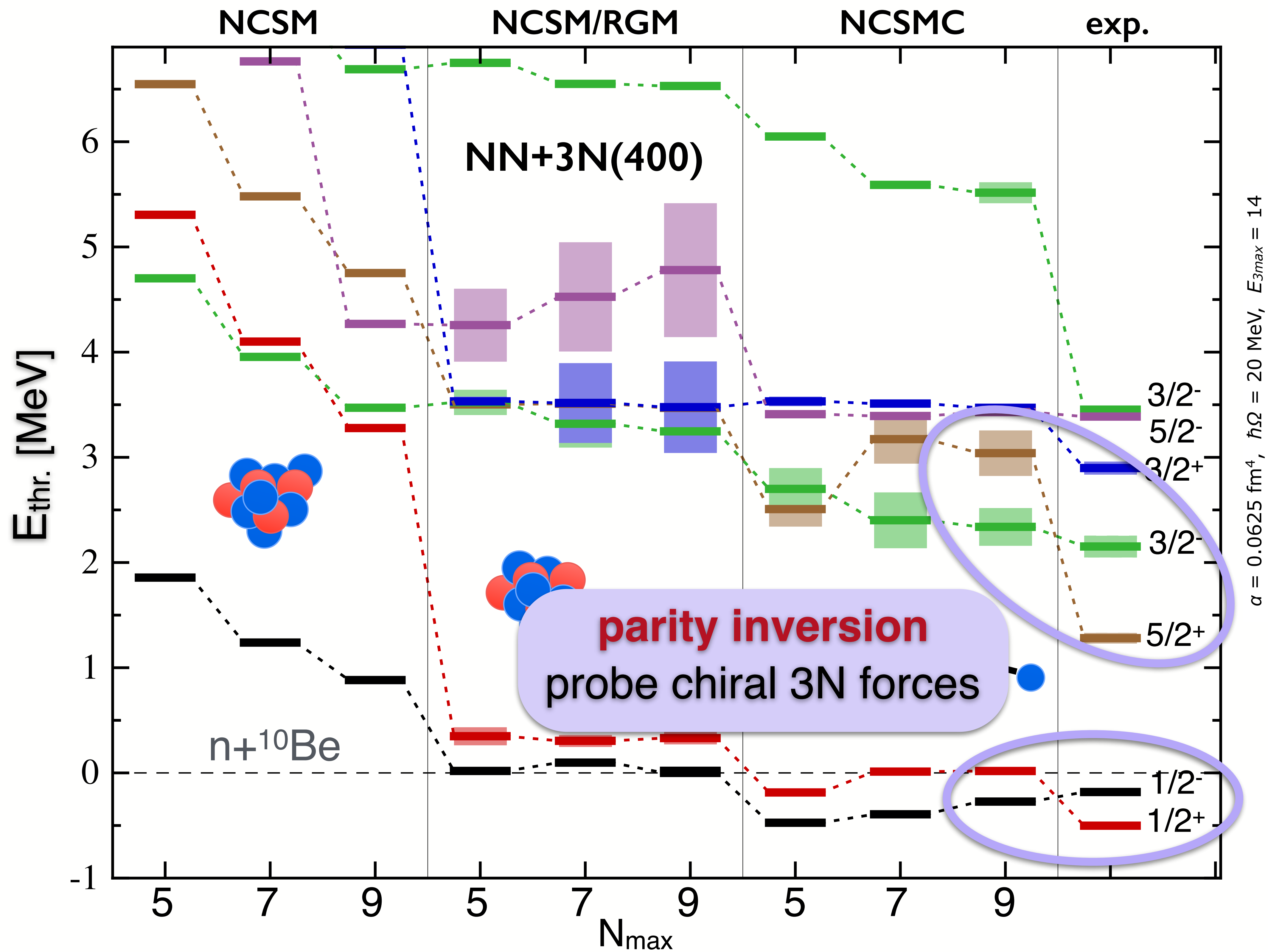
- **parity inversion**
  shell model predicts g.s. to be $J^{\pi}=1/2^-$



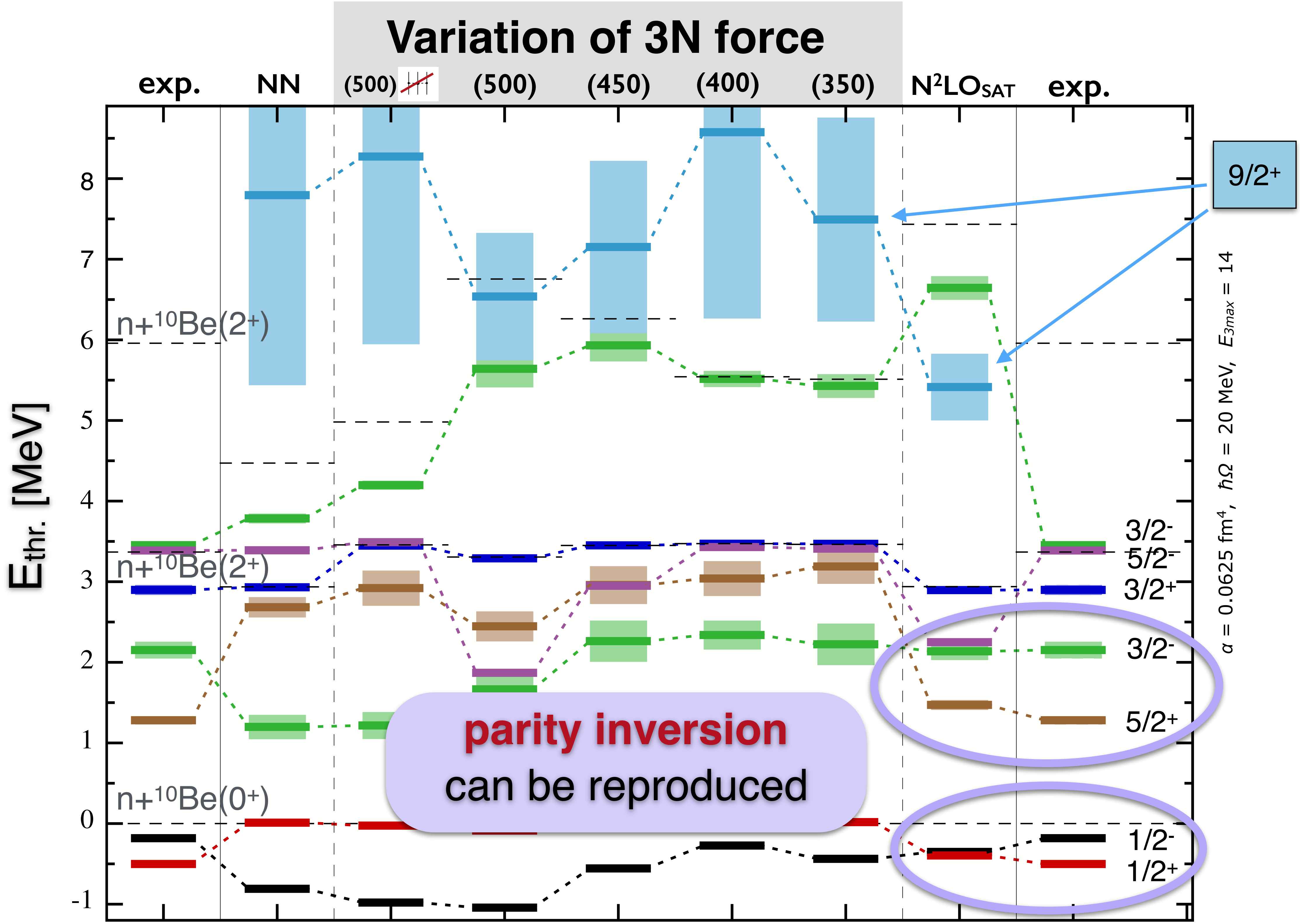
ab initio NCSMC

- include n-^{10}Be continuum (0^+,2^+,2^+ states of ^{10}Be)
- include 6 negative and 3 positive parity states of ^{11}Be

^{11}Be excitation spectrum

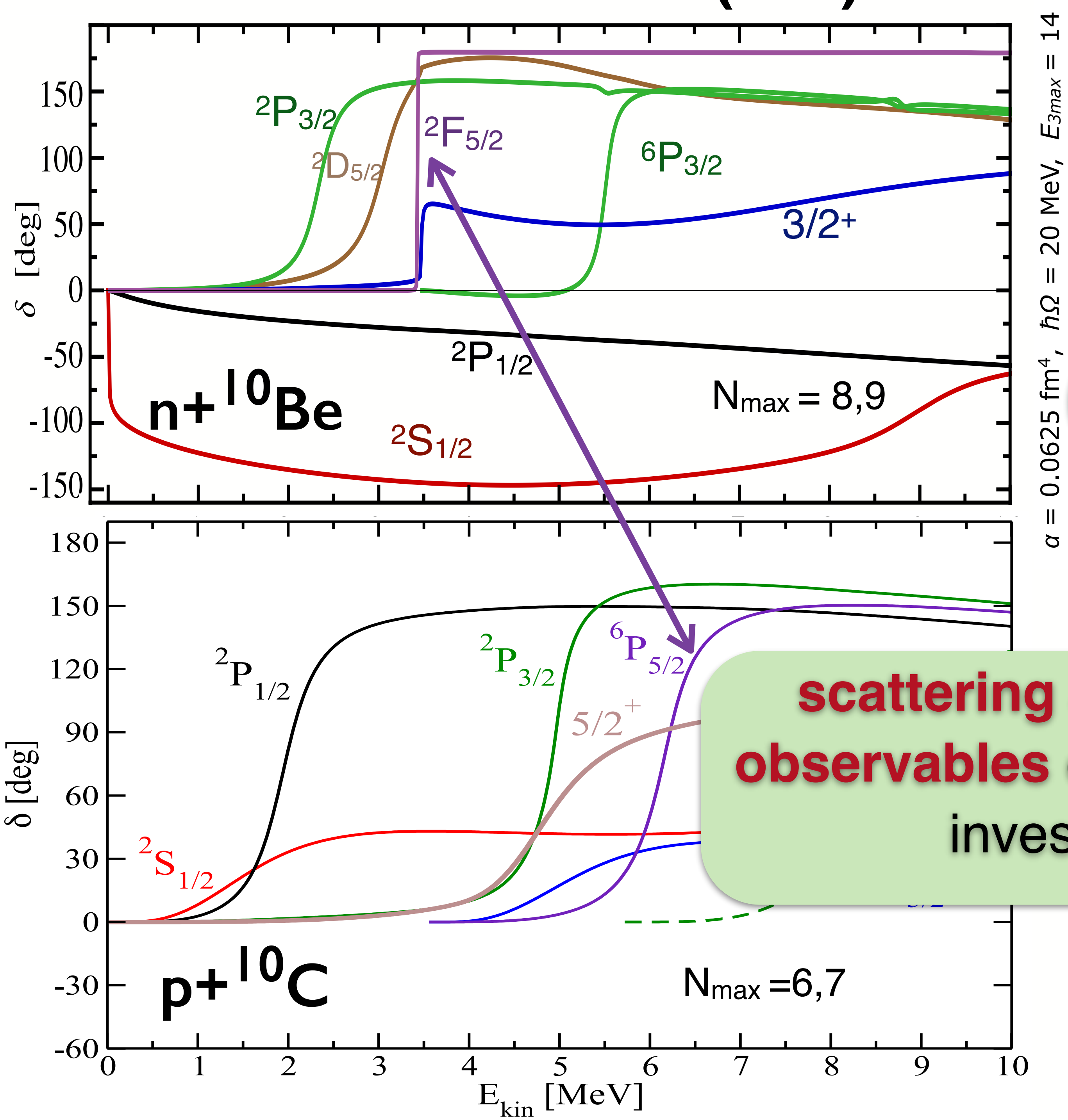


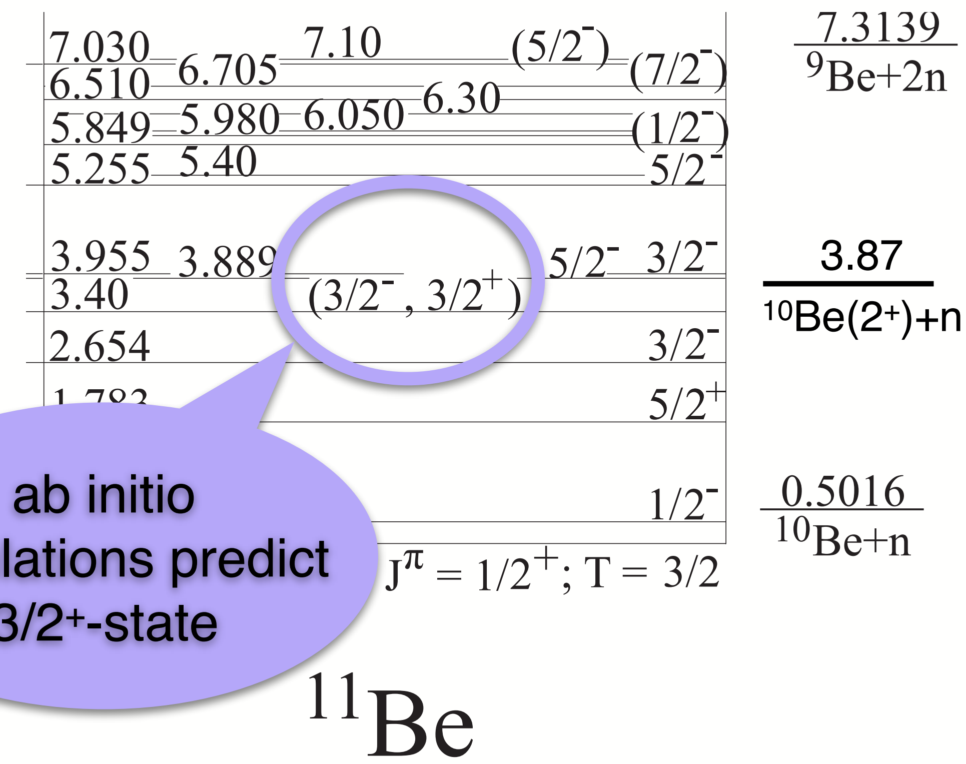
^{11}Be excitation spectrum



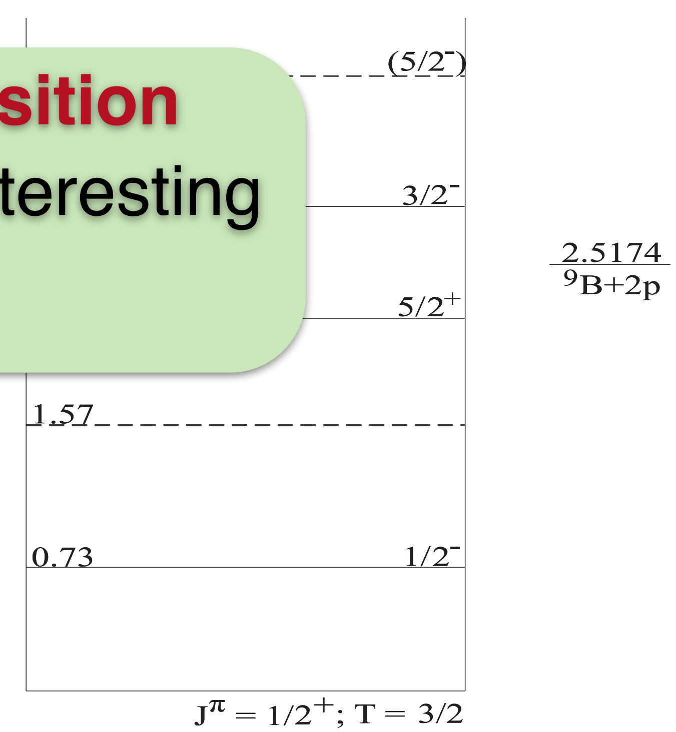
Mirror nuclei: ^{11}Be and ^{11}N

standard NN+3N(400)



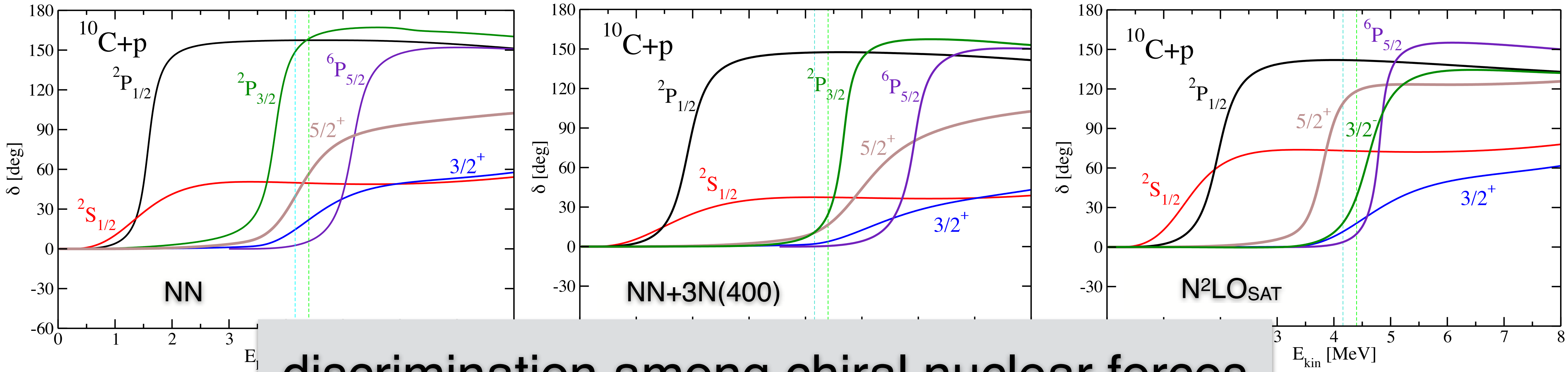


ab initio calculations predict 3/2+-state

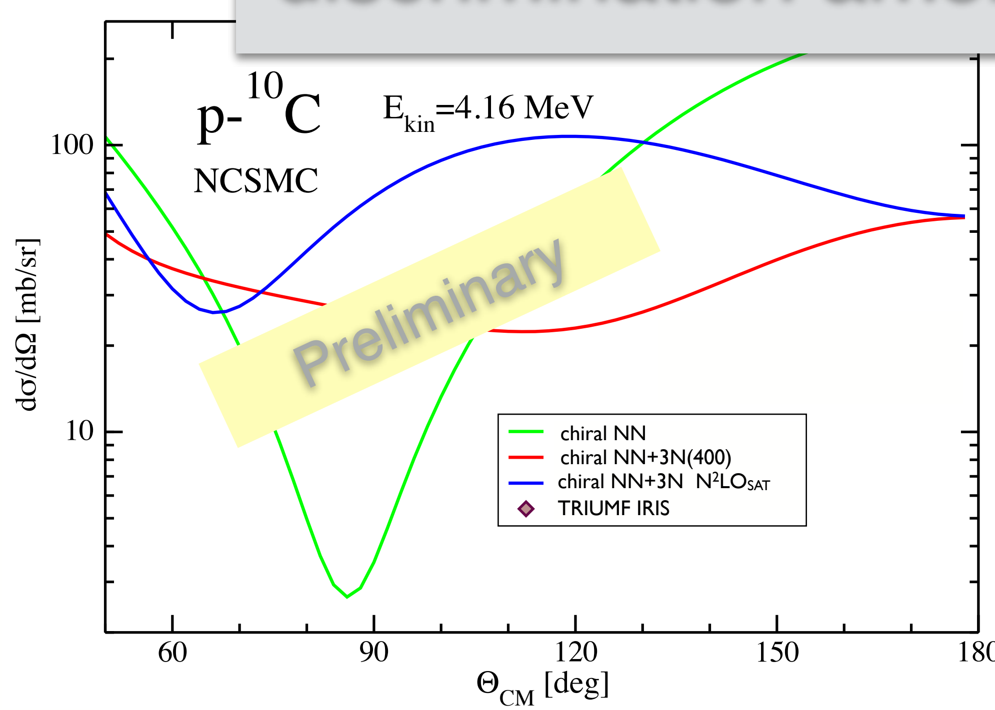


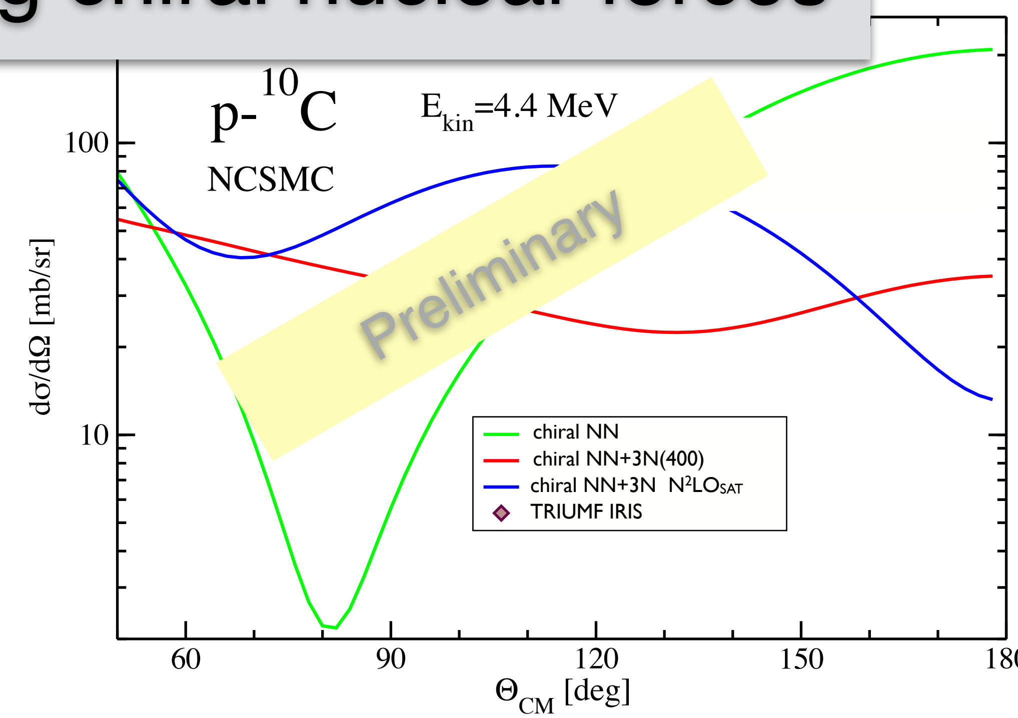
scattering and transition observables enable interesting investigations

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



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

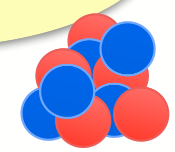
NCSMC with approximated 3N forces

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

NCSM with Continuum (NCSMC)

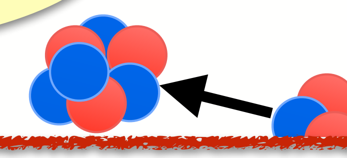
- representing $H\left|\Psi^{J\pi T}\right\rangle = E\left|\Psi^{J\pi T}\right\rangle$ using the **over-complete basis**

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



expansion in A-body (IT-)NCSM eigenstates

relative ... NCSM ...



- leads to NCSMC equation

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

inclusion of 3N is current bottleneck

- with 3N contributions in

H_{NCSM}: covered by (IT-)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

Normal-ordering (NO) approximation

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

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

see talk by Ragnar Stroberg on Thursday

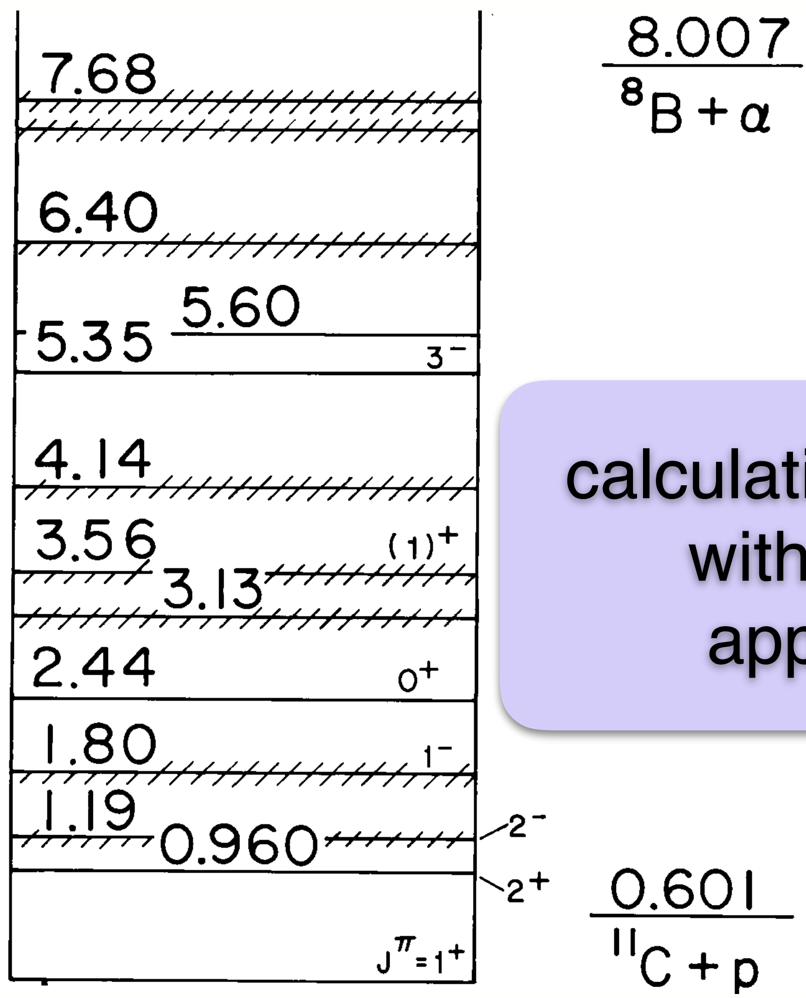
- interested in direct description of **open-shell systems**
  - multi-reference normal ordering (MR-NO)
  - generalization of wicks theorem [Kutzelnigg, Mukherjee]

NCSM/RGM kernels with MR-NO contributions

- reduces computational costs tremendously
- impressively accurate approximation

First application: ^{12}N

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



^{12}N

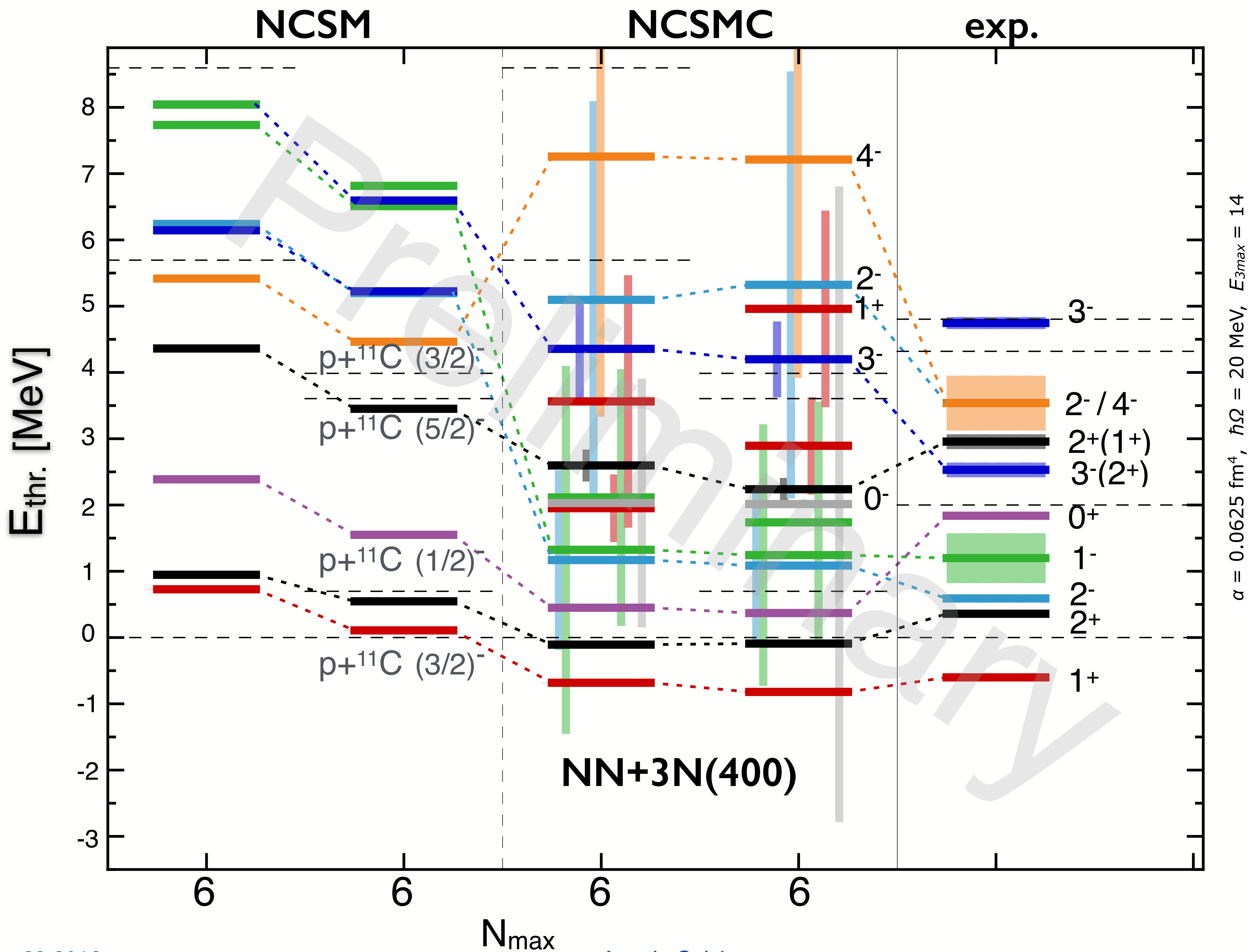
- some low lying resonances not measured precisely
- ^{11}C(p,ɣ)^{12}N can bypass triple-alpha process
- planed experiment at TUDA facility at TRIUMF

ab initio NCSMC

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

calculation out of range without MR-NO approximation

^{12}N with continuum effects



Outlook

- exciting **progress** in construction of **chiral forces**
  - **$N^2LO_{opt/sat/sim/sep}$** different strategies to fit LECs
  - **local interaction** up to N^2LO for quantum Monte Carlo
    Gezerlis, Tews, Epelbaum et al. Phys. Rev. C 90, 054323 (2014)
  - **minimally non-local NN** up to N^3LO include Δ in TPE component
    Piarulli, Girlanda, Marcucci et al. Phys. Rev. C 91, 024003 (2015)

  …

LENPIC Collaboration

- improved NN up to N^4LO
  Epelbaum et al. EPJ A 51, 5(2015); PRL 115, 122301(2015)
- **3N** up to N^3LO
  - allow to vary cutoff and chiral order to quantify uncertainty

Outlook

self-contained framework to employ **present and future chiral NN+3N +4N interactions** in a variety of many-body methods

- **p-shell spectra** provide powerful testbed for chiral potentials
  - constrain and benchmark nuclear forces
- inclusion of **continuum effects** and 3N forces crucial
  - **normal-ordering technique** enable heavier targets and **complex projectiles**

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Thank you! Merci!

- **thanks to my collaborators**
  - P. Navrátil, R. Stroberg, J. Holt, J. Dohet-Eraly
    TRIUMF Vancouver, Canada
  - R. Roth, K. Hebeler, E. Gebrerufael
    Institut für Kernphysik, TU Darmstadt
  - S. Binder
    University of Tennessee, Knoxville
  - J. Vary, P. Maris
    Iowa State University, USA
  - H. Hergert
    MSU, USA
  - S. Quaglioni, C. Romero-Redondo
    LLNL Livermore, USA
  - G. Hupin
    Université Paris-Sud, France

NRC·CNRC

NSERC CRSNG

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HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

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