Advances on NCSM, SRG & Chiral Interactions

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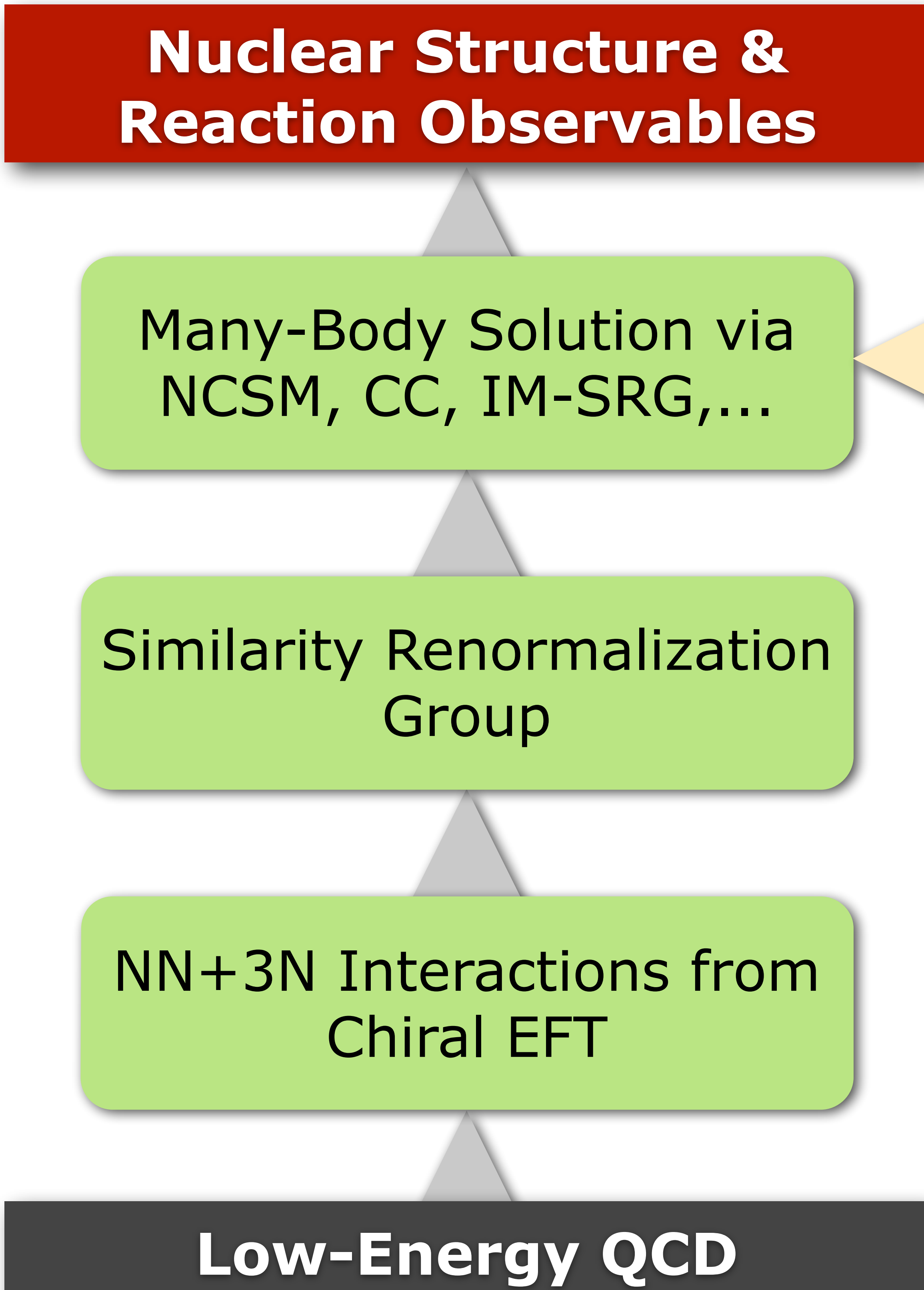
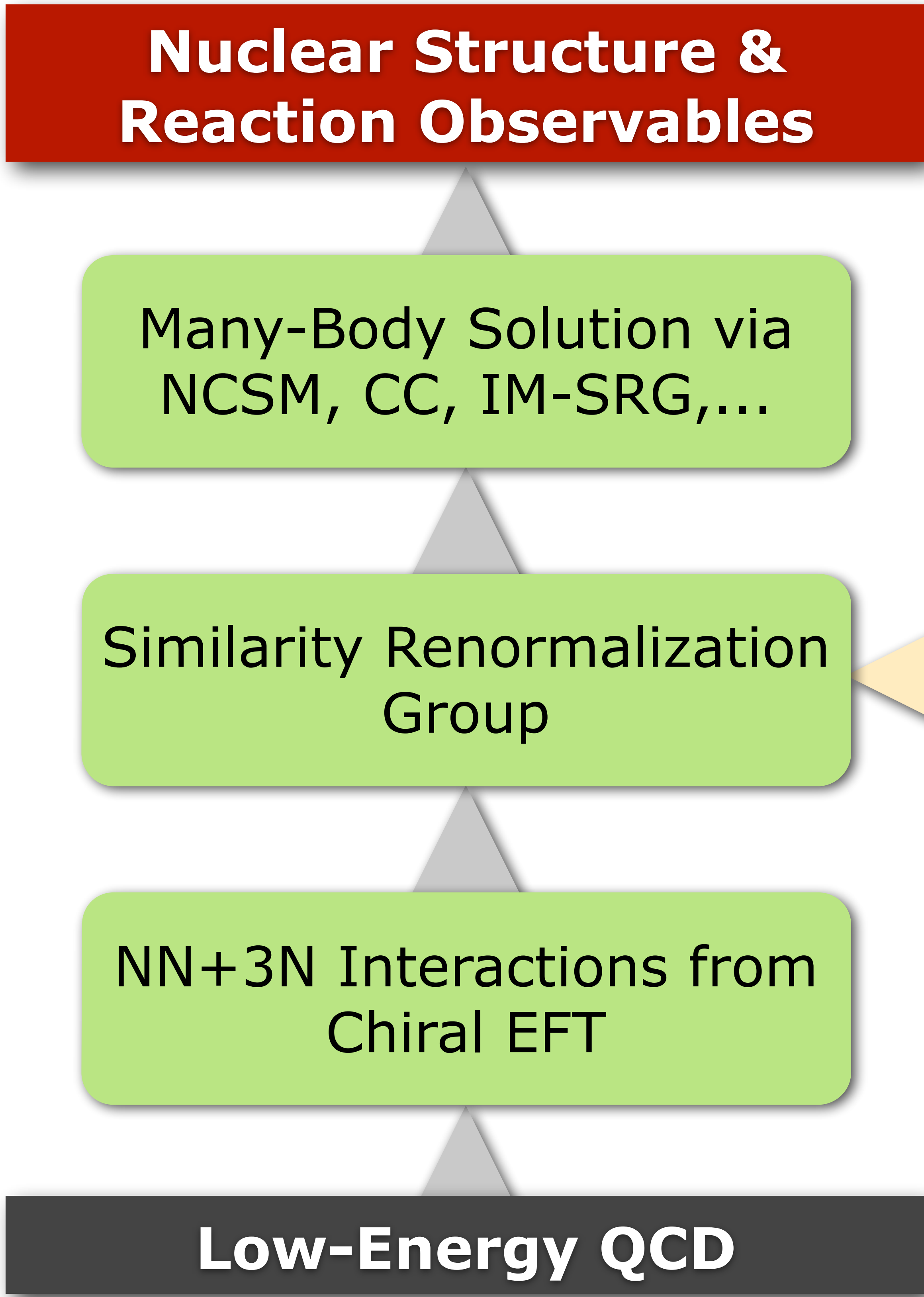
Ab Initio Workflow



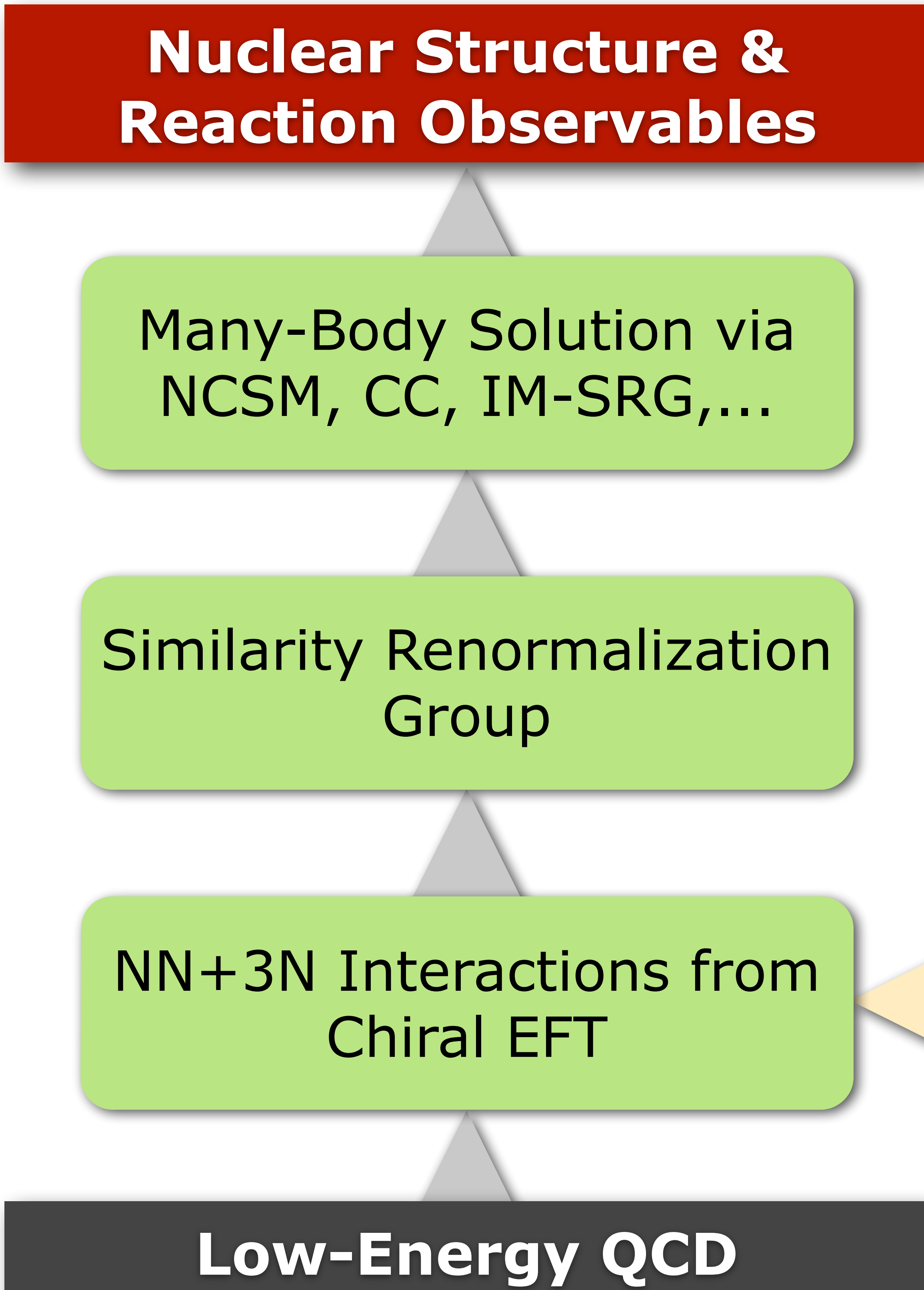
- initial formulation typically limited to bound-state basis
- description of continuum effects and observables not possible
- improvement: include continuum degrees of freedom explicitly
- here: **NCSM with Continuum**

Ab Initio Workflow



- drastically improves convergence but induces many-body forces
- induced beyond-3N interactions are a major limitation for many applications
- improvement: either include or suppress induced forces
- here: **Block Generators**

Ab Initio Workflow



- chiral EFT offers systematics, improvability and uncertainty estimation
- typically one "chiral interaction" is used in nuclear structure
- improved chiral EFT interactions offer opportunity to quantify uncertainties systematically
- here: **initial NCSM studies with NN from LO to N4LO**

NCSM with Continuum for the Structure of ^{9}Be

with
J. Langhammer, P. Navrátil,
S. Quaglioni, G. Hupin, A. Calci

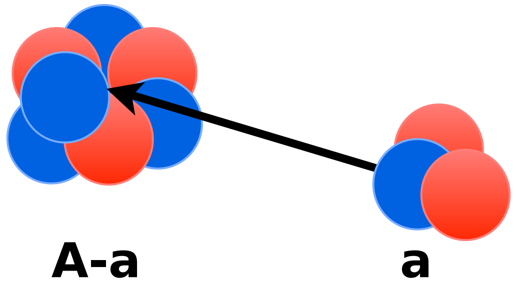
Phys. Rev. C 91, 021301(R) (2015)

NCSM with Continuum

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

comprehensive ab initio description of light nuclei

bound states
& spectroscopy



resonances
& scattering states

(IT-)NCSM
ab initio description of nuclear clusters

NCSMC

RGM
describing relative motion of clusters

focus on NCSMC with 3N interactions
for p-shell spectroscopy

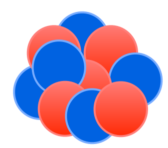
NCSMC with 3N Forces

Hupin, Langhammer, Navrátil, Quaglioni, Calci, Roth; Phys. Rev. C 88, 054622 (2013)

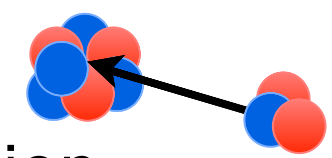
- representing $H|\psi^{J\pi T}\rangle = E|\psi^{J\pi T}\rangle$ using the **over-complete basis**

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

expansion in *A*-body (IT-)NCSM eigenstates



identical to the NCSM/RGM expansion



leads to the **NCSMC equations**

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

access targets beyond ^{4}He using uncoupled densities and on-the-fly algorithm

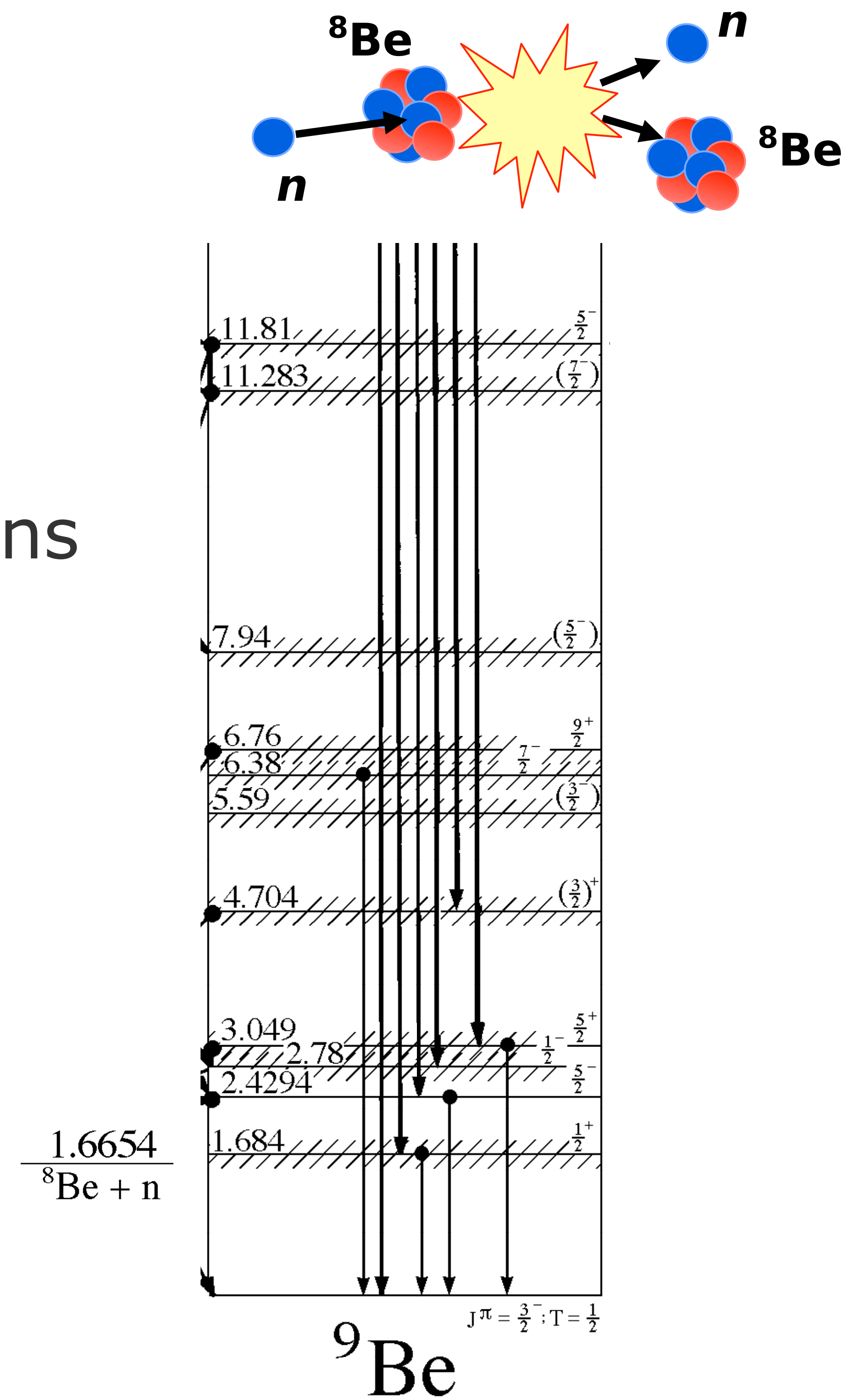
with 3N contributions in

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

Ab Initio Description of ^{9}Be

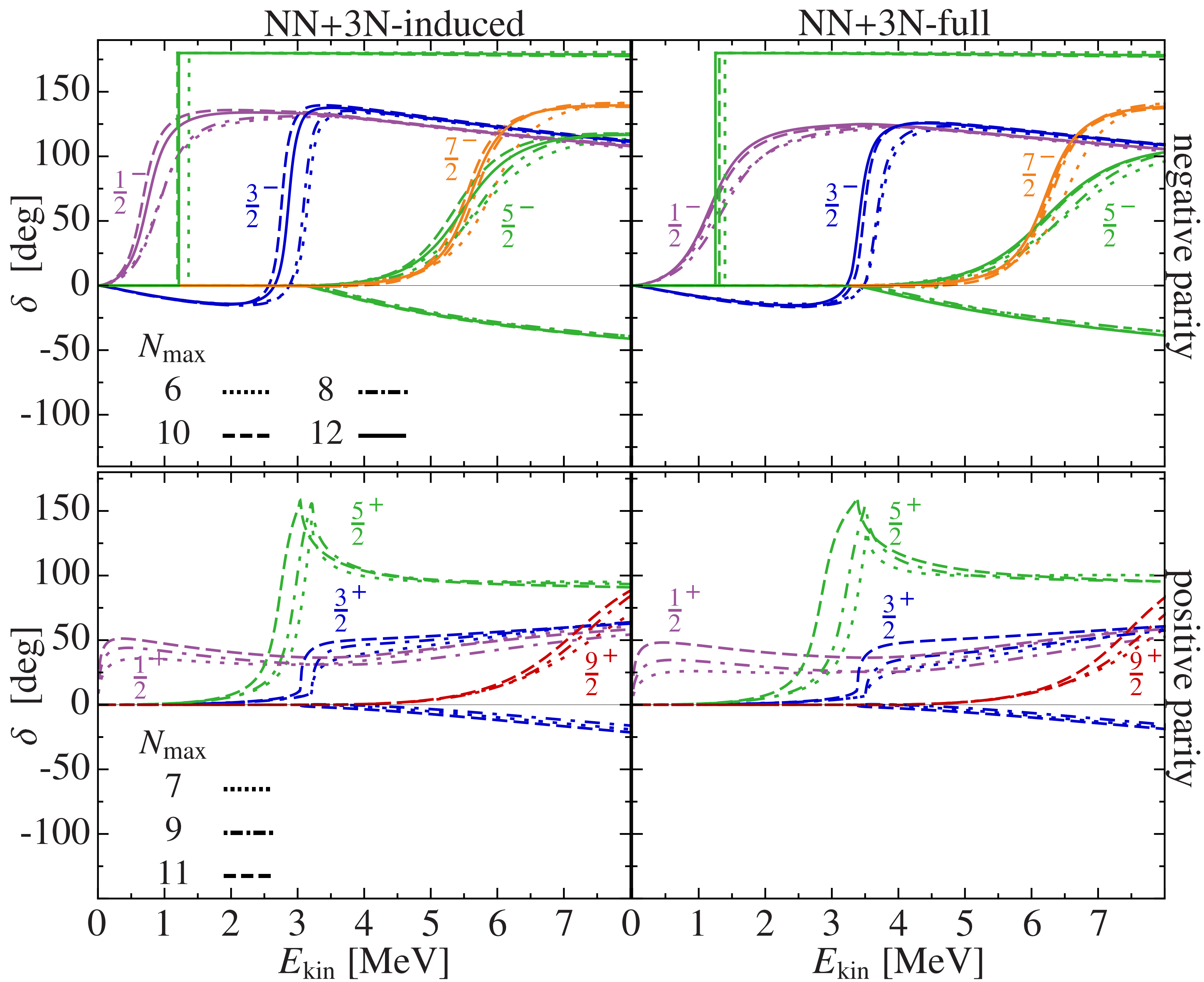
Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)

- ^{9}Be is excellent candidate to study continuum effects on spectra
- all excited states are resonances
- previous NCSM studies with NN interactions show clear discrepancies in spectrum: 3N or continuum effects?
- include n-^{8}Be continuum in NCSMC
- use standard NN+3N Hamiltonian:
  - NN: N3LO, Entem & Machleidt, 500 MeV cutoff
  - 3N: N2LO, Local, 500 MeV cutoff



^{9}Be: Convergence of Phase Shifts

Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)

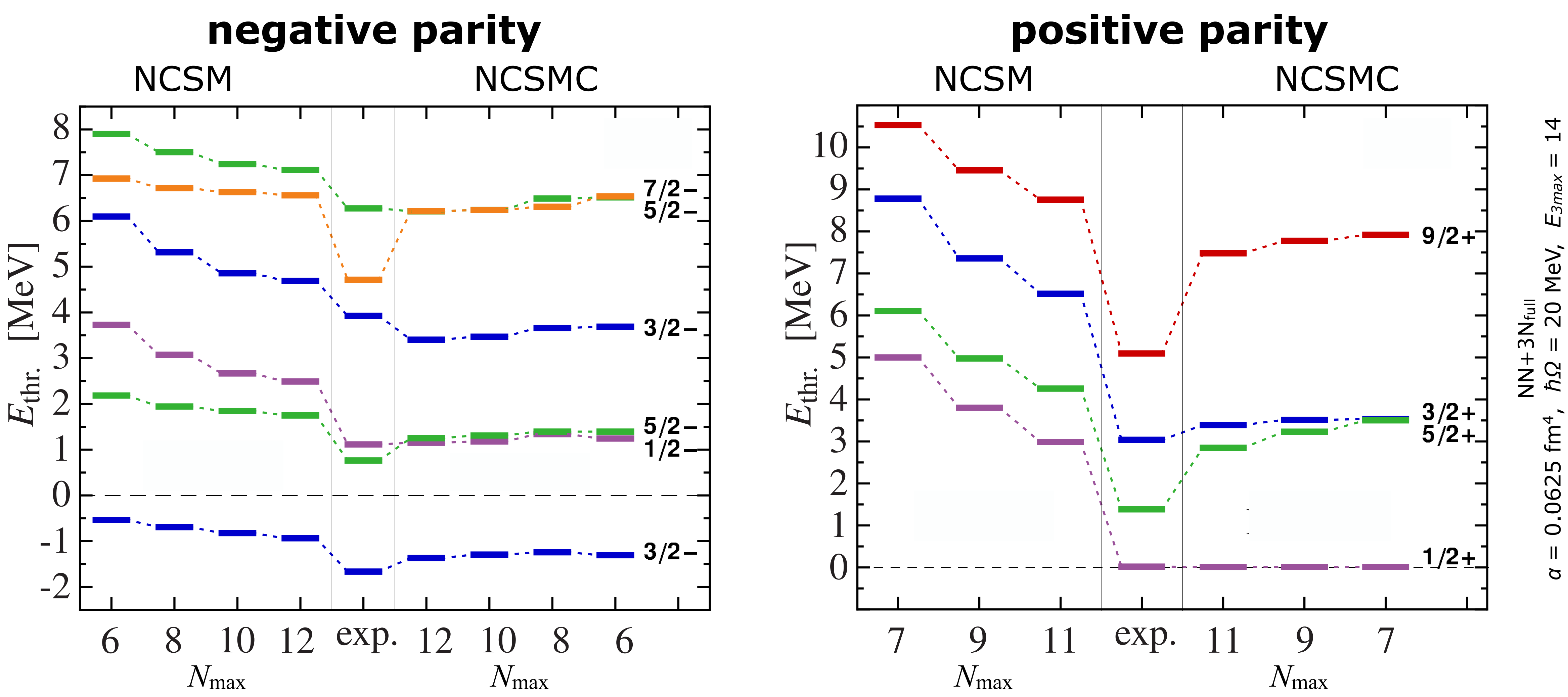


- include 0^+, 2^+ states of ^{8}Be
- include 6 negative and 4 positive parity states of ^{9}Be
- negative parity phase-shifts are well converged, positive parity more difficult
- extract resonance parameters from inflection point and derivative

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

^{9}Be: NCSM vs. NCSMC

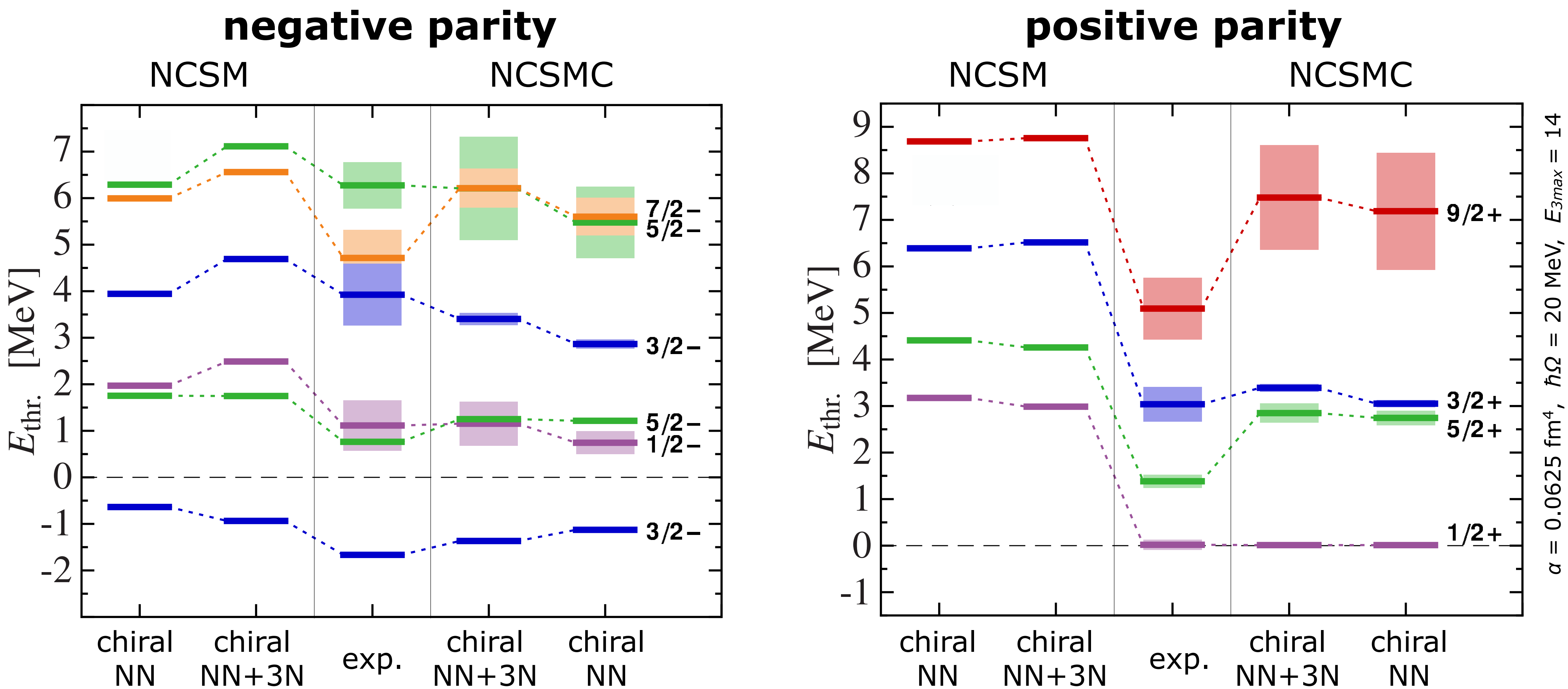
Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)



- NCSMC shows much better N_{max} convergence
- NCSM tries to capture continuum effects via large N_{max}
- drastic difference for the $1/2^+$ state right at threshold

^{9}Be: Spectrum

Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)



- continuum plays more important role than chiral 3N interaction
- NCSMC predictions for widths are in fair agreement with experiment

SRG with Block Generators

with
A. Calci, N. M. Dicaire, C. Omand, P. Navrátil,
T. Hüther, S. Schulz, K. Vobig

Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth, Navrátil...

continuous unitary transformation to **pre-diagonalize Hamiltonian** and thus improve model-space convergence

- **consistent unitary transformation** of Hamiltonian and observables

$$H_\alpha = U_\alpha^\dagger H\, U_\alpha \qquad\qquad O_\alpha = U_\alpha^\dagger O\, U_\alpha$$

- evolution equations for H_α and U

$$\frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \qquad\qquad \frac{d}{d\alpha} O_\alpha$$

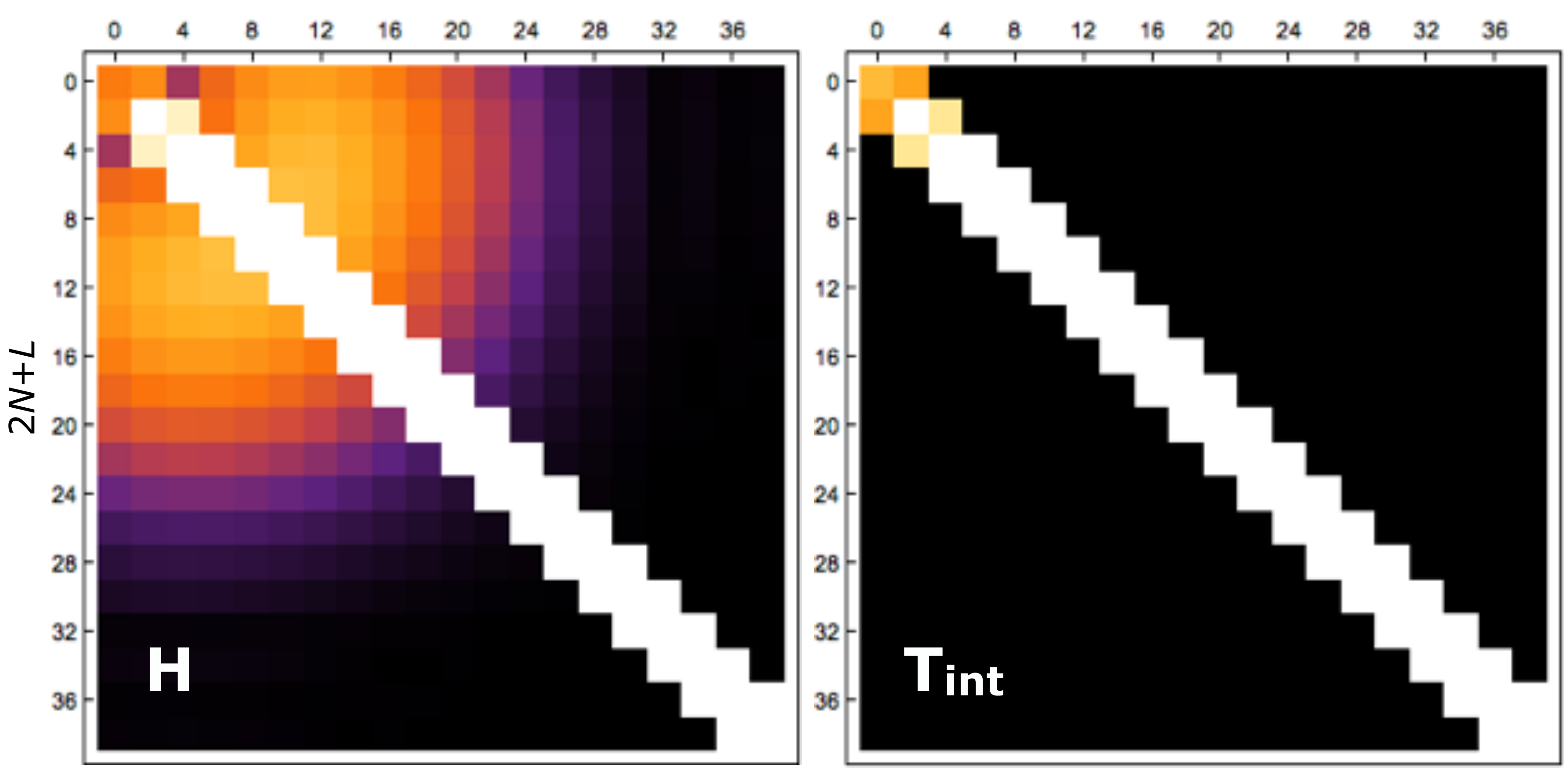
design G_α for optimum compromise between convergence & induced many-body forces

- **dynamic generator η_α** drives towards "diagonal" defined by G_α

$$\eta_\alpha = (2\mu)^2\, [G_\alpha, H_\alpha]$$

Choice of Generator: T_{int}

- standard choice for G_α is **intrinsic kinetic energy T_{int}**
- drives diagonalization everywhere, also for low-lying basis states that are covered explicitly by many-body model space
- rule of thumb: the **more diagonal** the **more induced many-body** interactions



HO matrix elements, $^1S_0$ channel, $\hbar\Omega$ = 24 MeV

Choice of Generator: Block Generators

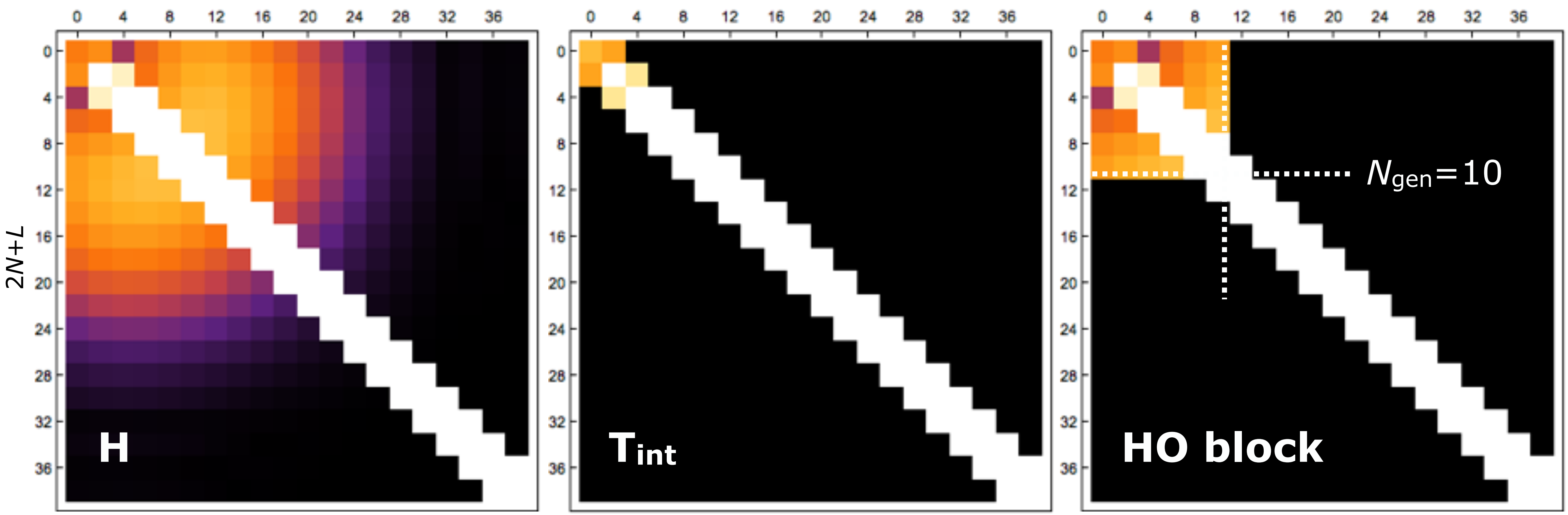
Dicaire, Omand, Navrátil; Phys. Rev. C 90, 034302 (2014)

- **HO block generator**: use H_α matrix elements for states below N_{gen} and T_{int} matrix elements above, i.e.,

$$G_\alpha = T_{int} + \Pi_{N_{gen}} V_\alpha \Pi_{N_{gen}}$$

with projection operator $\Pi_{N_{gen}}$ on rel. HO states with $2N + L \leq N_{gen}$

- generator has **explicit scale parameters**: N_{gen} & $\hbar\Omega$



HO matrix elements, $^1S_0$ channel, $\hbar\Omega$ = 24 MeV

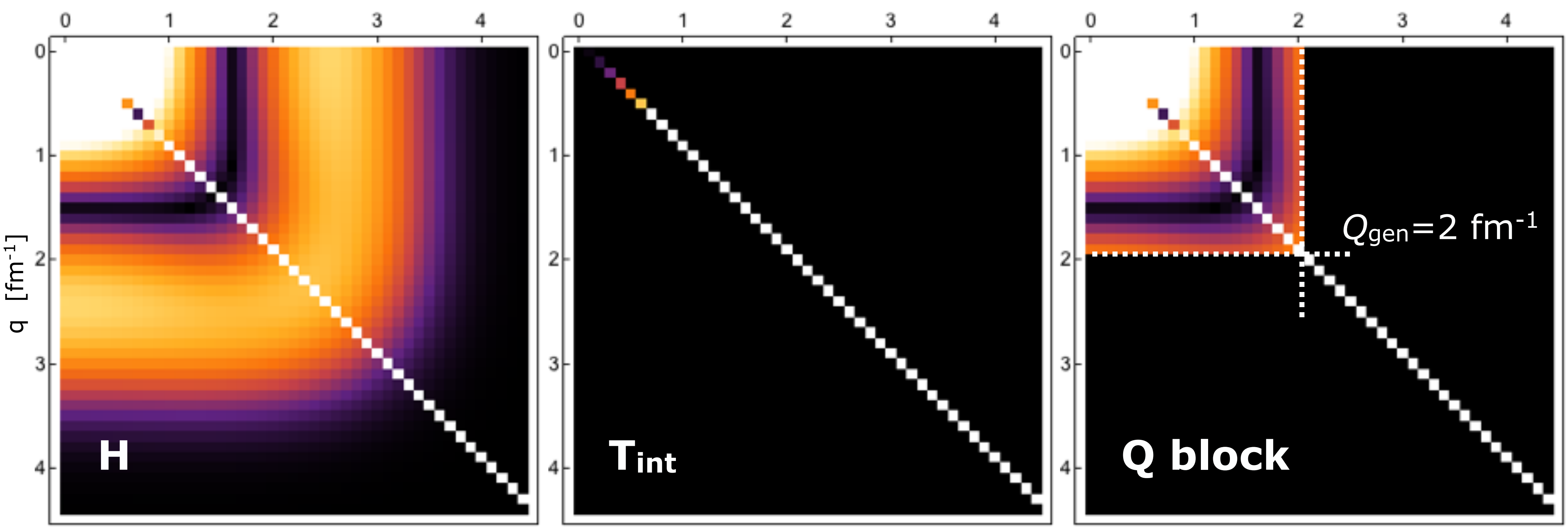
Choice of Generator: Block Generators

- **Q block generator**: use H_α matrix elements for states below Q_{gen} and T_{int} matrix elements above, i.e.,

$$G_\alpha = T_{int} + \Pi_{Q_{gen}} V_\alpha \Pi_{Q_{gen}}$$

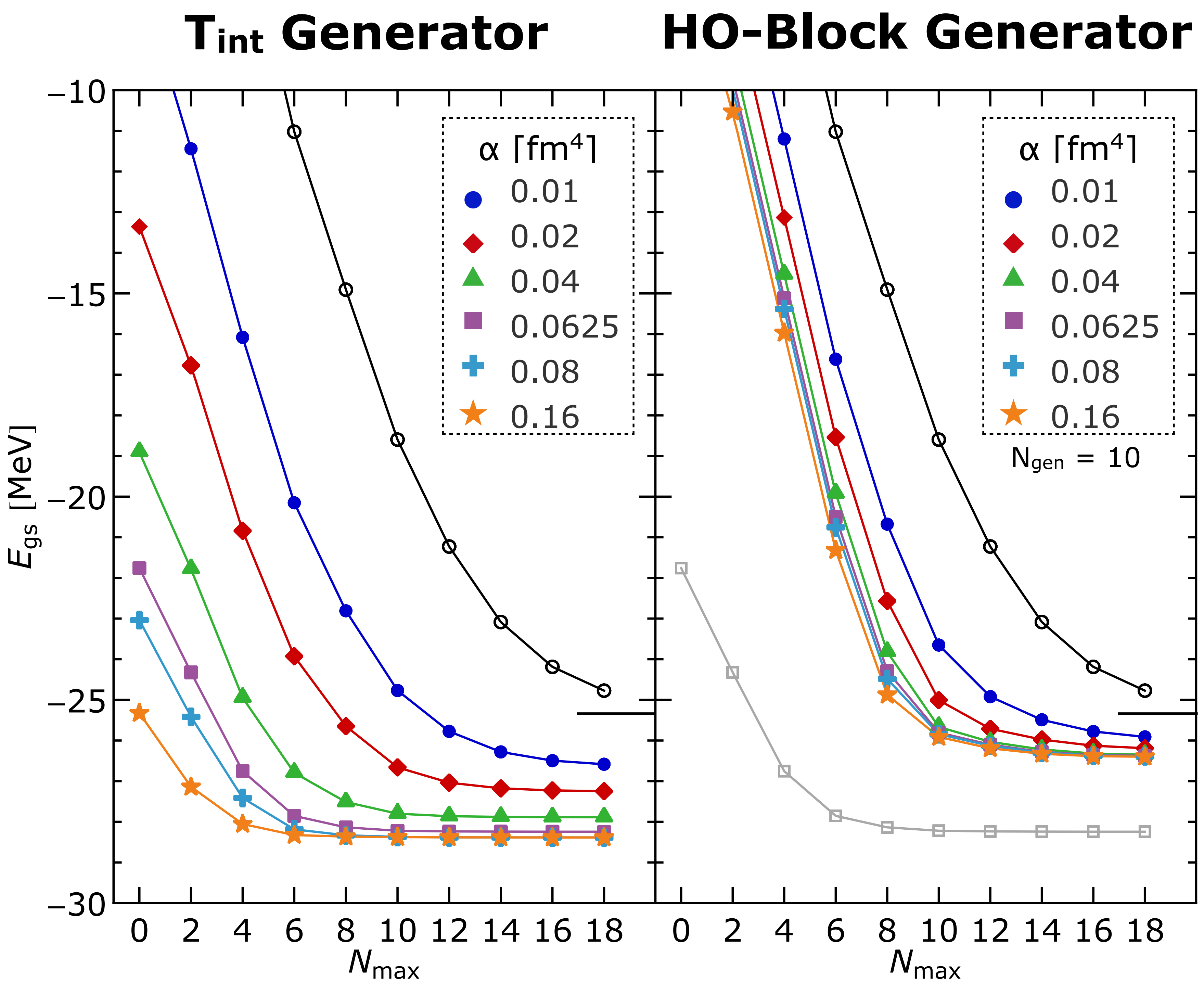
  with projection operator $\Pi_{Q_{gen}}$ on rel. momentum states with $q \leq Q_{gen}$

- generator has **explicit scale parameter**: Q_{gen}



momentum-space matrix elements, $^1S_0$ channel

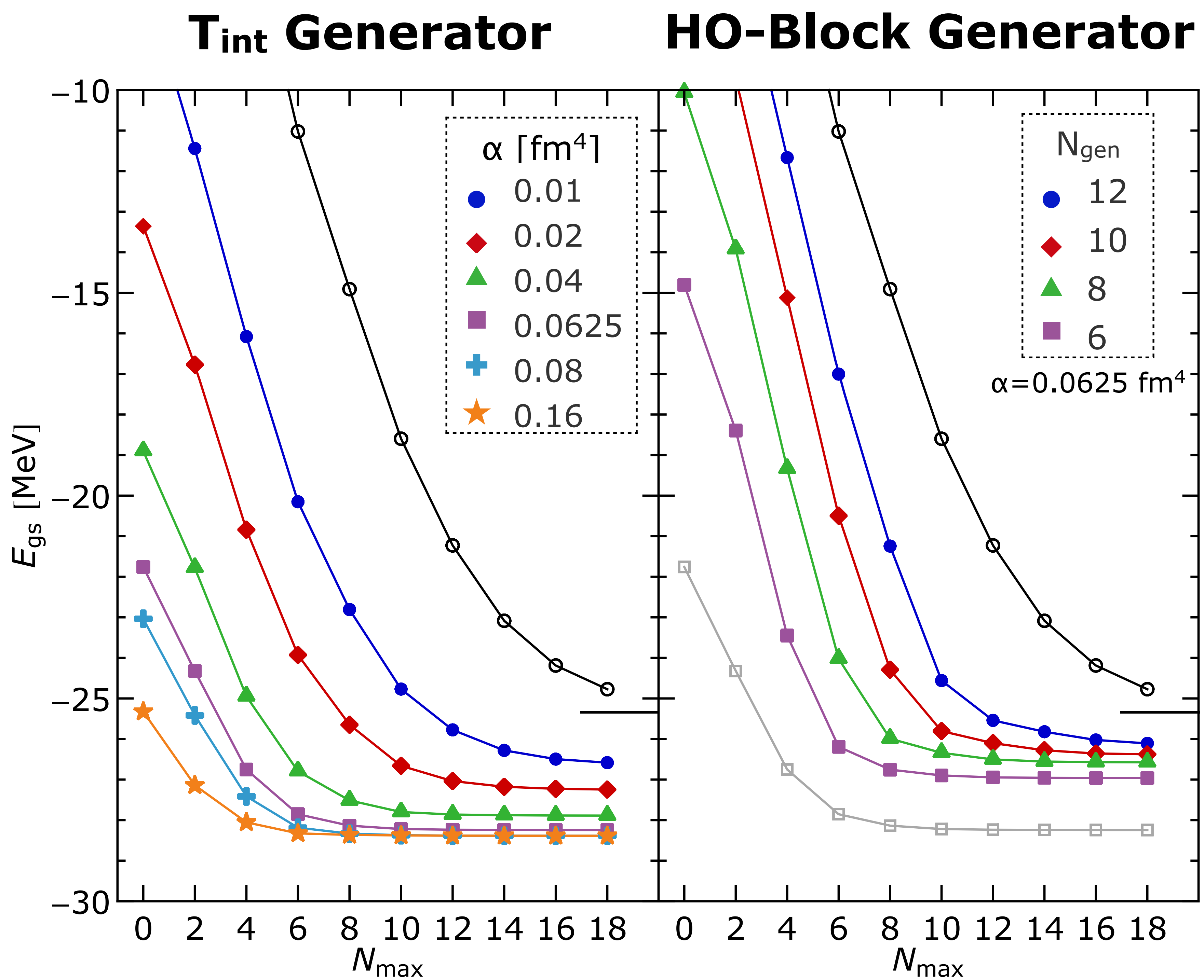
^{4}He: Convergence vs. Induced Many-Body



- α-dependence of block generator quickly saturates
- block protects low-lying matrix elements from further change

NN_{only}
$\hbar\Omega$ = 24 MeV
HO basis

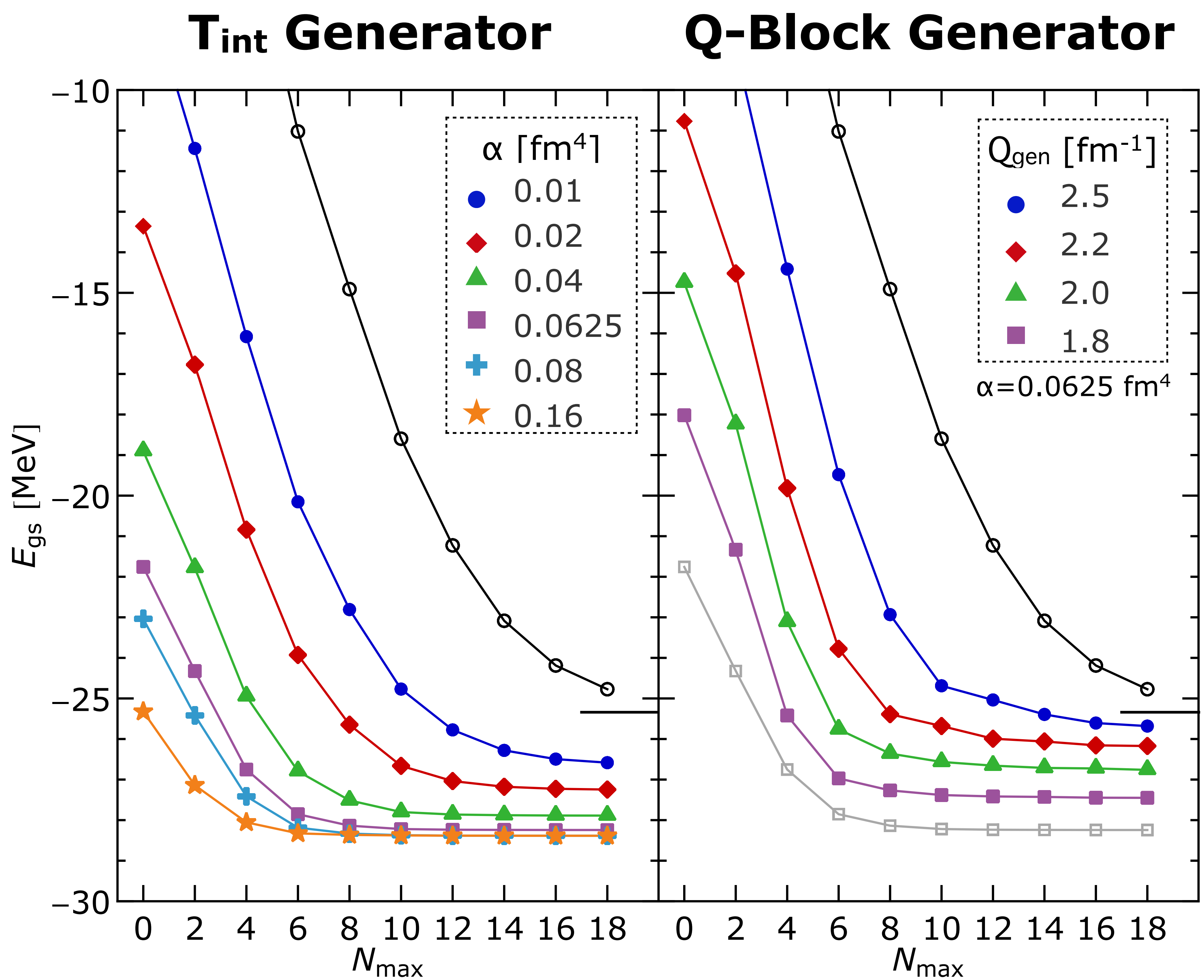
^{4}He: Convergence vs. Induced Many-Body



- N_{gen} controls convergence and induced many-body forces
- induced 3N appear smaller than with T_{int} generator

NN_{only}
$\hbar\Omega$ = 24 MeV
HO basis

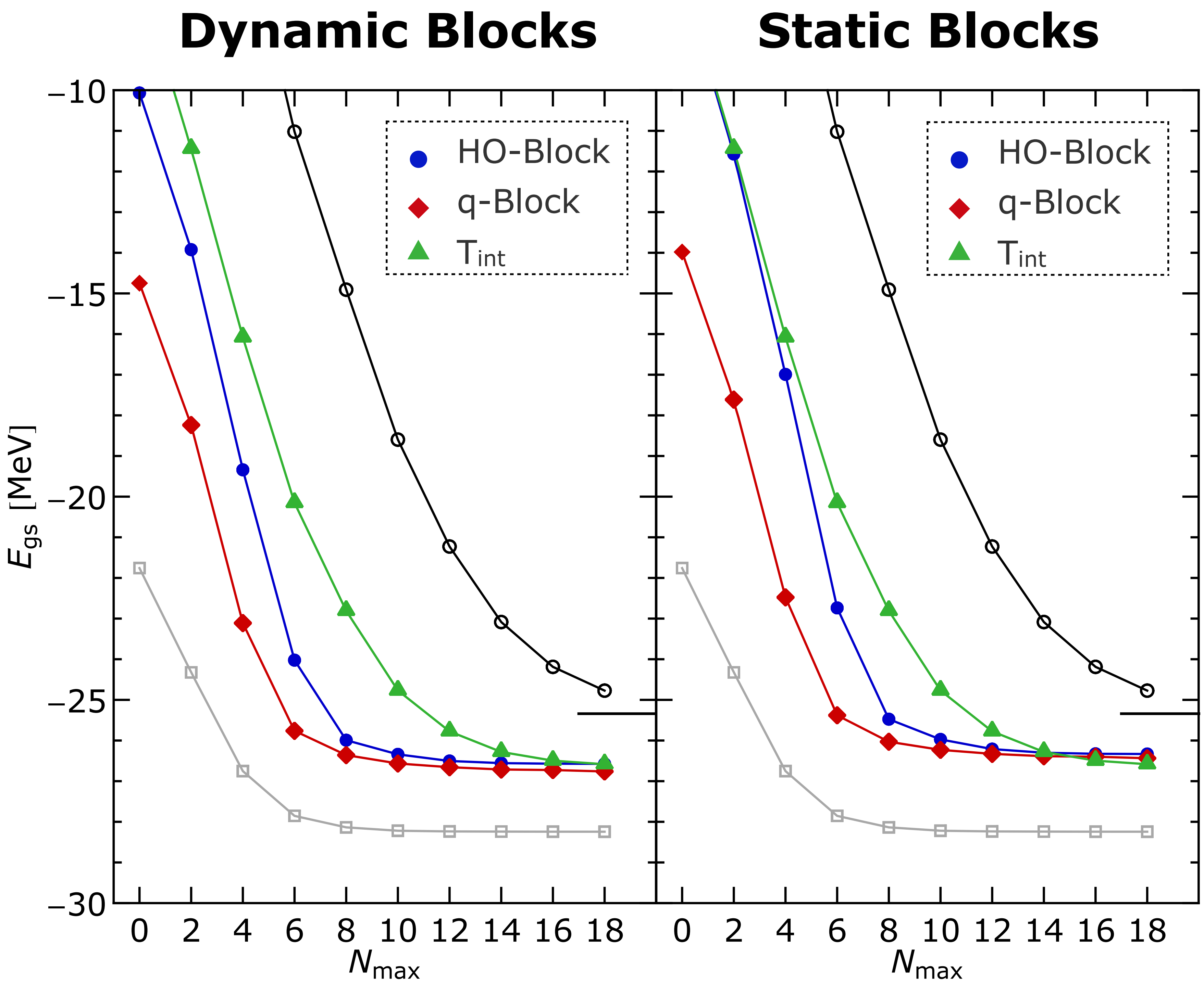
^{4}He: Convergence vs. Induced Many-Body



- Q-block generator exhibits similar behaviour
- typical $Q_{gen} \sim 2\ \text{fm}^{-1}$

NN_{only}
$\hbar\Omega$ = 24 MeV
HO basis

^{4}He: Efficiency Test



- efficiency test: dial same magnitude of induced 3N and compare convergence
- **Q- & HO-block give better convergence** than T_{int} for same induced 3N
- using static block generators ($G_\alpha = G_0$) gives similar results

NN_{only}
$\hbar\Omega$ = 24 MeV
HO basis

HO-block: N_{gen} = 8, α = 0.0625 fm^4 Q-block: Q_{gen} = 2.0 fm^{-1}, α = 0.0625 fm^4
T_{int}: α = 0.01 fm^4

Towards Many-Body Applications

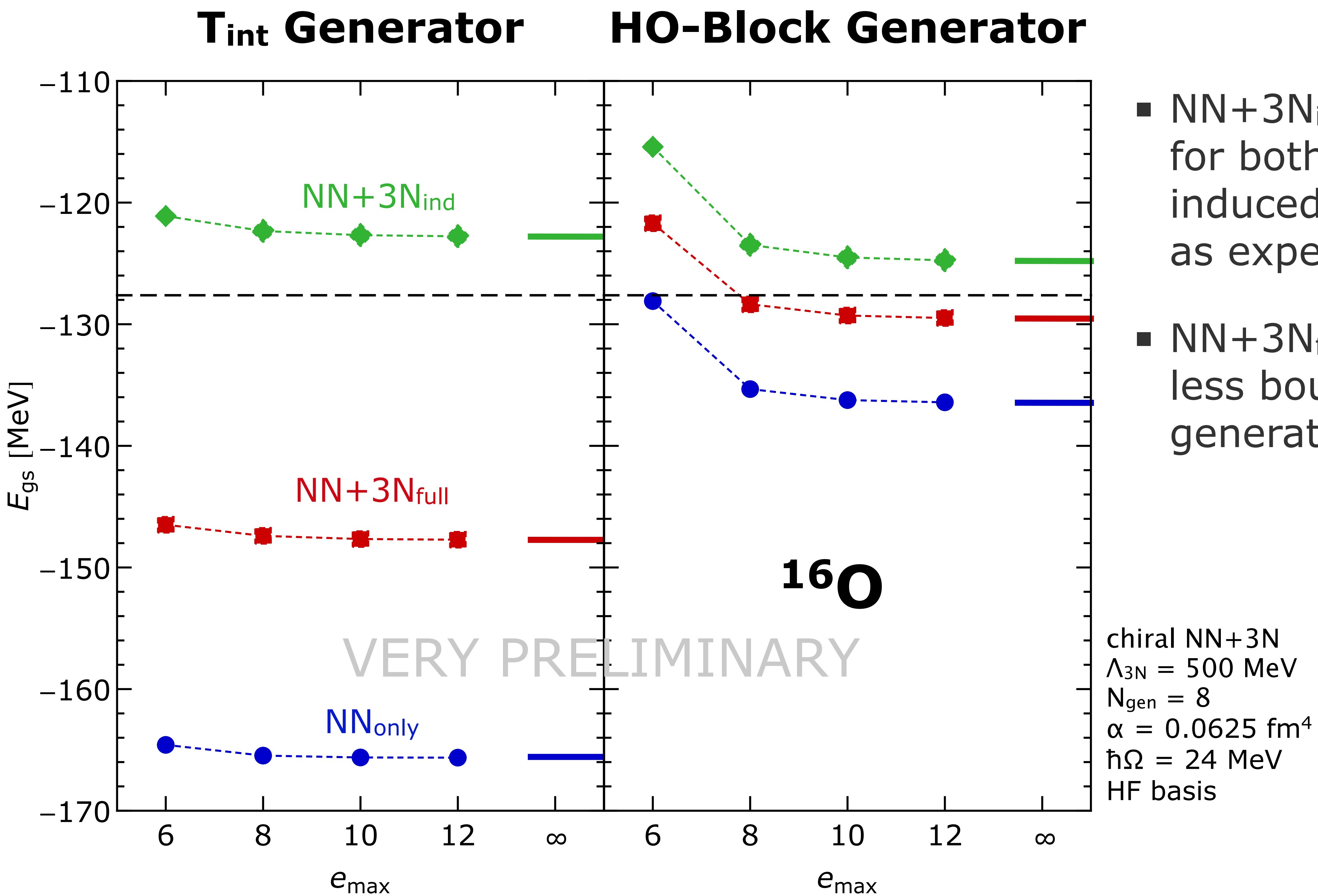
SRG Evolution in 3N

- extension of block generators to SRG evolution in three-body space *rather* straight forward (with static generators)
- careful with embedding and generalisation of scale definition
- first results for HO-block generator available

Many-Body Solution

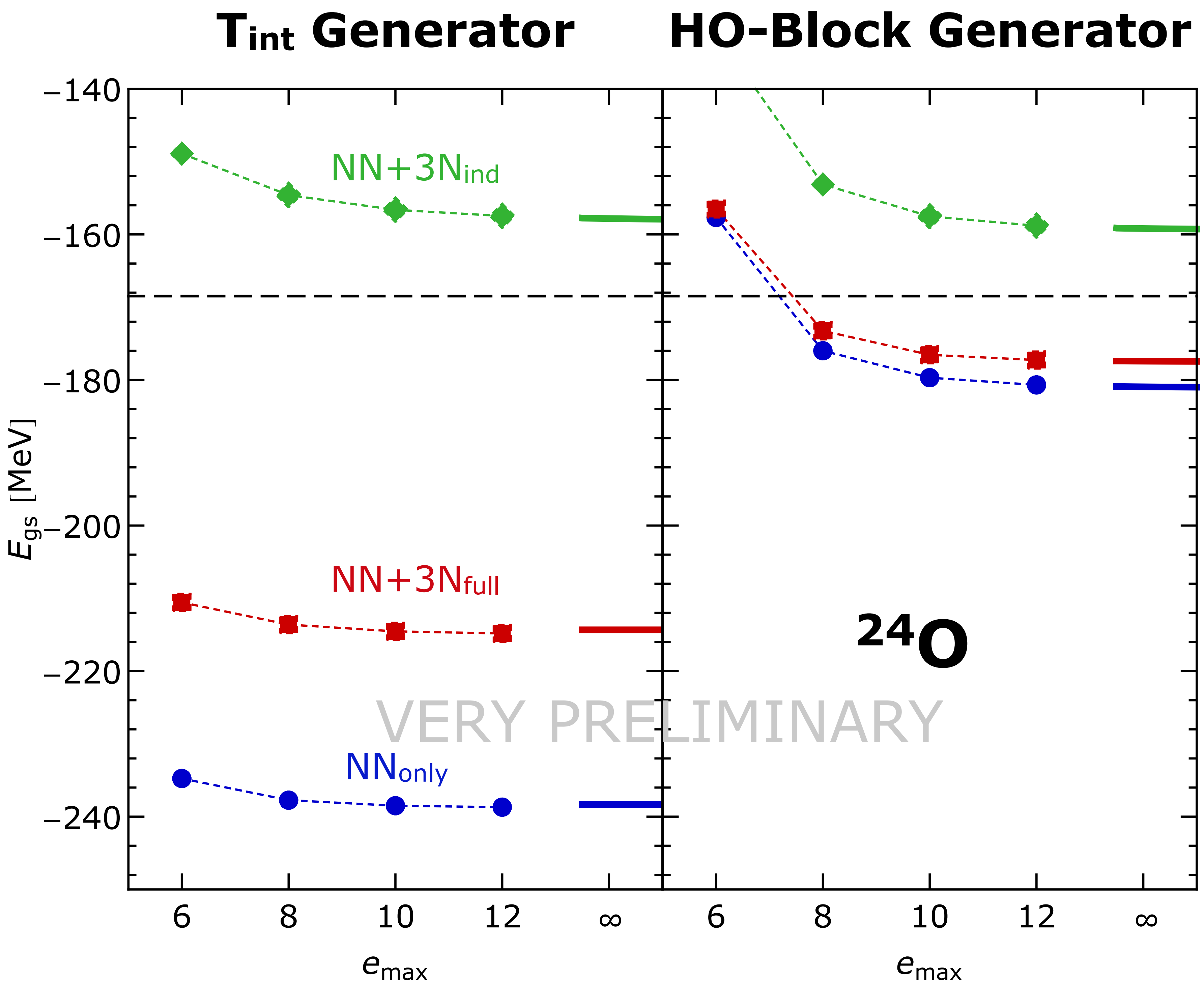
- any many-body approach will do, i.e., not restricted to N_{max} truncated NCSM space
- first results from In-Medium SRG available
- using HF basis and including 3N contributions included in NO2B approximation

IM-SRG Results



- NN+3N$_{ind}$ agrees well for both generators: induced 4N are small as expected
- NN+3N$_{full}$ is much less bound with block generator

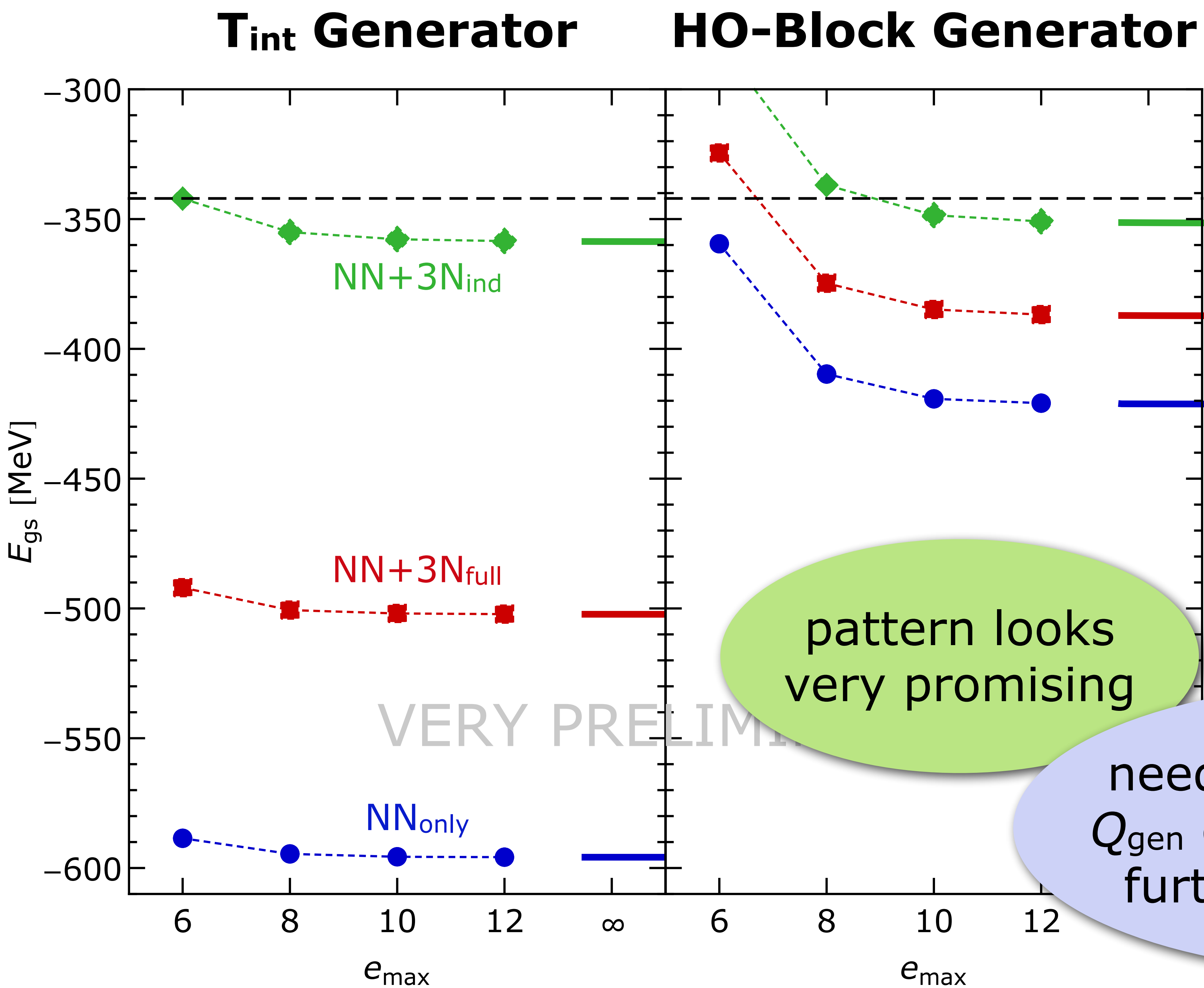
IM-SRG Results



- NN+$3N_{ind}$ agrees well for both generators: induced 4N are small as expected
- NN+$3N_{full}$ is much less bound with block generator

chiral NN+3N
Λ_{3N} = 500 MeV
N_{gen} = 8
α = 0.0625 fm^4
$\hbar\Omega$ = 24 MeV
HF basis

IM-SRG Results



- $NN+3N_{ind}$ agrees well for both generators: induced 4N are small as expected
- $NN+3N_{full}$ is much less bound with block generator

pattern looks very promising

need to study N_{gen} and Q_{gen} dependence and do further IT-NCSM runs

Improved Chiral NN Interactions

with the
LENPIC Collaboration

E. Epelbaum, H. Krebs, U.-G. Meißner, S. Binder, K. Hebeler, J. Langhammer,
J. Golak, R. Skibiński, K. Topolnicki, H. Witała, P. Maris, H. Potter, J. Vary, A. Nogga,
H. Kamada, D. Furnstahl, V. Bernard, A. Calci

Improved Chiral NN Interactions

- family of improved chiral NN interactions from LO to N4LO with (semi)local regulators [talk by Hermann Krebs]

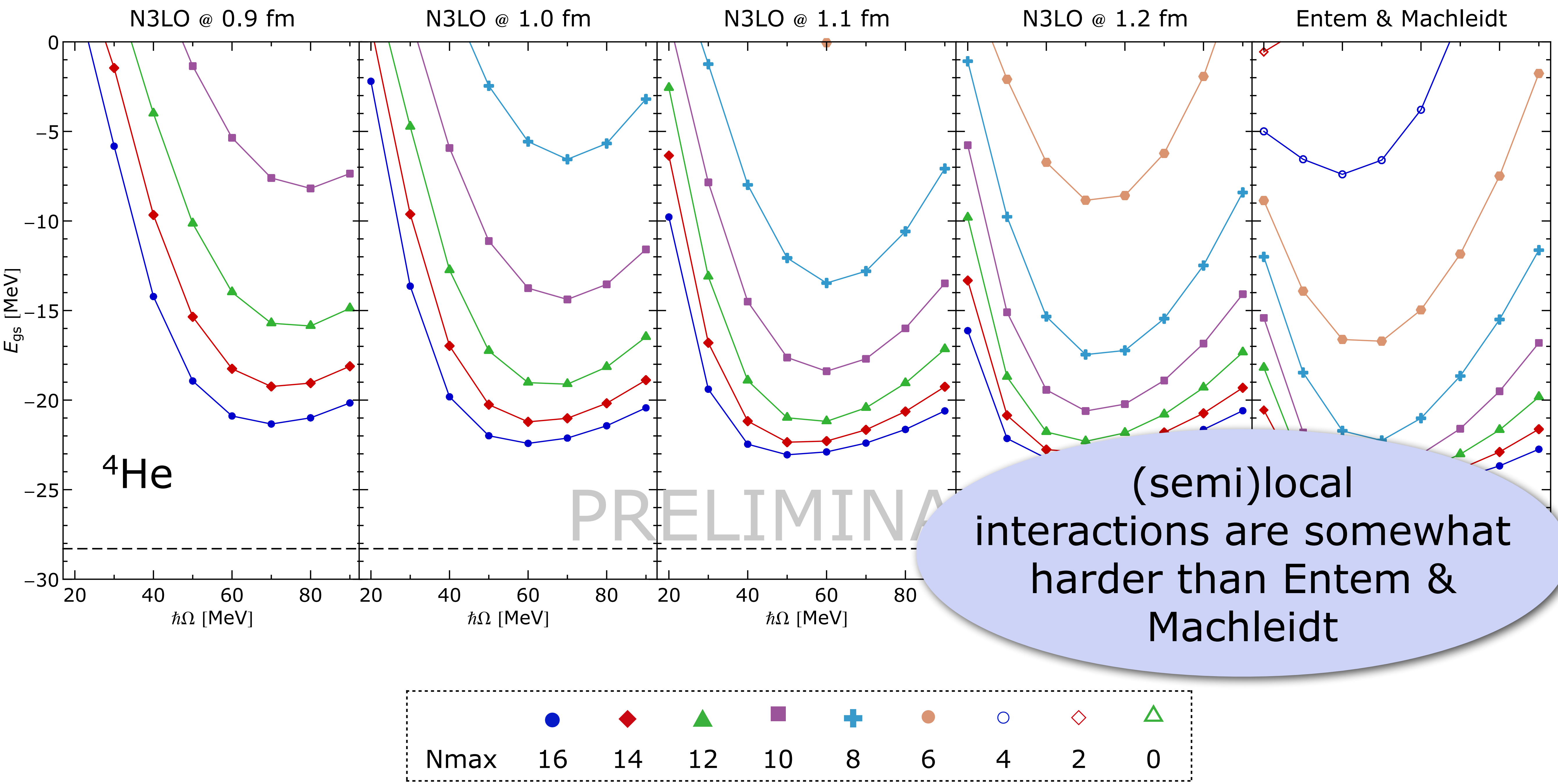
  Epelbaum, Krebs, Meißner, arXiv:1412.0142 & 1412.4623

- matrix elements of corresponding 3N interactions up to N3LO are being generated [talk by Kai Hebeler]

- initial **questions from many-body perspective**:
  - how do (semi)local regulators affect convergence?
  - what is the order-by-order systematics of observables and convergence?
  - uncertainty estimation from order-by-order at fixed cutoff feasible?
  - do the interactions behave well under SRG transformation?

^{4}He: Cutoff Dependence @ N3LO

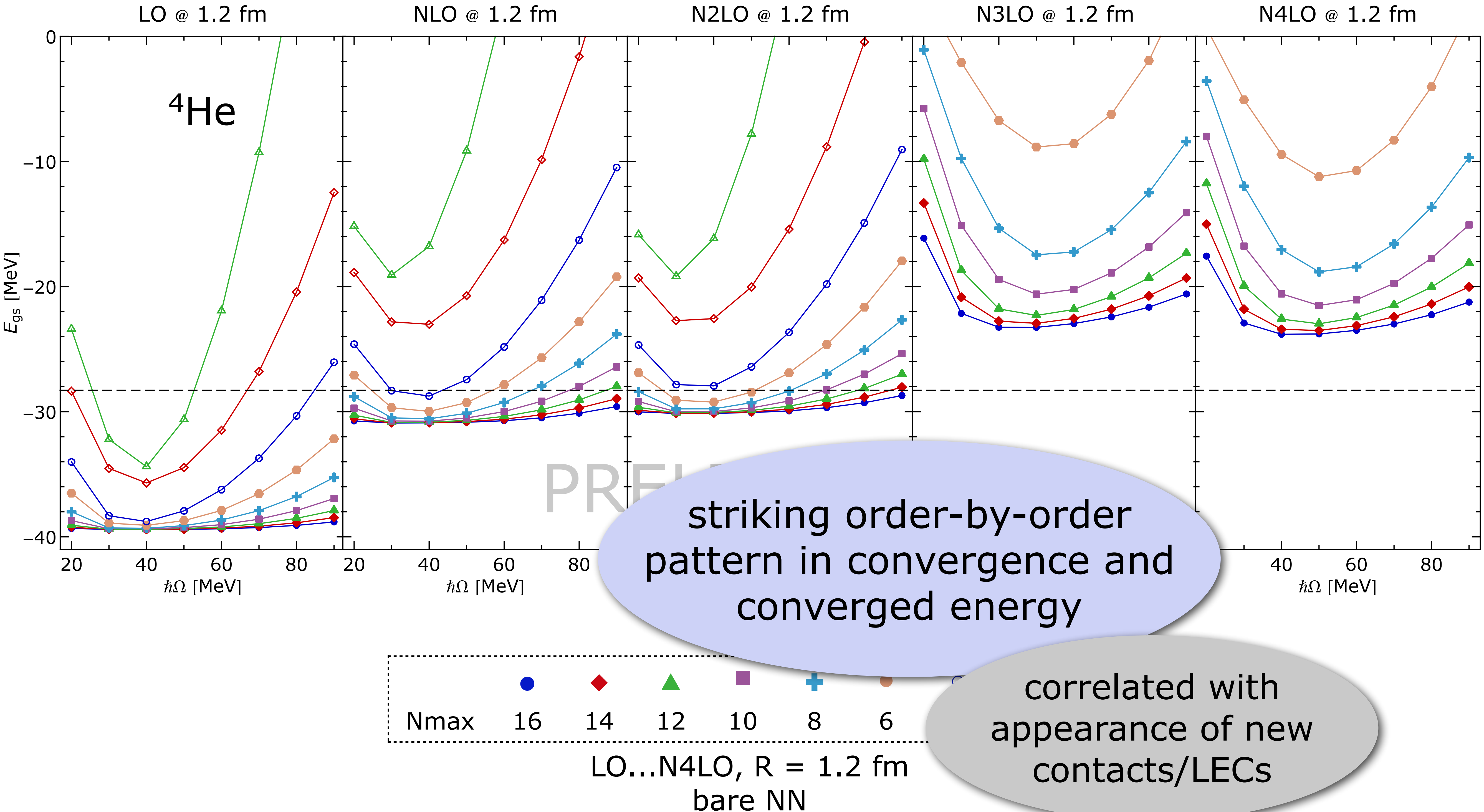
LENPIC Collaboration, in prep.



N3LO, R = 0.9...1.2 fm
bare NN

^{4}He: Order-by-Order @ 1.2 fm

LENPIC Collaboration, in prep.



striking order-by-order pattern in convergence and converged energy

correlated with appearance of new contacts/LECs

Epilogue

- **thanks to my group and my collaborators**
  - J. Braun, E. Gebrerufael, T. Hüther, J. Langhammer, S. Schulz, H. Spiess, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
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    Oak Ridge National Laboratory
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    NSCL / Michigan State University
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    Iowa State University
  - S. Quaglioni, G. Hupin
    Lawrence Livermore National Laboratory
  - E. Epelbaum, H. Krebs & the LENPIC Collaboration
    Universität Bochum, ...

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EDISON — NERSC

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