

Exotic Nuclei and Beyond

- An Ab Initio Theory Perspective -

Robert Roth

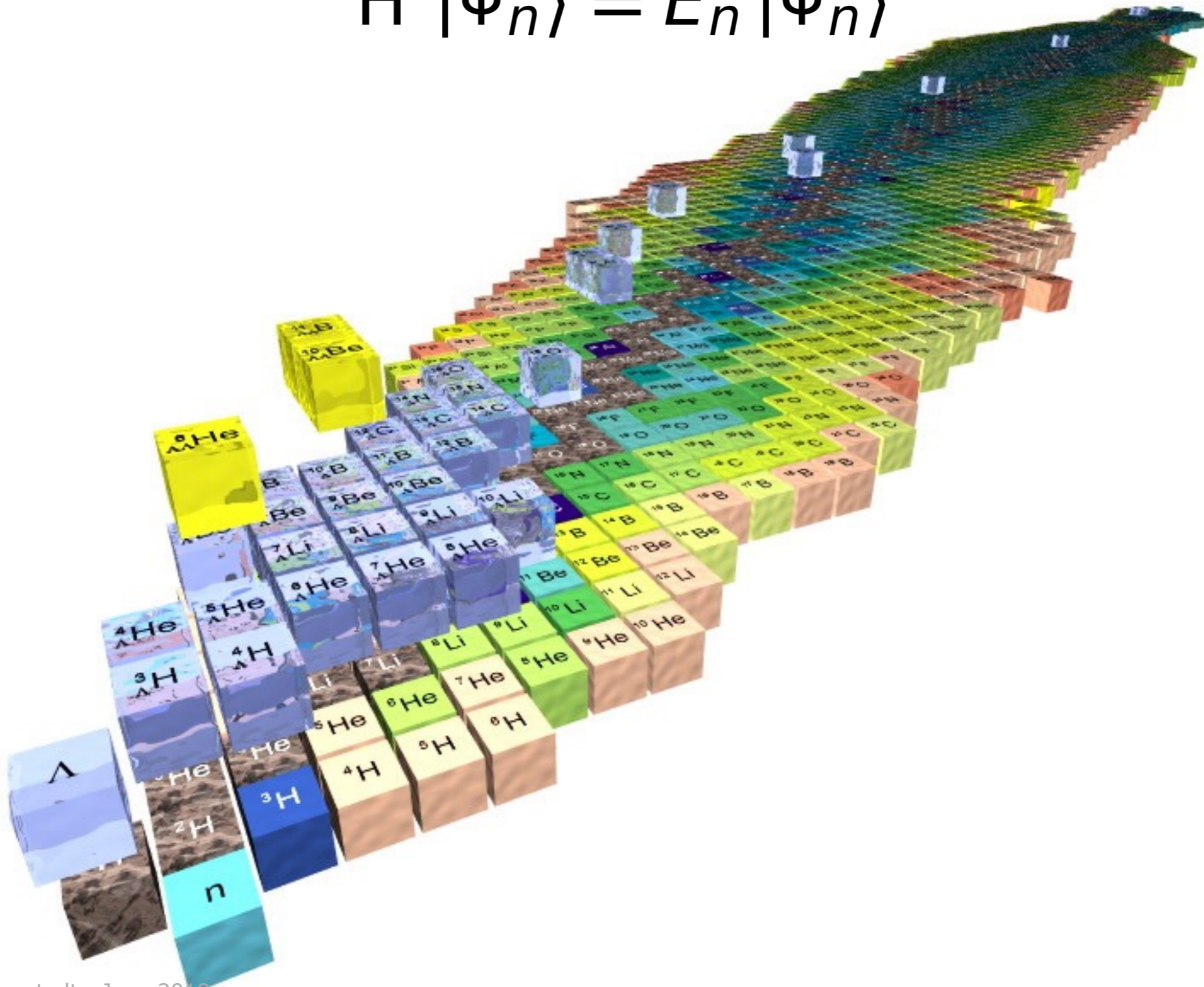


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Ab Initio Nuclear Structure Theory

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



Ab Initio Nuclear Structure Theory

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

**solve nuclear many-body problem
based on realistic interactions
using controlled and improvable truncations
with quantified theoretical uncertainties**

Ab Initio Nuclear Structure Theory

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

What is the nuclear Hamiltonian?

nuclear forces,
chiral effective field theory,
three-body interactions,
consistency and convergence,...

What about these many-body states?

degrees of freedom,
Hilbert space and truncations,
single-particle basis,
bound states vs. continuum,...

How to solve this equation?

large-scale diagonalization,
decoupling approaches,
truncations and convergence,
uncertainty quantification...

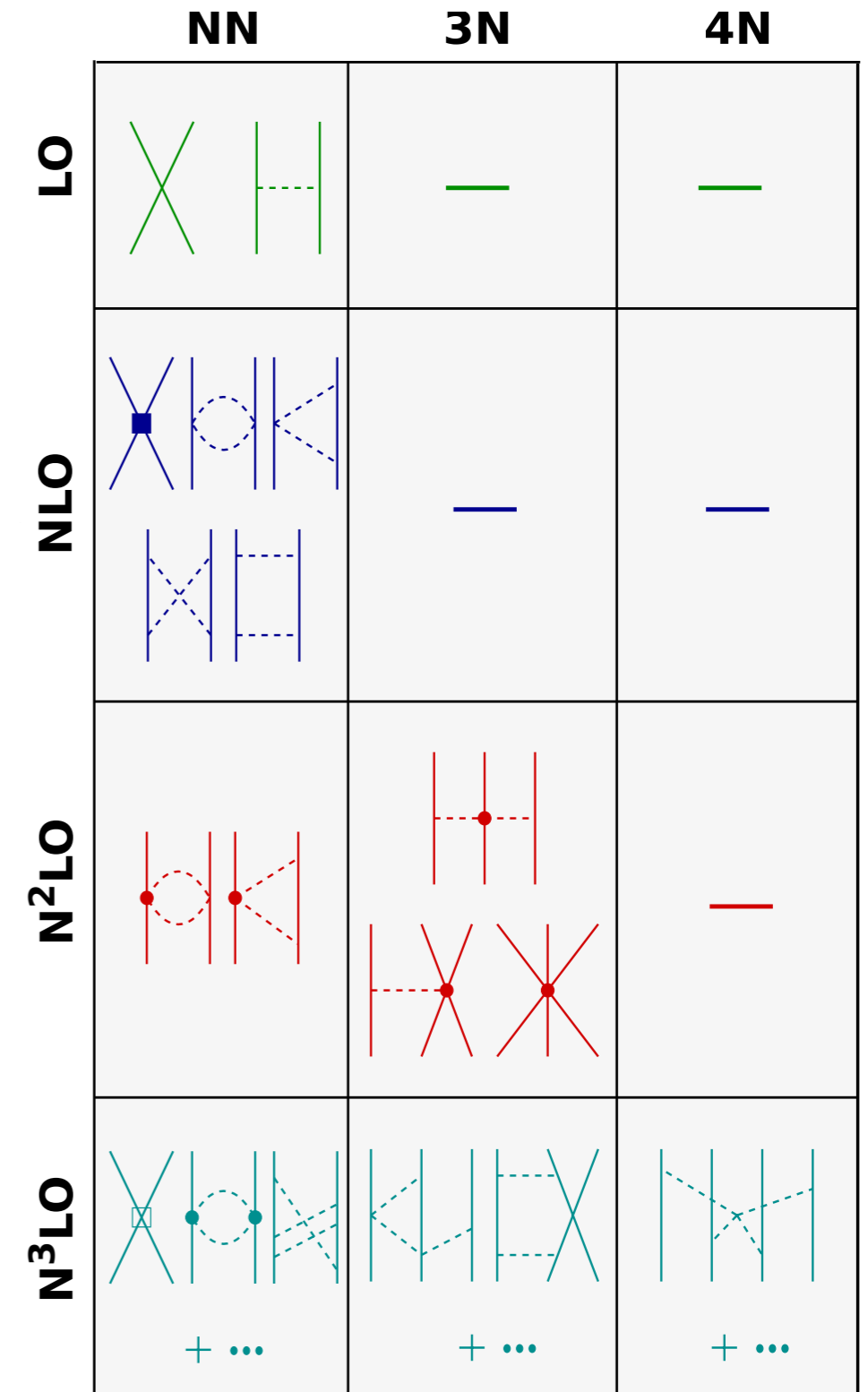
Hamiltonian

$$H = T - T_{\text{cm}} + V_{\text{NN}} + V_{\text{3N}} + \dots$$

Nuclear Interactions from Chiral EFT

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

- low-energy **effective field theory** for relevant degrees of freedom (π, N) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- hierarchy of **consistent NN, 3N, 4N, ...** interactions and electroweak operators
- many **recent developments**
 - improved NN up to N4LO+
 - 3N interaction up to N3LO
 - 4N interaction at N3LO
 - improved fits and error analysis
 - order-by-order uncertainty quantification



Ab Initio Nuclear Structure Theory

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Unitary Transformations



ELSEVIER

Nuclear Physics A 632 (1998) 61–95

NUCLEAR
PHYSICS A

A unitary correlation operator method

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Received 22 September 1997; accepted 12 December 1997

Abstract

The short range repulsion between nucleons is treated by a unitary correlation operator which shifts the nucleons away from each other whenever their uncorrelated positions are within the repulsive core. By formulating the correlation as a transformation of the relative distance between particle pairs, general analytic expressions for the correlated wave functions and correlated op-

Unitary Transformations

- eigenvalue problem of H and expectation value of observable O

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle \qquad O_n = \langle \Psi_n | O | \Psi_n \rangle$$

- invent a **unitary operator U** with $U U^\dagger = 1$ and use it

$$U^\dagger H U U^\dagger |\Psi_n\rangle = E_n U^\dagger |\Psi_n\rangle \qquad O_n = \langle \Psi_n | U U^\dagger O U U^\dagger | \Psi_n \rangle$$

- identify **transformed operators and states** and rewrite equations

$$|\tilde{\Psi}_n\rangle = U^\dagger |\Psi_n\rangle, \quad \tilde{H} = U^\dagger H U, \quad \tilde{O} = U^\dagger O U$$

$$\tilde{H} |\tilde{\Psi}_n\rangle = E_n |\tilde{\Psi}_n\rangle \qquad O_n = \langle \tilde{\Psi}_n | \tilde{O} | \tilde{\Psi}_n \rangle$$

Unitary Transformations

- eigenvalue problem of H and expectation value of observable O

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

$$O_n = \langle \Psi_n | O | \Psi_n \rangle$$

- in many-body systems, unitary transformations change the structure of the Hamiltonian and the many-body states without changing the observables

1 and use it

$$O_n = \langle \Psi_n | U U^\dagger O U U^\dagger | \Psi_n \rangle$$

- identify **transformed operator**

design a unitary transformation that simplifies the solution of the many-body problem

$$|\tilde{\Psi}_n\rangle = U^\dagger |\Psi_n\rangle, \quad \tilde{H} = U^\dagger H U, \quad \tilde{O} = U^\dagger O U$$

$$\tilde{H} |\tilde{\Psi}_n\rangle = E_n |\tilde{\Psi}_n\rangle$$

$$O_n = \langle \tilde{\Psi}_n | \tilde{O} | \tilde{\Psi}_n \rangle$$

Korrelierte Wellenfunktion (Index l m weggelassen)

$$r X(x) = \left(\frac{dR_-}{dx} \right)^{1/2} R_-(x) \psi(R_-(x))$$

$$\left. \begin{aligned} R_-(x) &:= R(Y(x)-1) \\ R_+(r) &:= R(Y(r)+1) \end{aligned} \right\} \leadsto \begin{cases} R_-(R_+(r)) = r \\ R_+(R_-(x)) = x \end{cases} \quad R_+ \text{ invers zu } R_- \quad \checkmark$$

$$\left. \begin{aligned} R'_-(x) &:= \frac{dR_-(x)}{dx} = \frac{S(R_-(x))}{S(x)} \\ R'_+(r) &:= \frac{dR_+(r)}{dr} = \frac{S(R_+(r))}{S(r)} \end{aligned} \right\} \leadsto R'_-(x) = \frac{1}{R'_+(r)} \quad \text{wobei } r = R_-(x)$$

Koordinatentransformation:

$$r = R_-(x)$$

$$x = R_+(r) \quad dx = R'_+(r) dr \quad ; \quad \frac{d}{dx} = \frac{1}{R'_+(r)} \frac{d}{dr}$$

Unitary Correlation Operator Method

Feldmeier, Neff, Roth, Schnack,...

unitary transformation designed to imprint central and tensor correlations into nuclear many-body states

- **explicit ansatz for unitary operator** with central and tensor correlations

$$U = C_{\Omega} C_r = \exp\left(-i \sum_{j < k} g_{\Omega, jk}\right) \exp\left(-i \sum_{j < k} g_{r, jk}\right)$$

- **central correlations**: generated by distance-dependent shift in the relative coordinate of a nucleon pair

$$g_r = \frac{1}{2} [s(r) q_r + q_r s(r)] \quad q_r = \frac{1}{2} \left[\frac{\vec{r}}{r} \cdot \vec{q} + \vec{q} \cdot \frac{\vec{r}}{r} \right]$$

- **tensor correlations**: alignment of spatial orientation of nucleon pair depending on spin direction and orientation

$$g_{\Omega} = \frac{3}{2} \vartheta(r) \left[(\vec{\sigma}_1 \cdot \vec{q}_{\Omega})(\vec{\sigma}_2 \cdot \vec{r}) + (\vec{q}_{\Omega} \leftrightarrow \vec{r}) \right] \quad \vec{q}_{\Omega} = \vec{q} - \frac{\vec{r}}{r} q_r$$

Similarity Renormalization Group

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

continuous unitary transformation of Hamiltonian towards diagonal form with respect to uncorrelated basis

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

$$H_\alpha = U_\alpha^\dagger H U_\alpha \quad O_\alpha = U_\alpha^\dagger O U_\alpha$$

- evolution equations for H_α and U_α with continuous **flow parameter α**

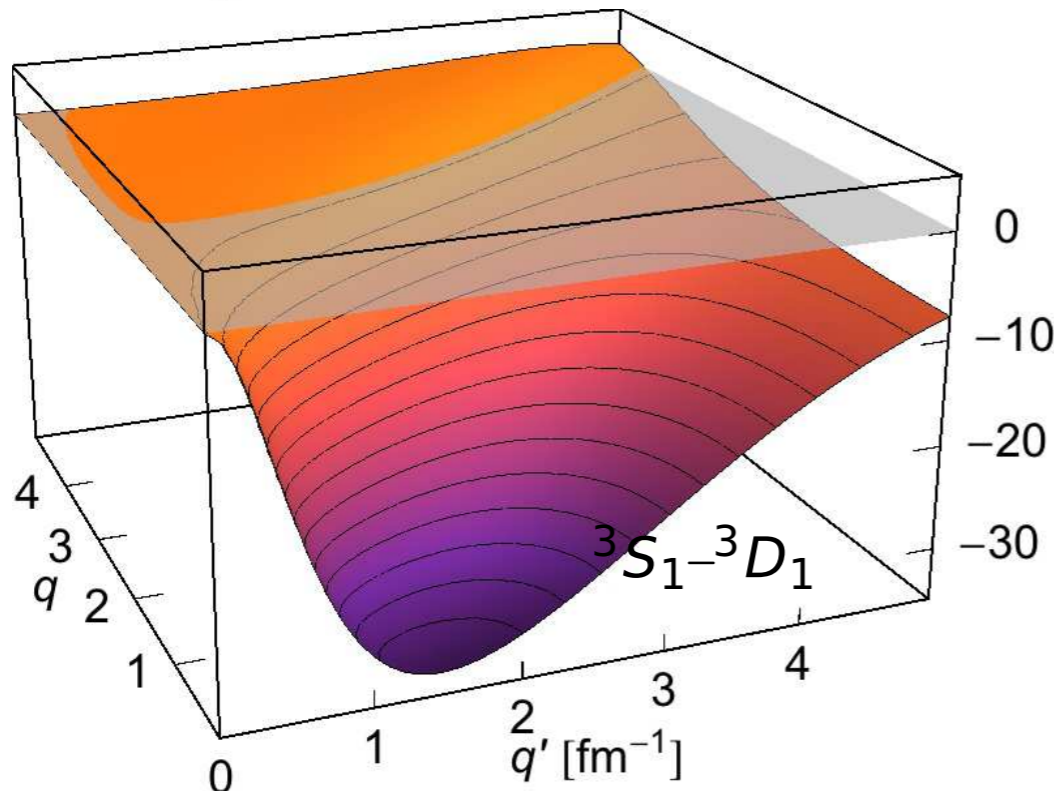
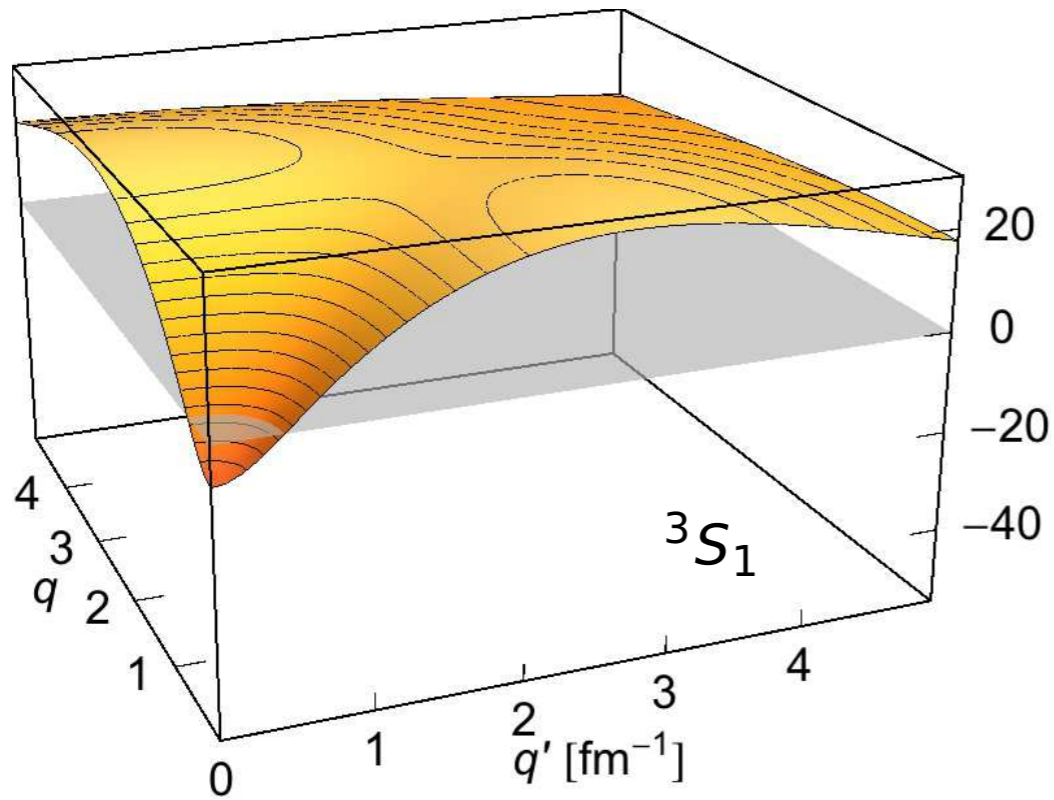
$$\frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \quad \frac{d}{d\alpha} O_\alpha = [\eta_\alpha, O_\alpha] \quad \frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha$$

- physics-guided choice **dynamic generator η_α** , e.g. for momentum pre-diagonalization

$$\eta_\alpha = (2\mu)^2 [T_{\text{int}}, H_\alpha]$$

SRG Evolution in Two-Body Space

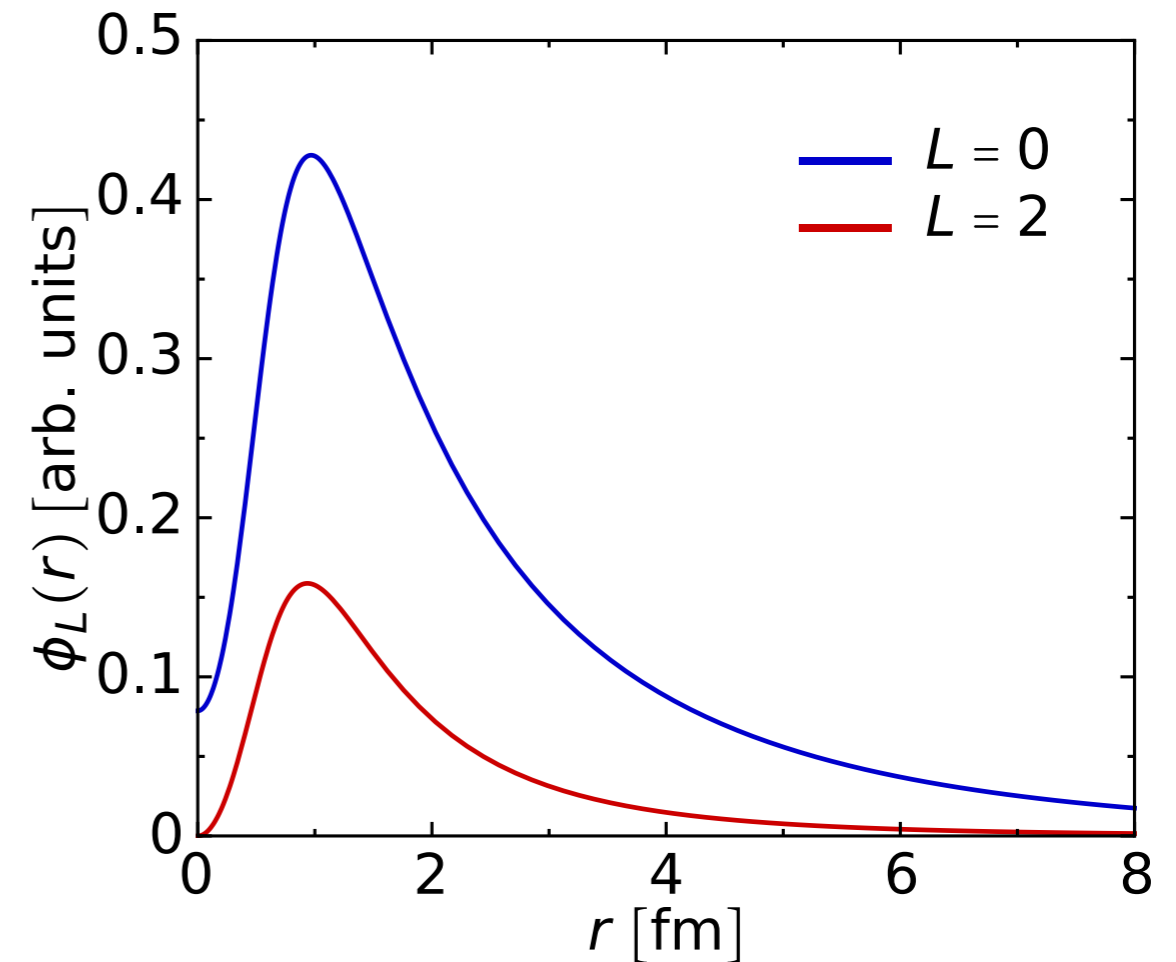
momentum-space matrix elements



Argonne V18

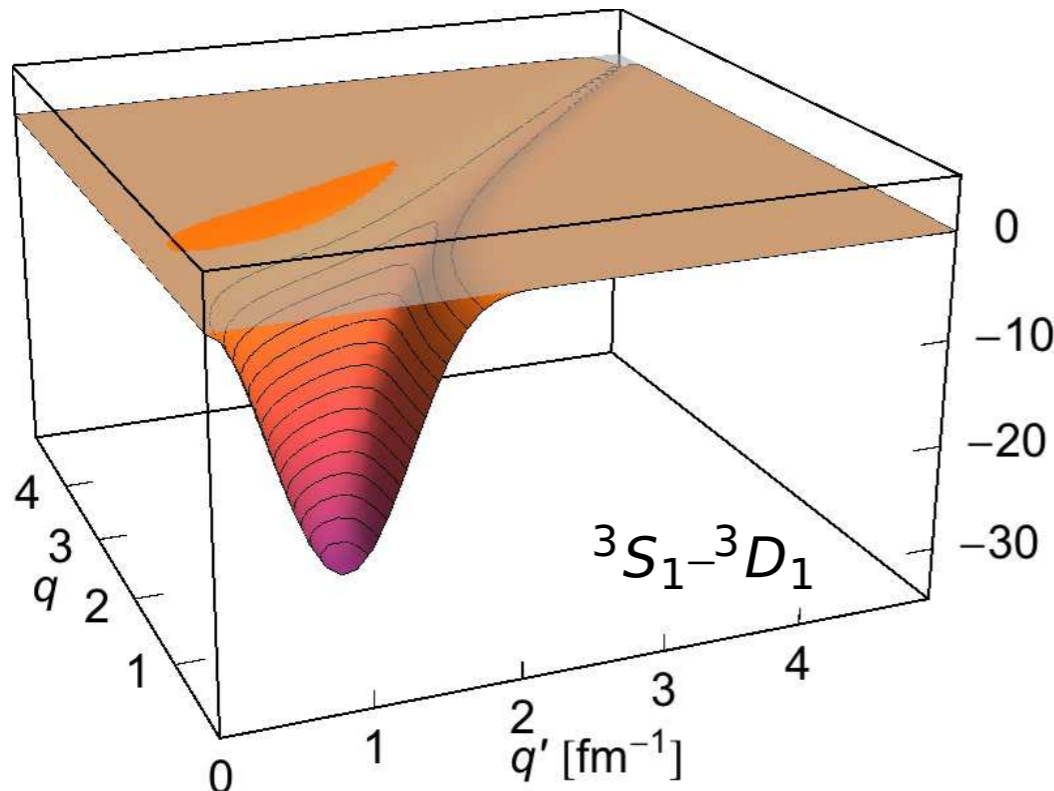
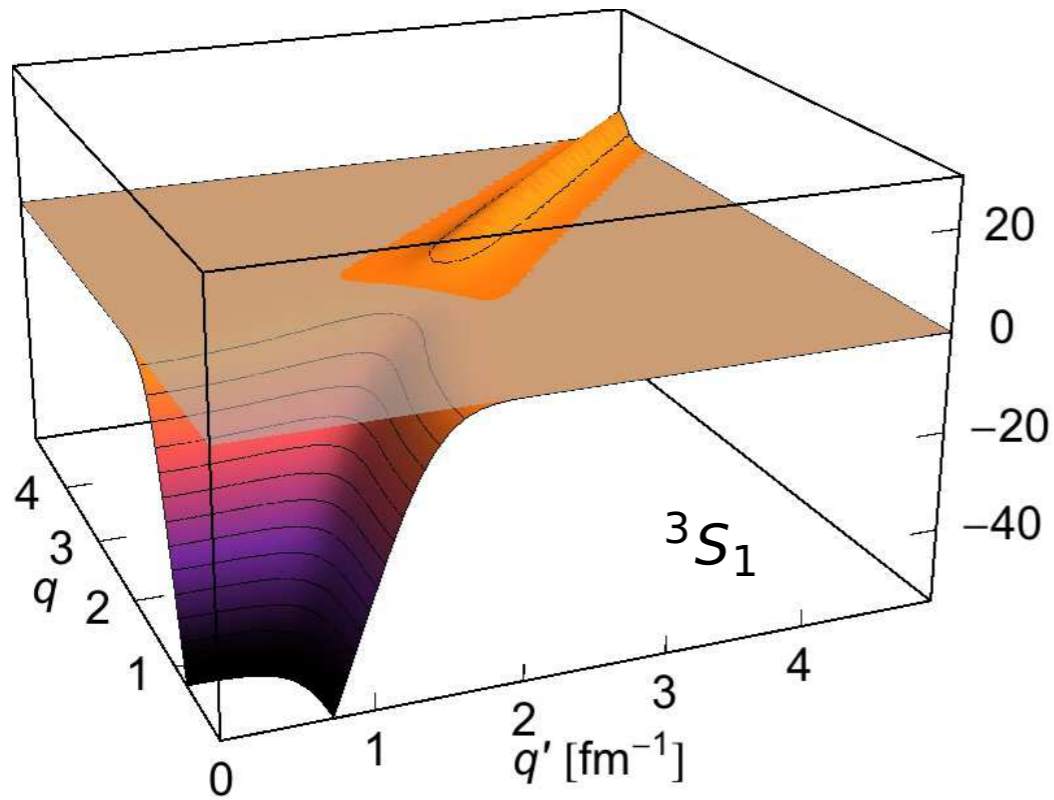
$$J^\pi = 1^+, T = 0$$

deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements

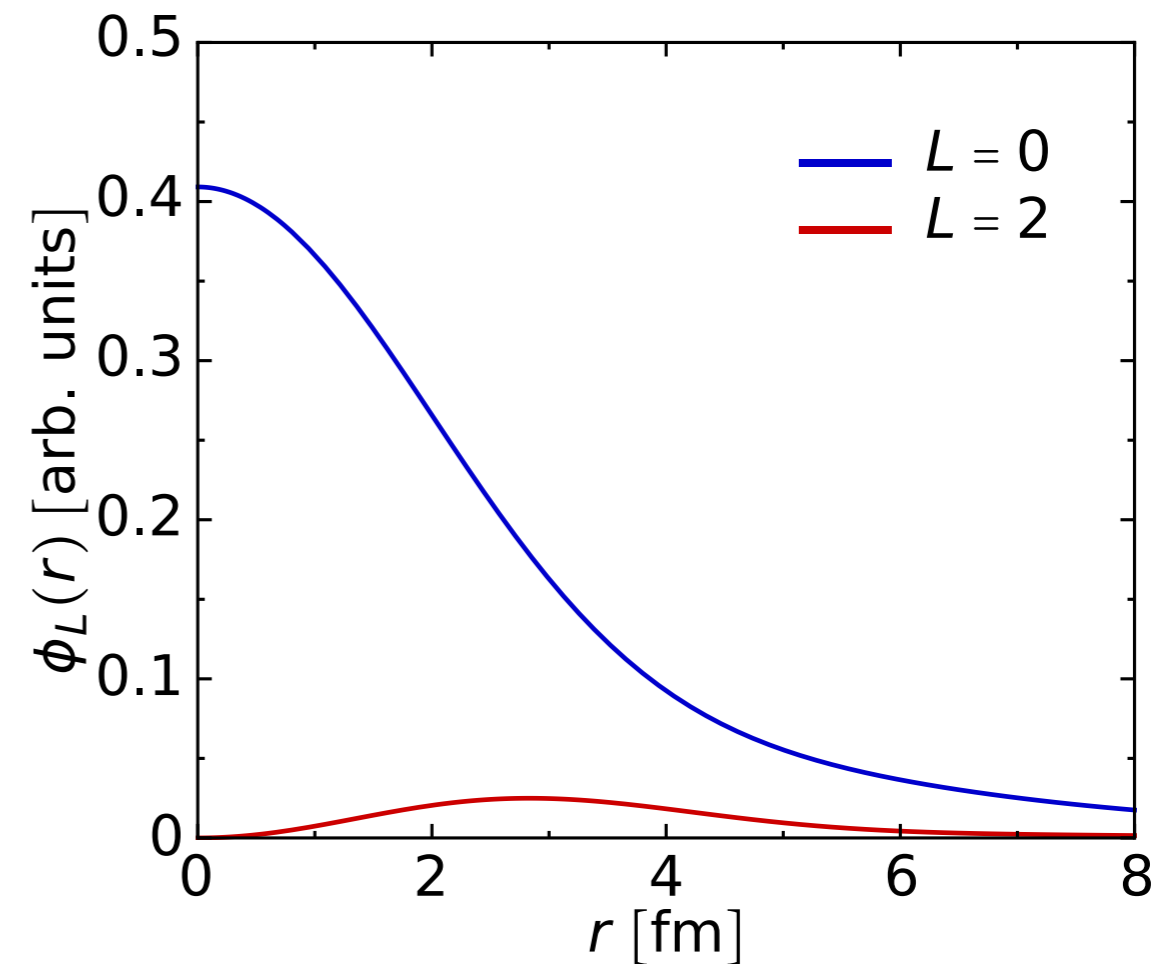


$$\alpha = 0.320 \text{ fm}^4$$

$$\Lambda = 1.33 \text{ fm}^{-1}$$

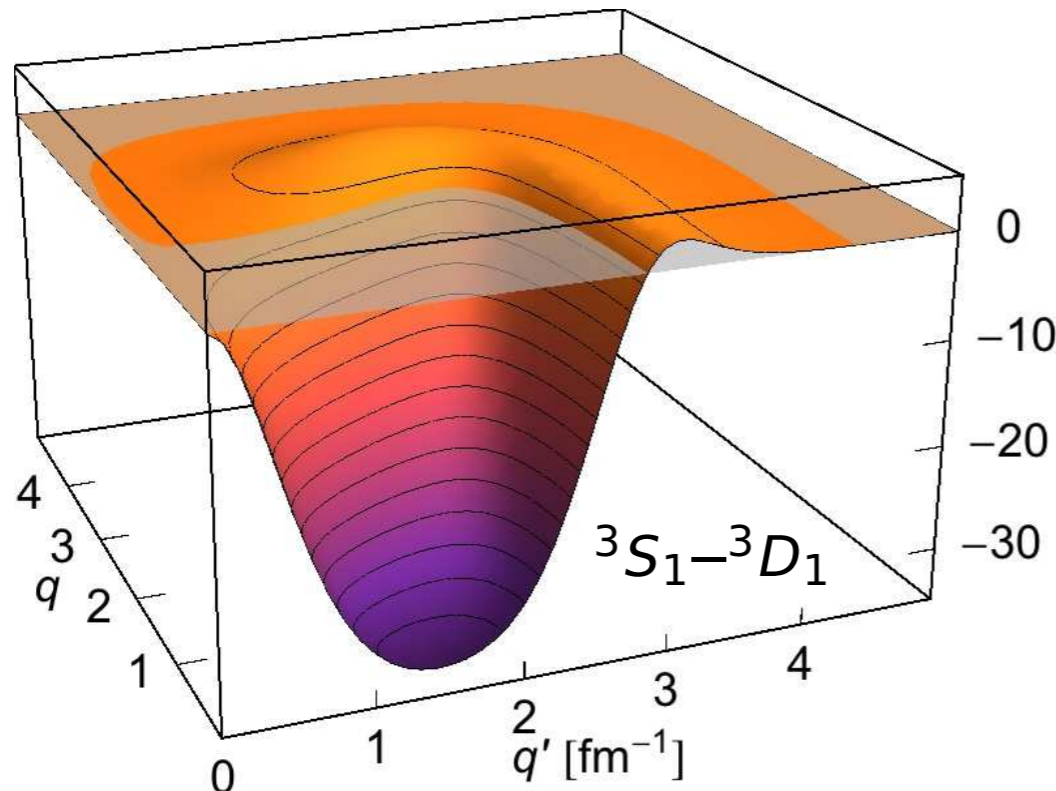
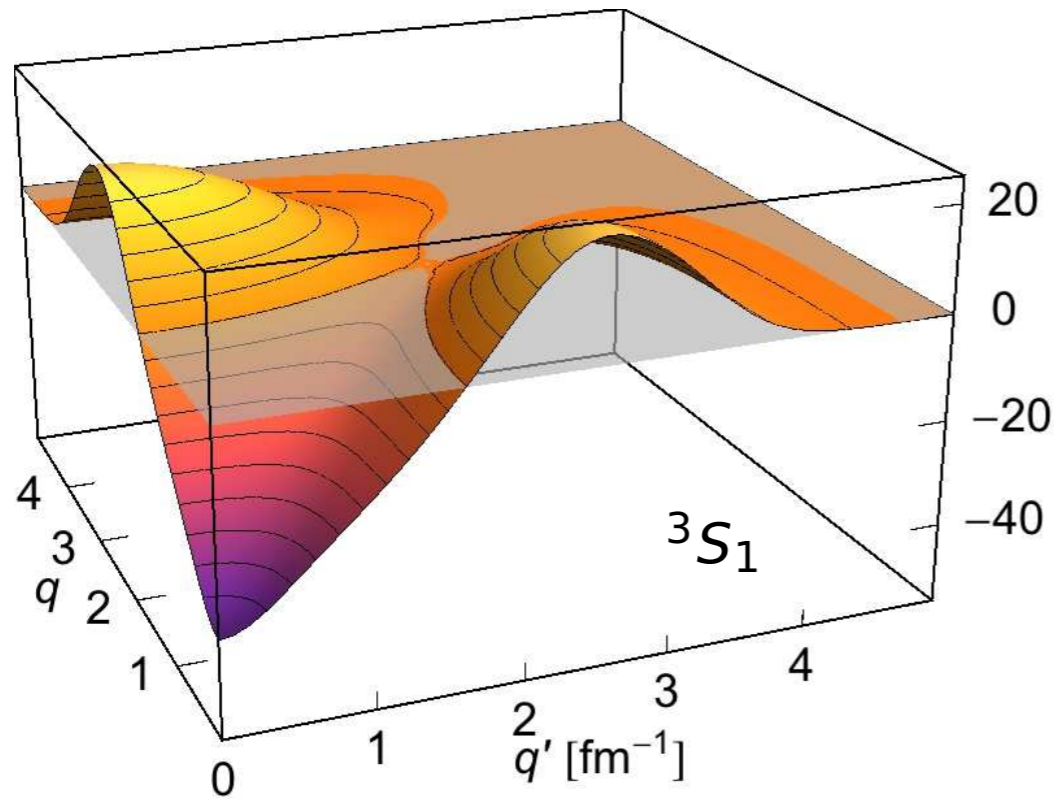
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SRG Evolution in Two-Body Space

momentum-space matrix elements

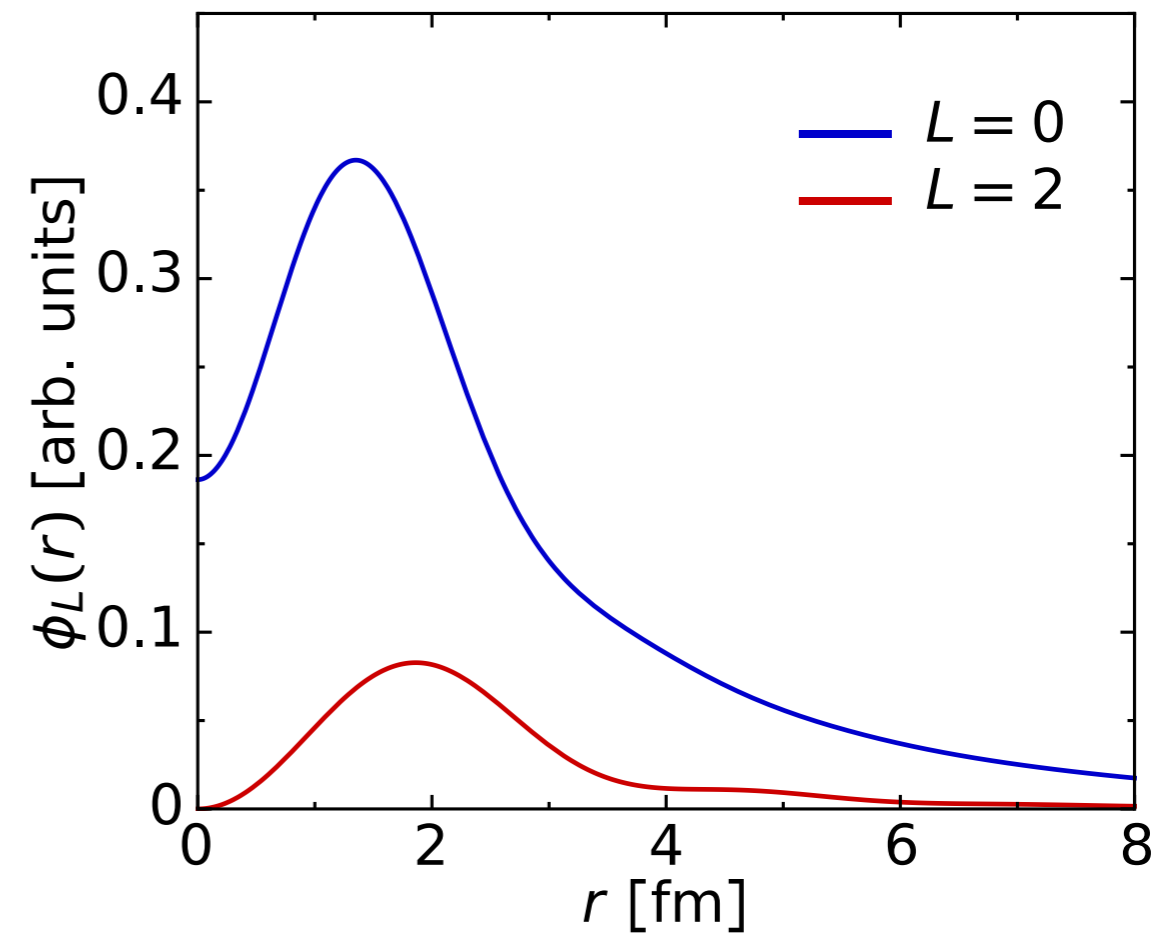


chiral NN

Entem & Machleidt. N 3 LO, 500 MeV

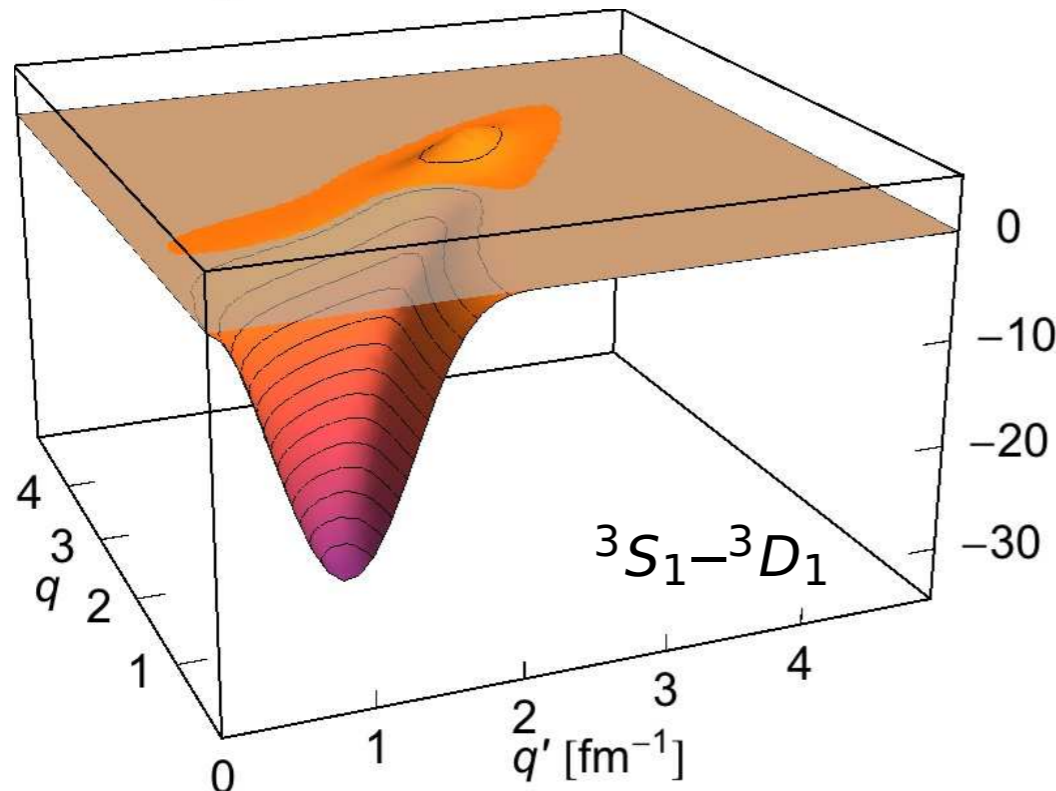
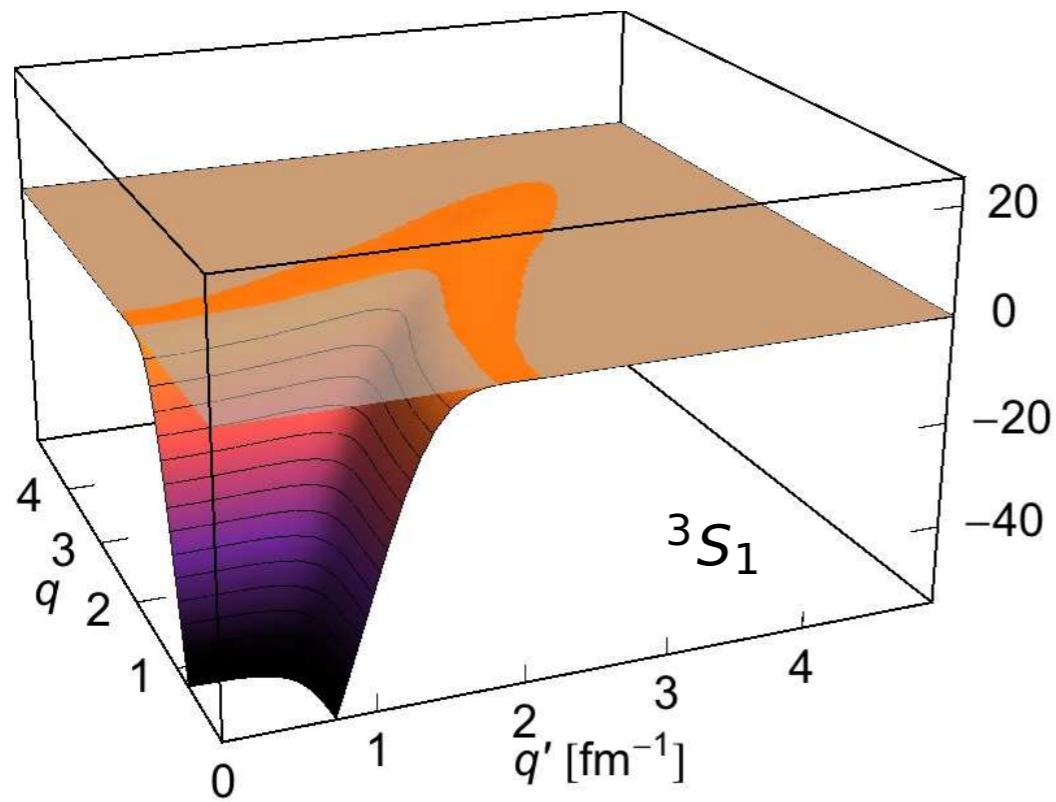
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SRG Evolution in Two-Body Space

momentum-space matrix elements

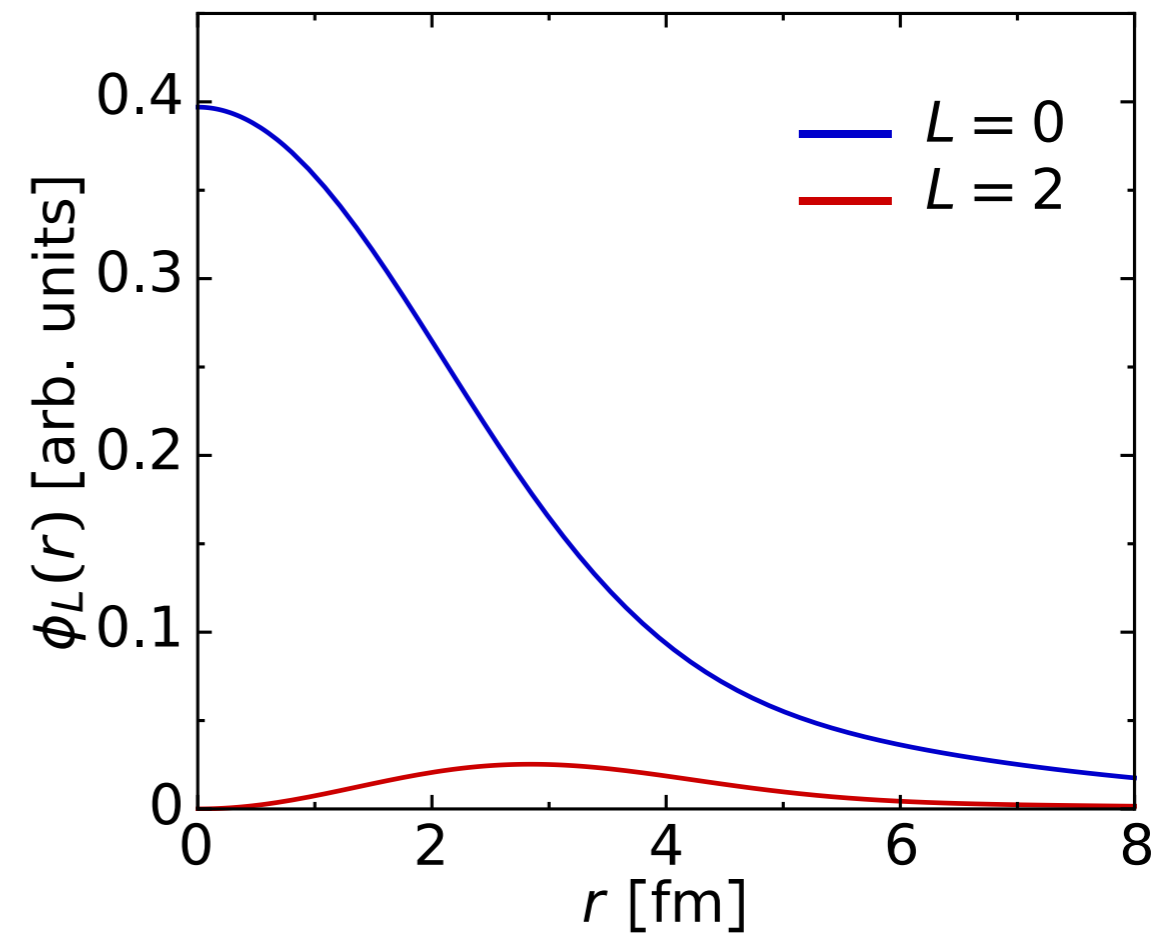


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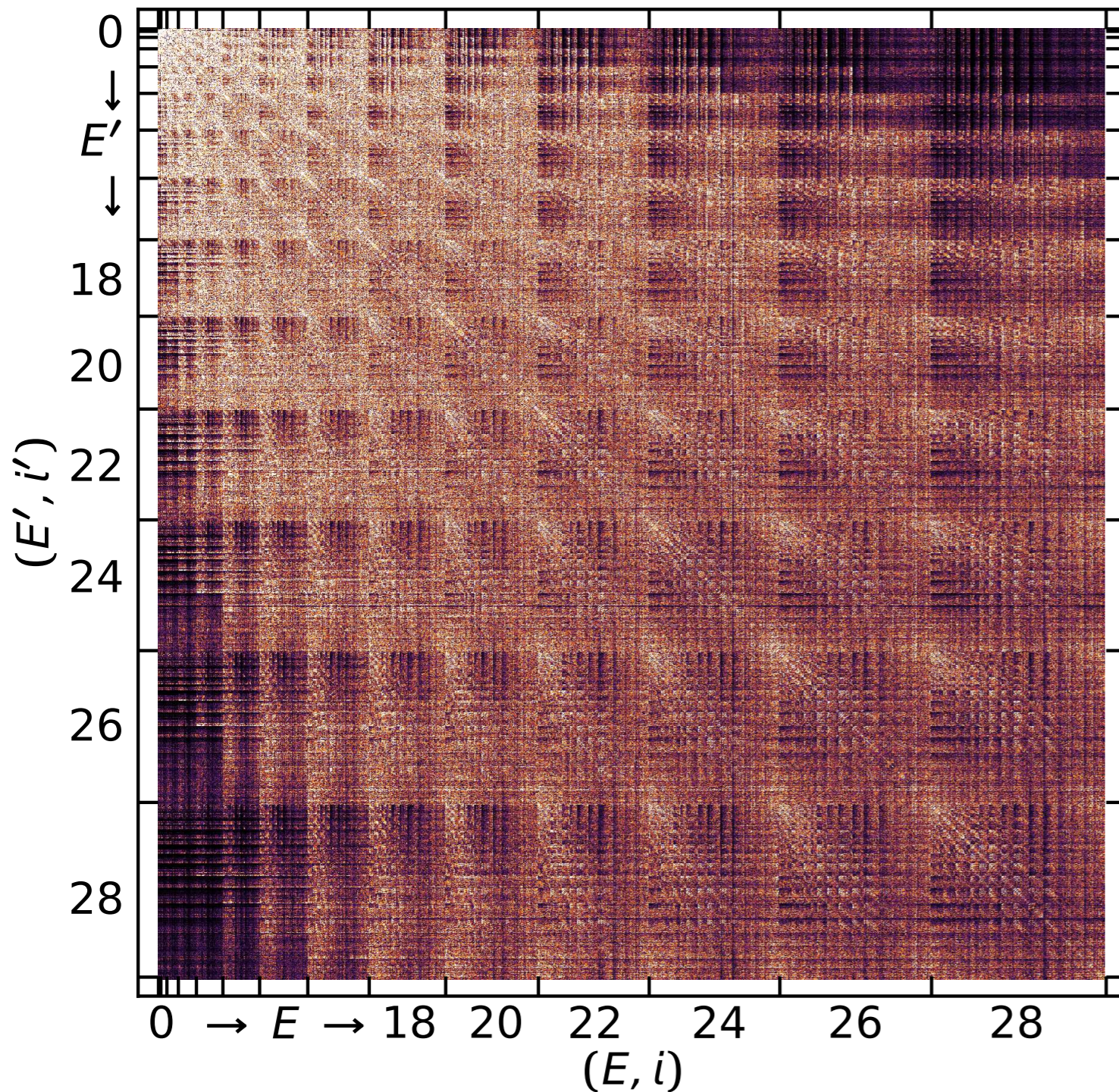
$$J^\pi = 1^+, T = 0$$

deuteron wave-function



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

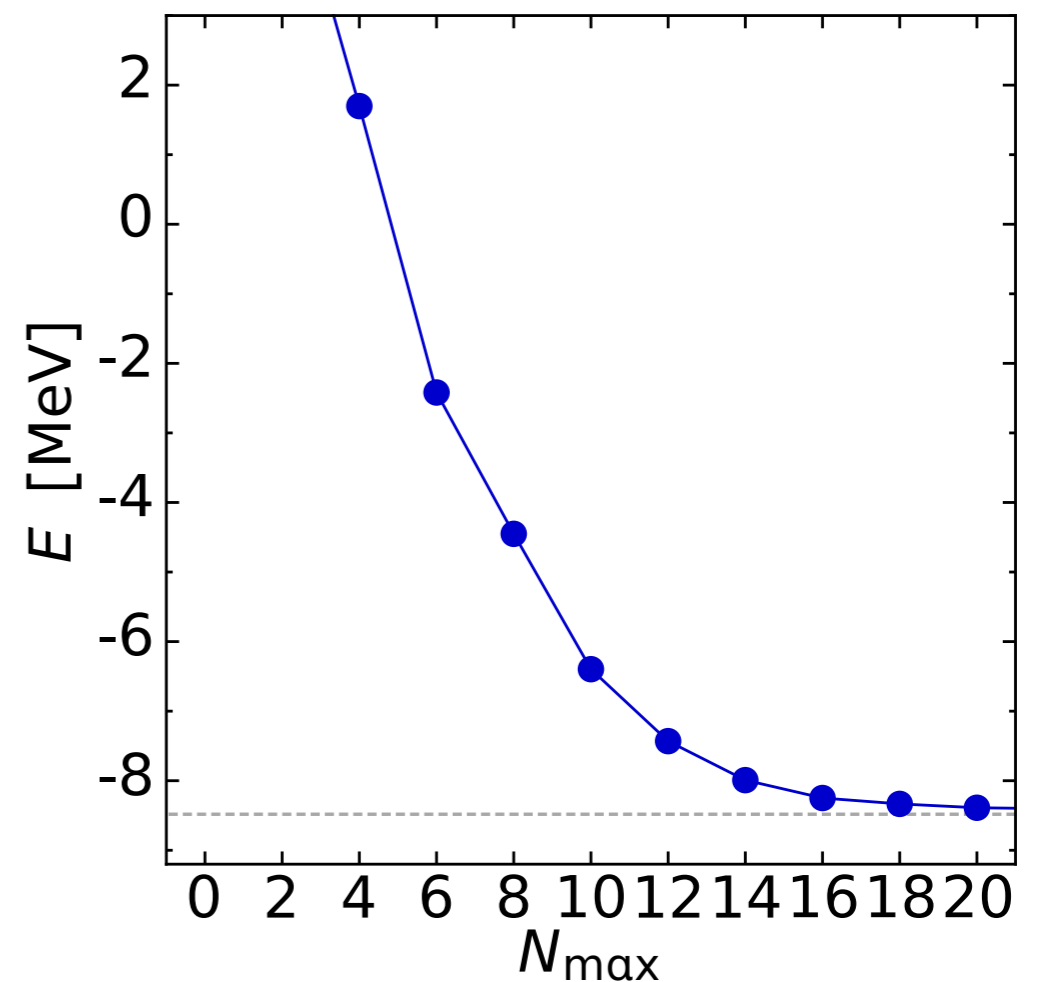


chiral NN+3N

$N^3\text{LO} + N^2\text{LO}$, triton-fit, 500 MeV

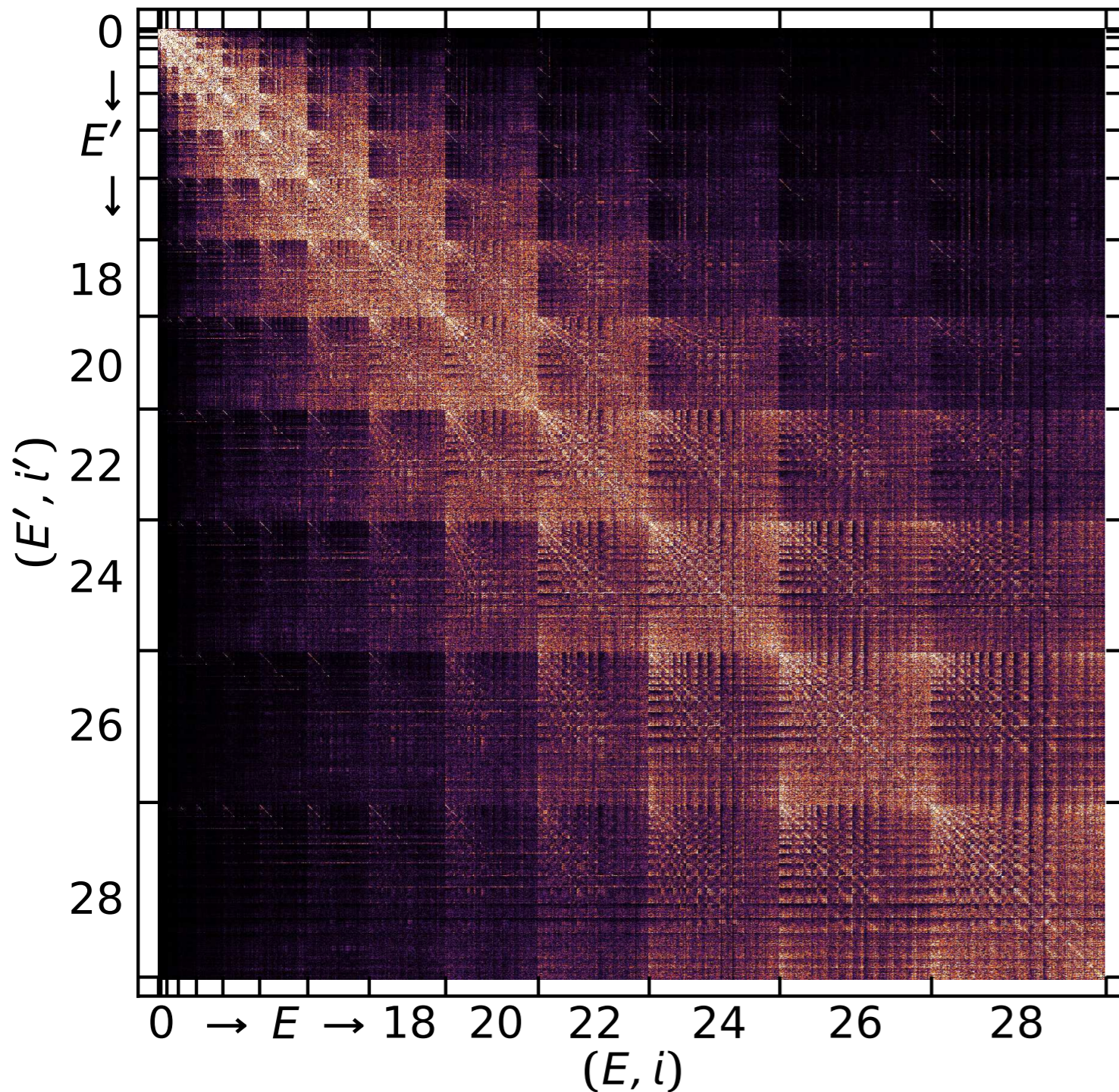
$$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV}$$

NCSM ground state ${}^3\text{H}$



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

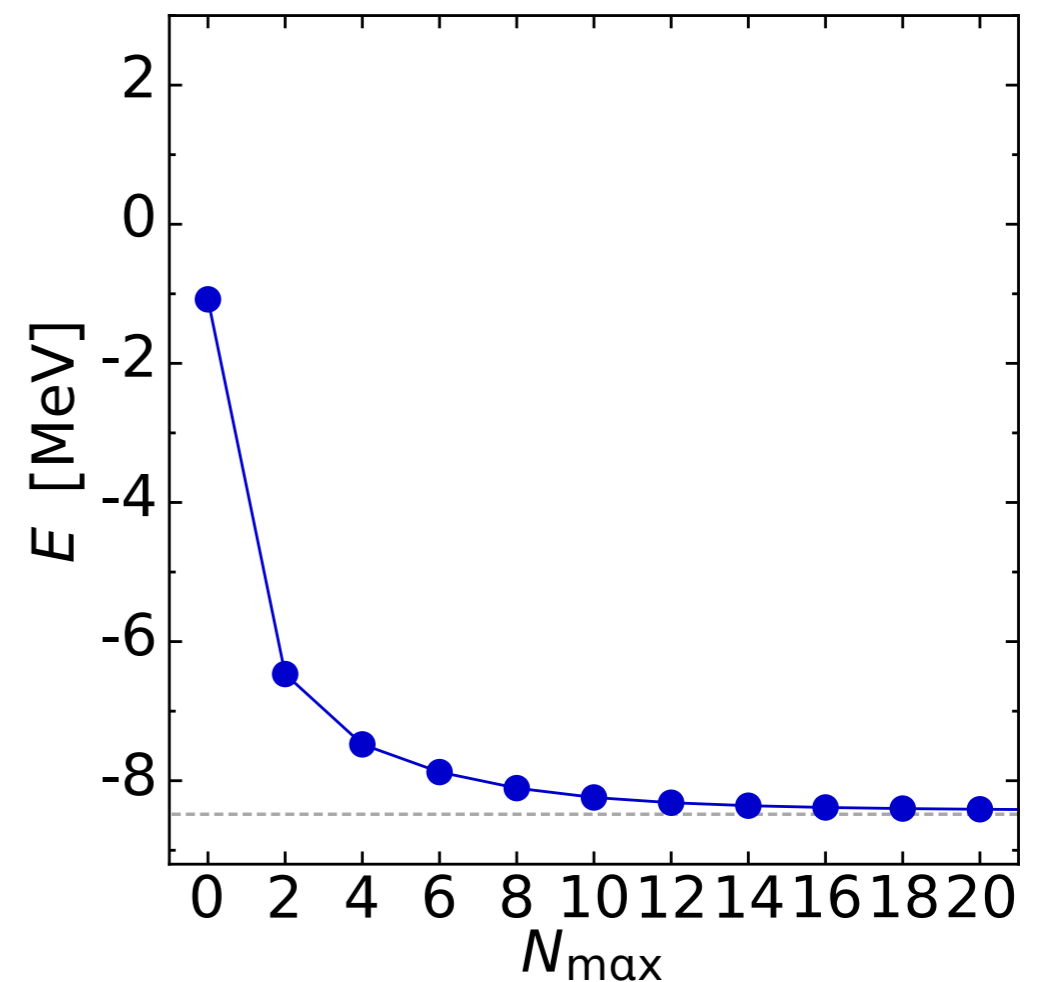


$$\alpha = 0.320 \text{ fm}^4$$

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$$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV}$$

NCSM ground state ${}^3\text{H}$



CLUSTER - ENTWICKLUNG

Versuchszustand: $|Q\rangle = e^{-i\tilde{S}} |Q_0\rangle$
↑ Statedeterminante

$\tilde{S} = \tilde{S}^\dagger$ Teilchenzahlerhaltung

Effektiver Operator:

$$\tilde{Q}_{eff} := e^{i\tilde{S}} \tilde{Q} e^{-i\tilde{S}}$$

Erwartungswert:

$$\langle Q | \tilde{Q} | Q \rangle = \langle Q_0 | e^{i\tilde{S}} \tilde{Q} e^{-i\tilde{S}} | Q_0 \rangle = \langle Q_0 | \tilde{Q}_{eff} | Q_0 \rangle$$

Cluster Entwicklung von \tilde{Q}_{eff}

$$\tilde{Q}_{eff} = \sum_{n=0}^{\infty} \tilde{Q}_{eff}^{(n)}$$

Produktzustände

$$\tilde{Q}_{eff}^{(n)} := \frac{1}{n!} \sum_{k_1, k_2, \dots, k_n} \langle k_1 k_2 \dots k_n | \tilde{Q}_{eff} - \sum_{m=0}^{n-1} \tilde{Q}_{eff}^{(m)} | l_1 l_2 \dots l_n \rangle a_{k_1}^\dagger a_{k_2}^\dagger \dots a_{k_n}^\dagger a_{l_n} \dots a_{l_2} a_{l_1}$$

Hamiltonian in A-Body Space

- evolution **induces n -body contributions $H_\alpha^{[n]}$** to Hamiltonian

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + \dots$$

- **truncation of cluster series** formally destroys unitarity and invariance of observables (independence of α)
- flow-parameter variation provides **diagnostic tool** to assess neglected contributions of higher particle ranks

SRG-Evolved Hamiltonians

NN_{only} : use initial NN, keep evolved NN

NN+3N_{ind} : use initial NN, keep evolved NN+3N

NN+3N_{full} : use initial NN+3N, keep evolved NN+3N

NN+3N_{full}+4N_{ind} : use initial NN+3N, keep evolved NN+3N+4N

Many-Body Problem

No-Core Shell Model

Barrett, Vary, Navrátil, Maris, Nogga, Roth,...

no-core shell model is the most universal and powerful ab initio approach for light nuclei (up to $A \approx 25$)

- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max} \hbar \Omega$

$$\left(\begin{array}{c} \text{[Matrix of blue dots with a diagonal band of yellow and green dots]} \end{array} \right) \begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_i^{(n)} \\ \vdots \end{pmatrix}$$

No-Core Shell Model

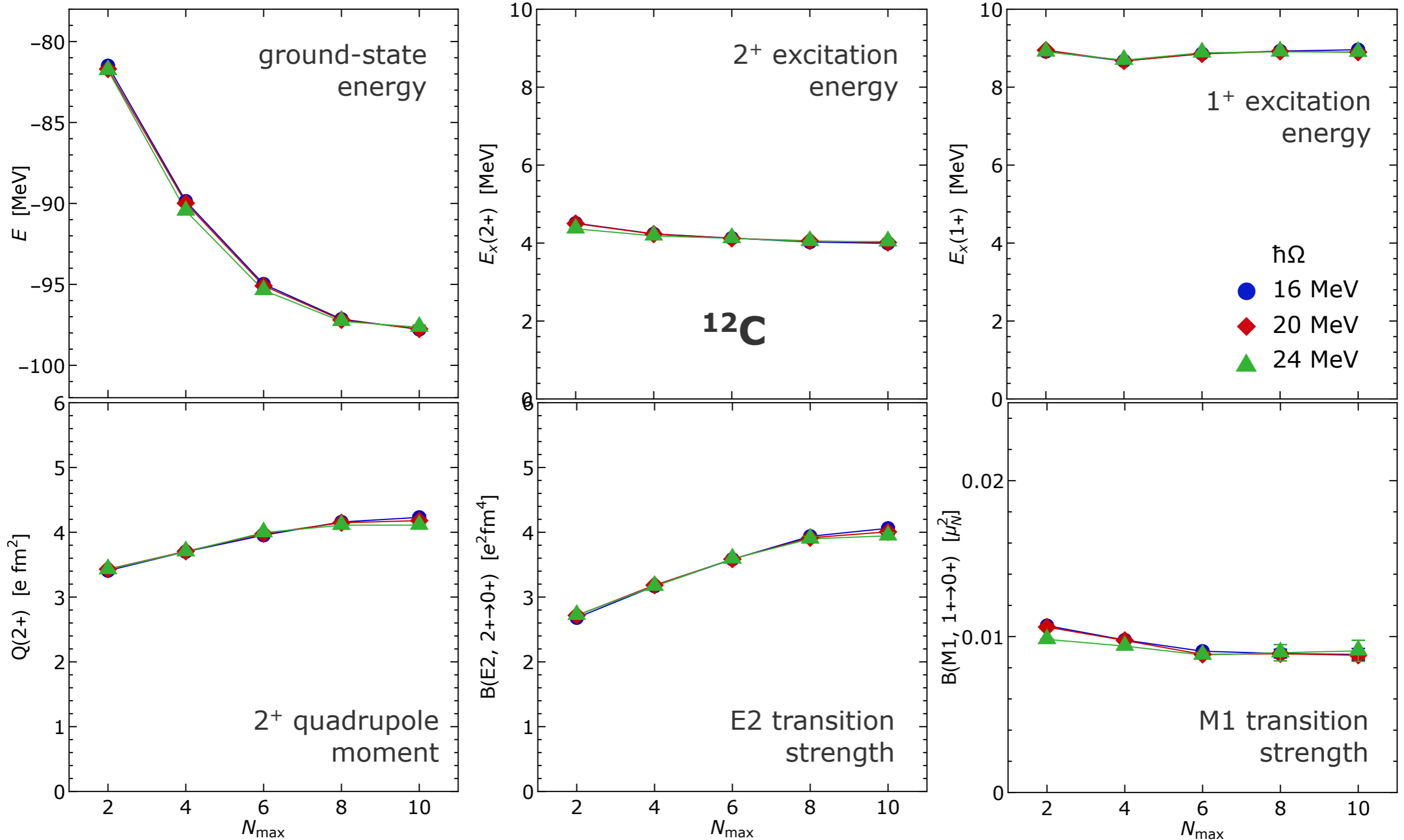
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- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max} \hbar \Omega$
 - convergence of observables w.r.t. N_{\max} is the only limitation and source of uncertainty
- **importance truncation**: reduce NCSM model space to physically relevant basis states and extrapolate to full space a posteriori
 - increases the range of applicability of NCSM significantly
- **alternative basis**: optimize basis to enhance model-space convergence or to include continuum physics
 - single-particle basis: natural orbitals, Gamow states
 - many-body basis: resonating group method with binary clusters

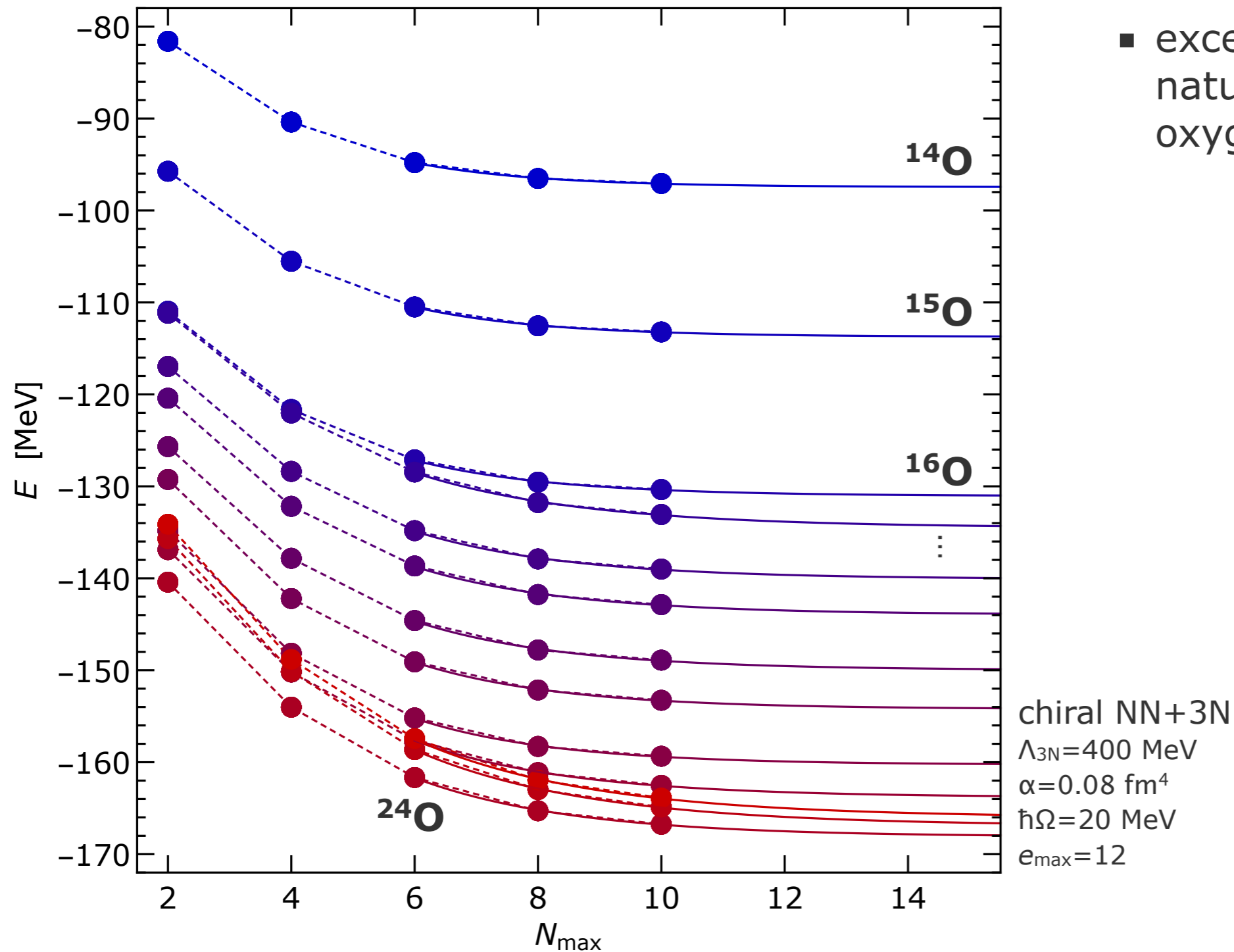
NCSM: Convergence - Natural Orbitals

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



NCSM: Oxygen Isotopes

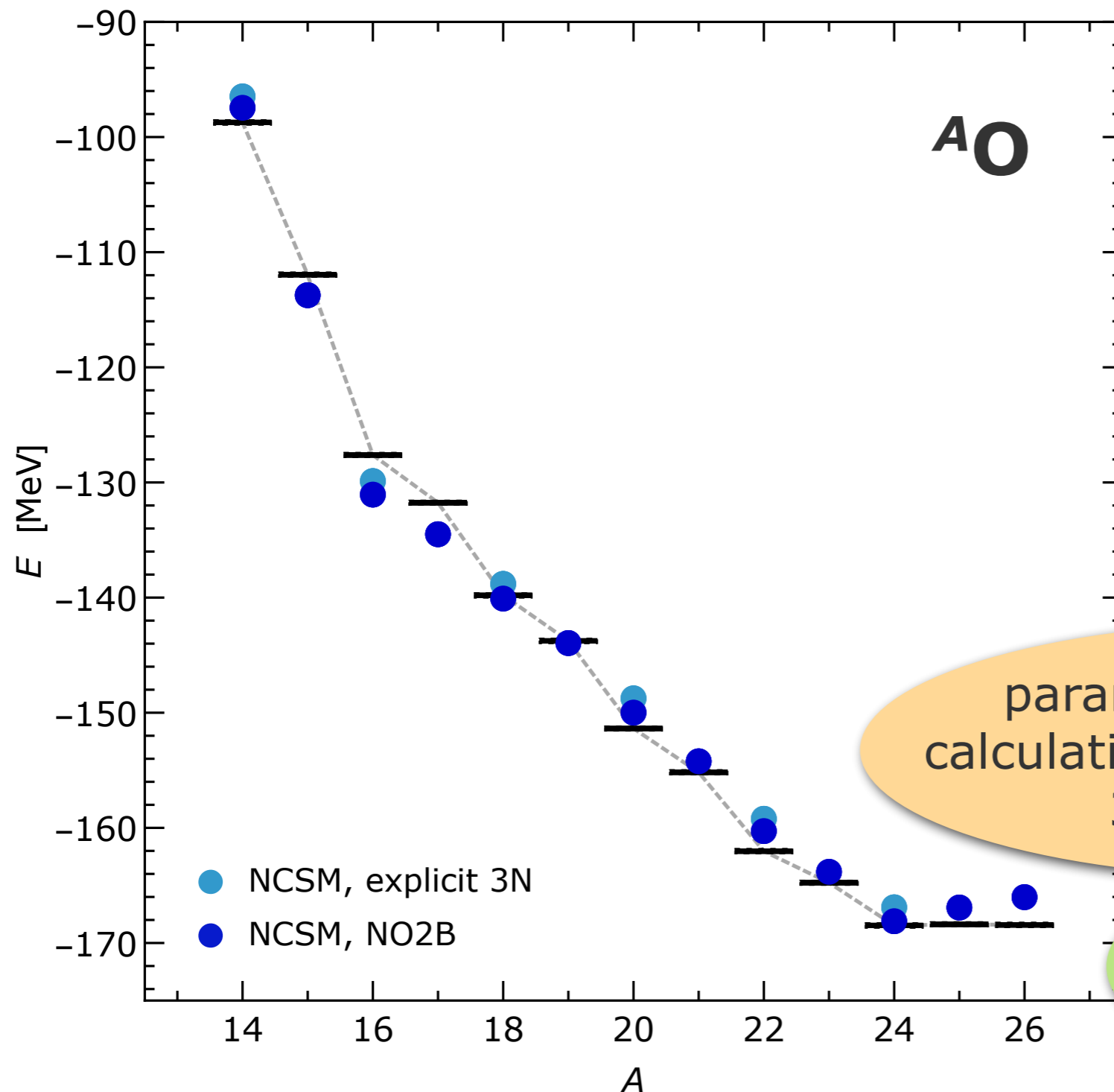
J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



- excellent convergence with natural-orbital basis for all oxygen isotopes

NCSM: Oxygen Isotopes

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



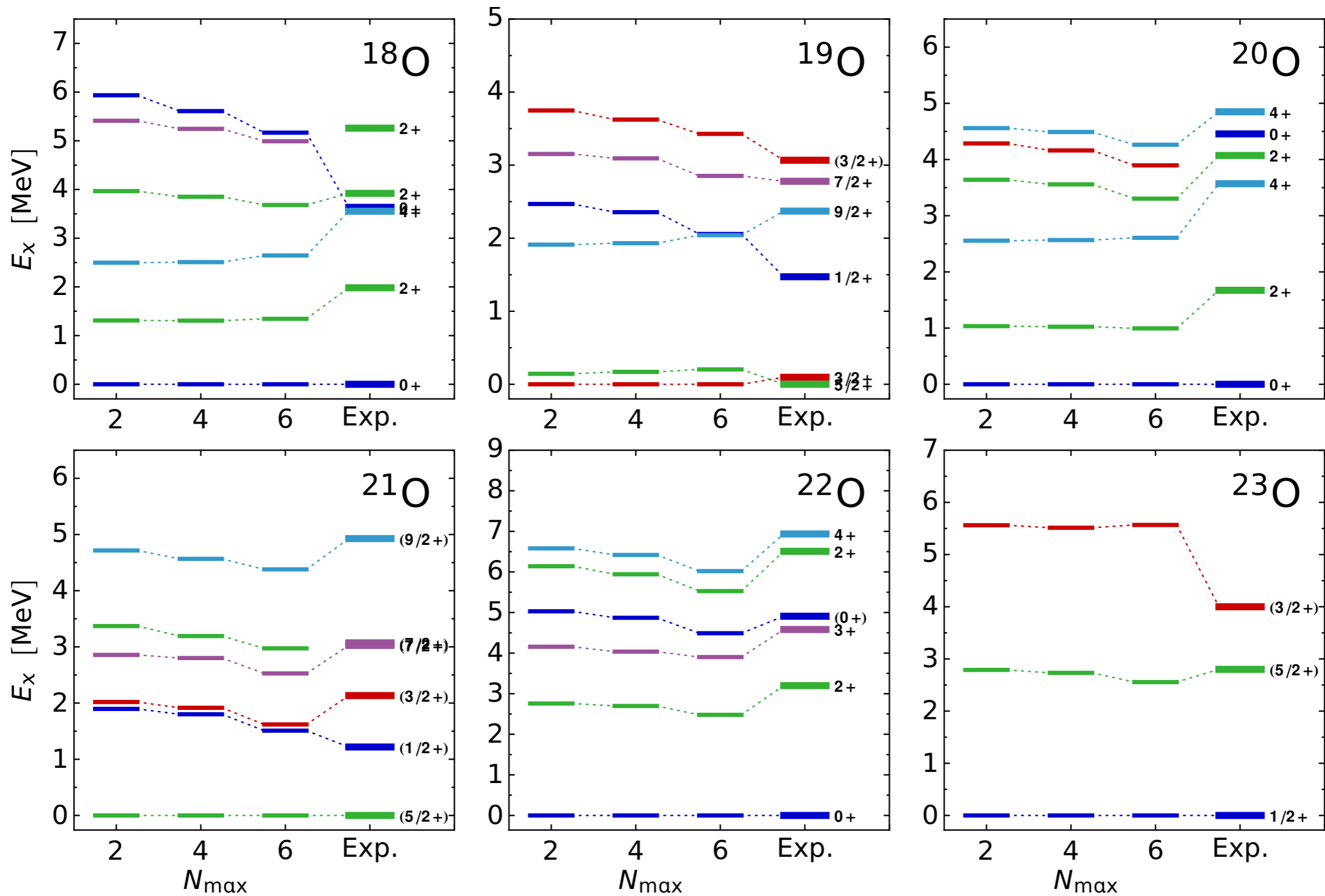
- excellent convergence with natural-orbital basis for all oxygen isotopes
- very good agreement with experimental systematics and dripline
- NO2B instead of explicit 3N causes $\sim 1\%$ overbinding

parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

Spectra of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013) & in prep.

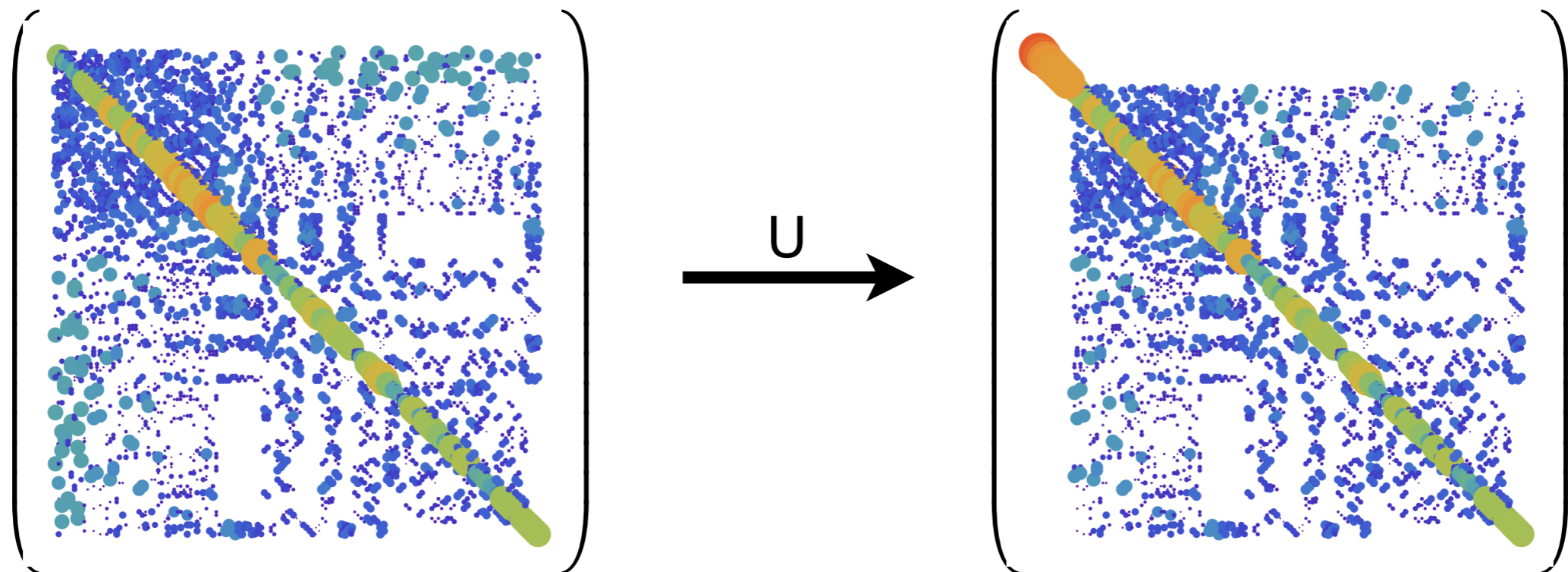


NN+3N_{full} (chiral NN+3N)
 $\Lambda_{3N} = 400 \text{ MeV}$, $\alpha = 0.08 \text{ fm}^4$, $\hbar\Omega = 16 \text{ MeV}$

Decoupling Methods

advent of novel ab initio approaches
targeting the ground state of medium-mass nuclei
very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian



Decoupling Methods

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- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian

Tsukiyama, Bogner, Schwenk, Hergert,...

- **In-Medium Similarity Renormalisation Group**: decouple many-body reference state from particle-hole excitations by SRG transformation

- normal-ordered A-body Hamiltonian truncated at the two-body level
- open and closed-shell nuclei can be targeted directly

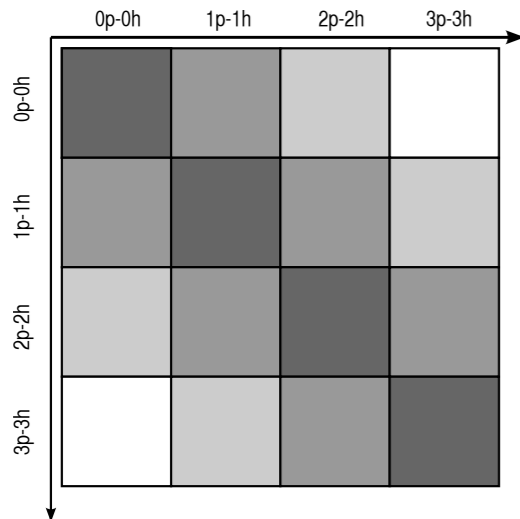
Hagen, Papenbrock, Dean, Piecuch, Binder,...

- **Coupled-Cluster Theory**: ground-state is parametrised by exponential wave operator acting on single-determinant reference state

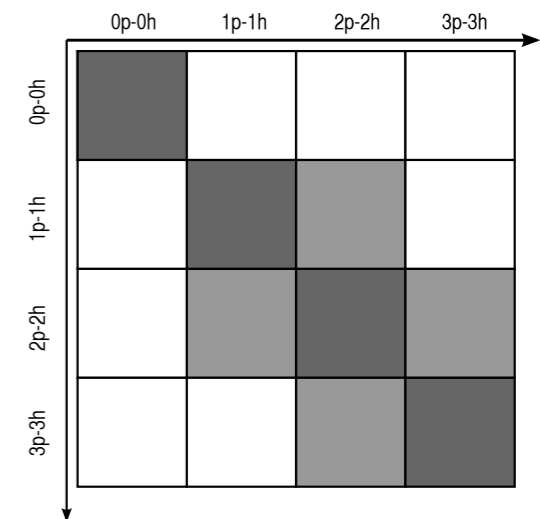
- truncation at doubles level (CCSD) with corrections for triples contributions
- directly applicable for closed-shell nuclei, equations-of-motion methods for open-shell

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,...



use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations



$$\frac{d}{ds}H(s) = [\eta(s), H(s)]$$

- Hamiltonian and generator in normal order with respect to single or multi-determinant reference state, omit residual three-body piece

$$H(s) = E(s) + \sum_{ij} f_j^i(s) \tilde{A}_j^i + \frac{1}{4} \sum_{ijkl} \Gamma_{kl}^{ij}(s) \tilde{A}_{kl}^{ij} + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk}(s) \tilde{A}_{lmn}^{ijk}$$

- define generator to suppress off-diagonal contributions that couple reference state to ph excitations

$$\eta(s) = [H(s), H^d(s)] = [H^{od}(s), H^d(s)]$$

In-Medium NCSM

Gebrerufael, Vobig, Hergert, Roth,...

NCSM
Reference State

- ground-state from NCSM at small N_{\max} as reference state for multi-reference IM-SRG
- access to all open-shell nuclei and systematically improvable

IM-SRG
Many-Body Decoupling

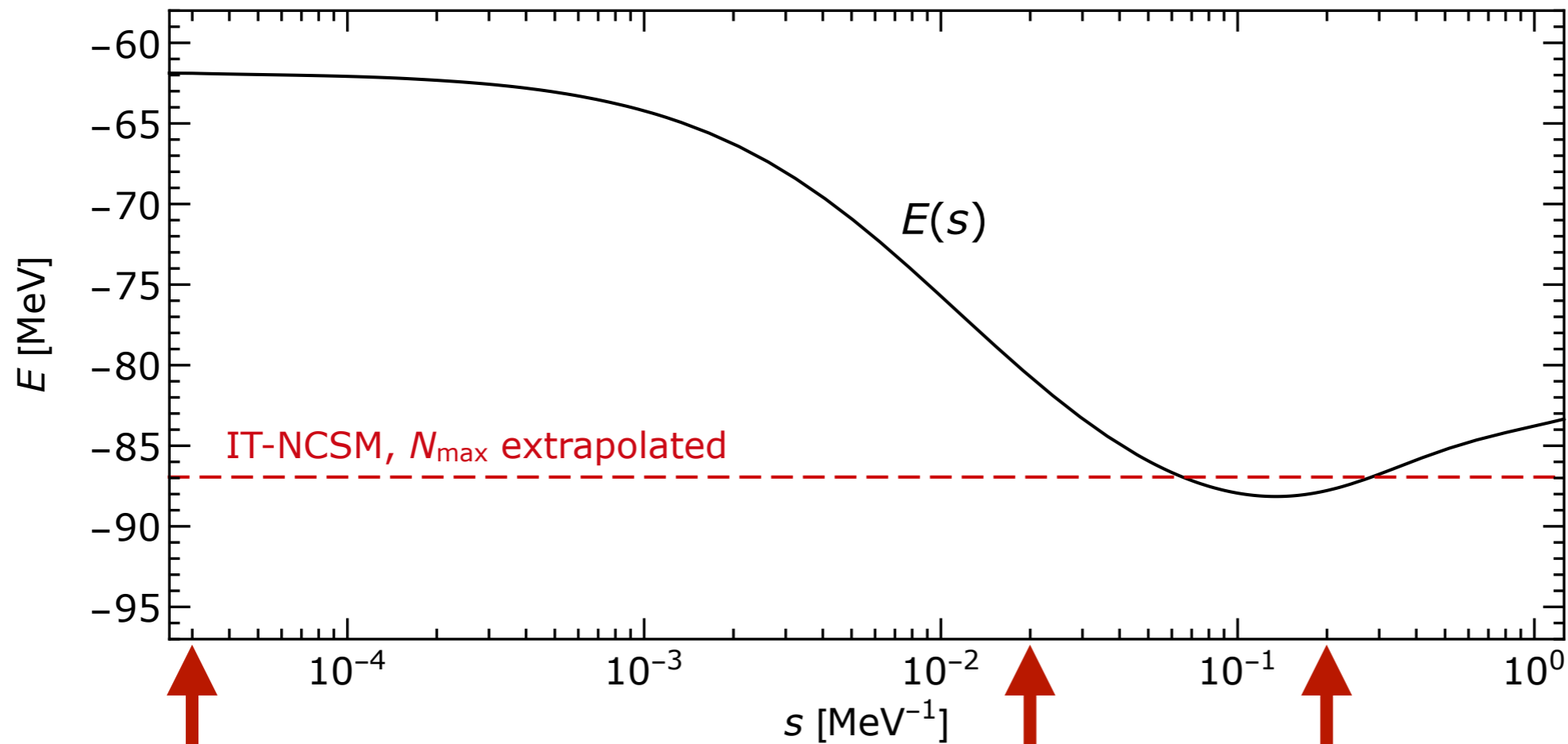
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in A -body space

NCSM
Observables

- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

In-Medium NCSM

Gebrerufael, et al.; PRL 118, 152503 (2017)



^{12}C

chiral NN+3N

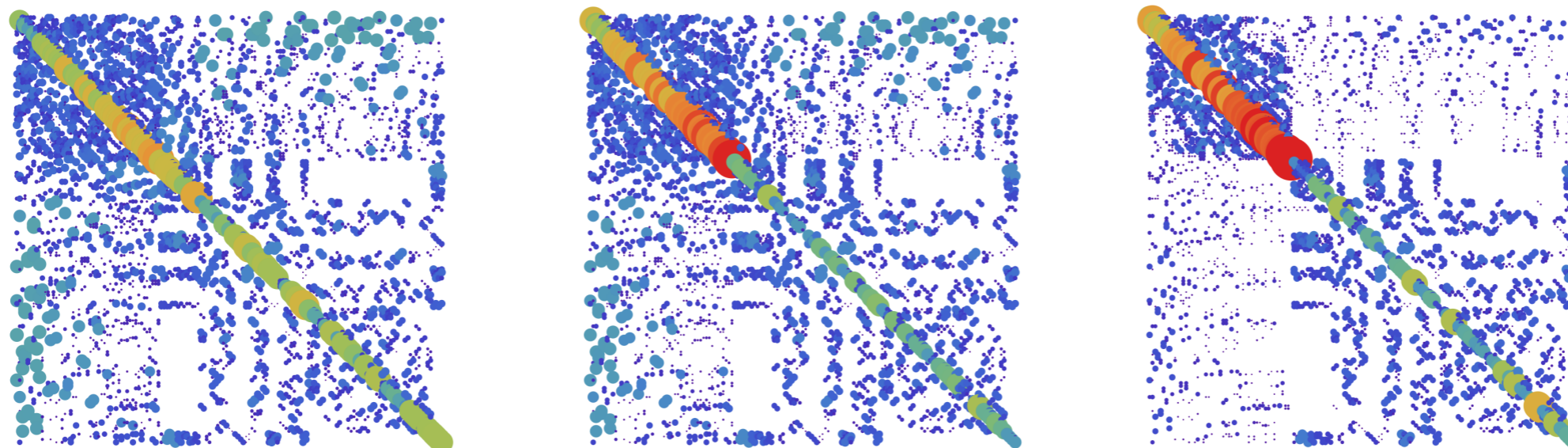
$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

$e_{\text{max}}=12$

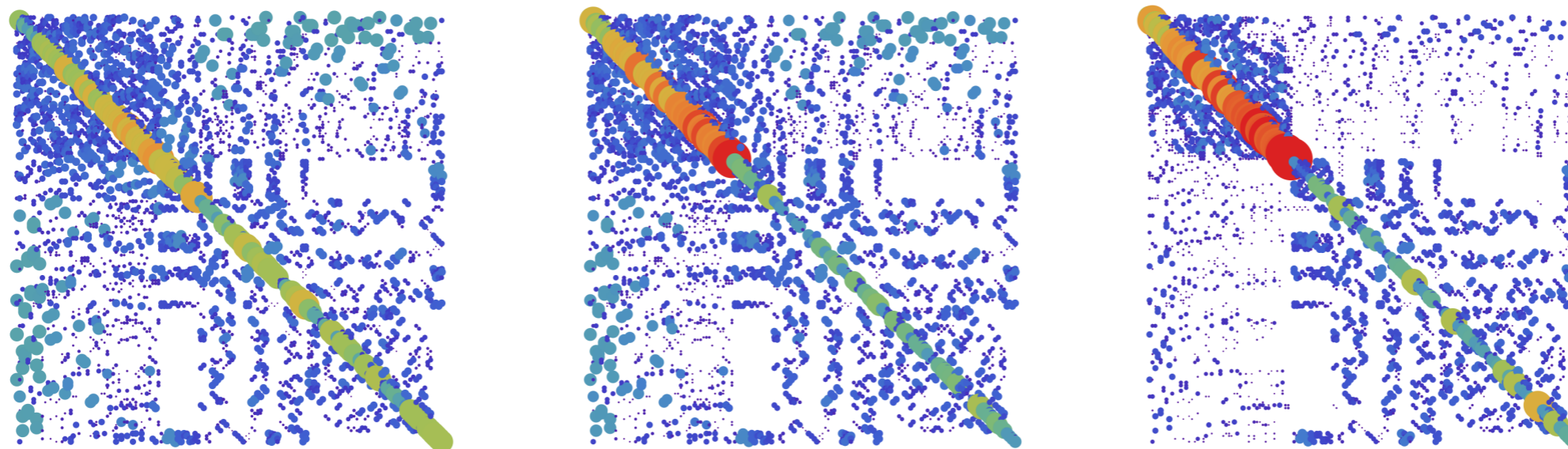
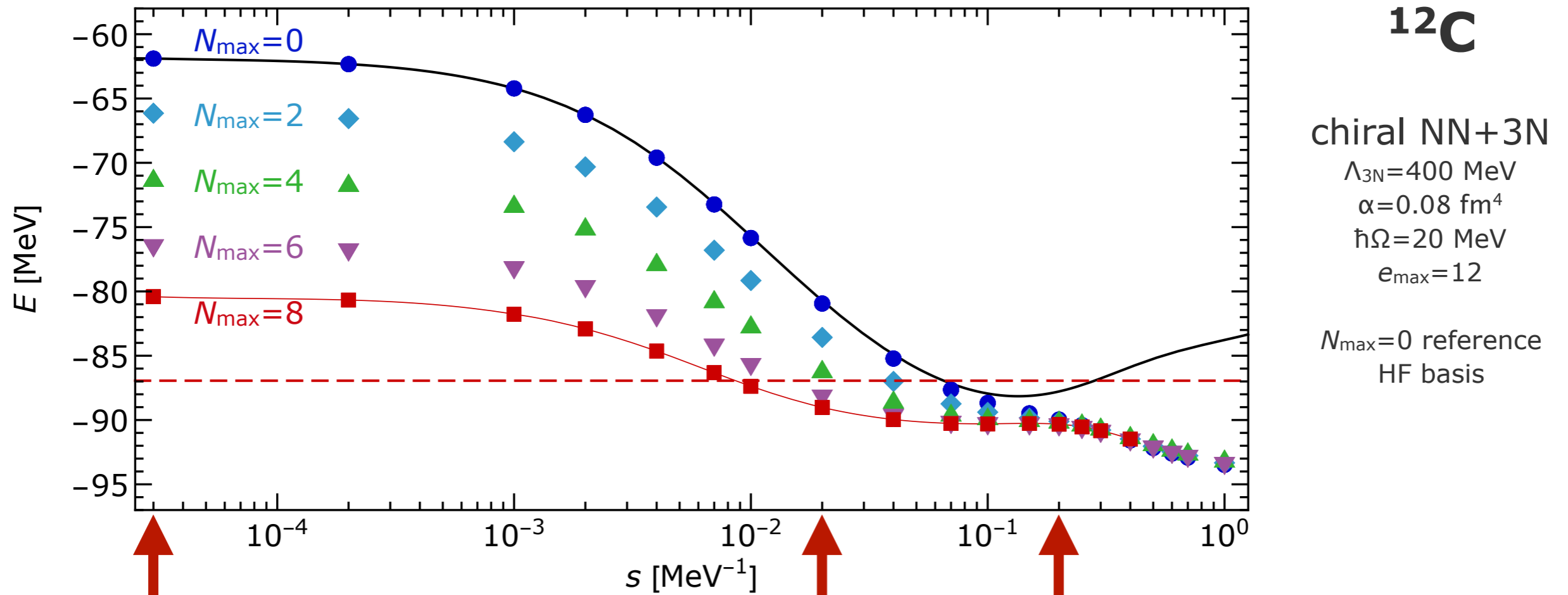
$N_{\text{max}}=0$ reference
HF basis



Hamilton
matrix in
 $N_{\text{max}}=2$
space

In-Medium NCSM

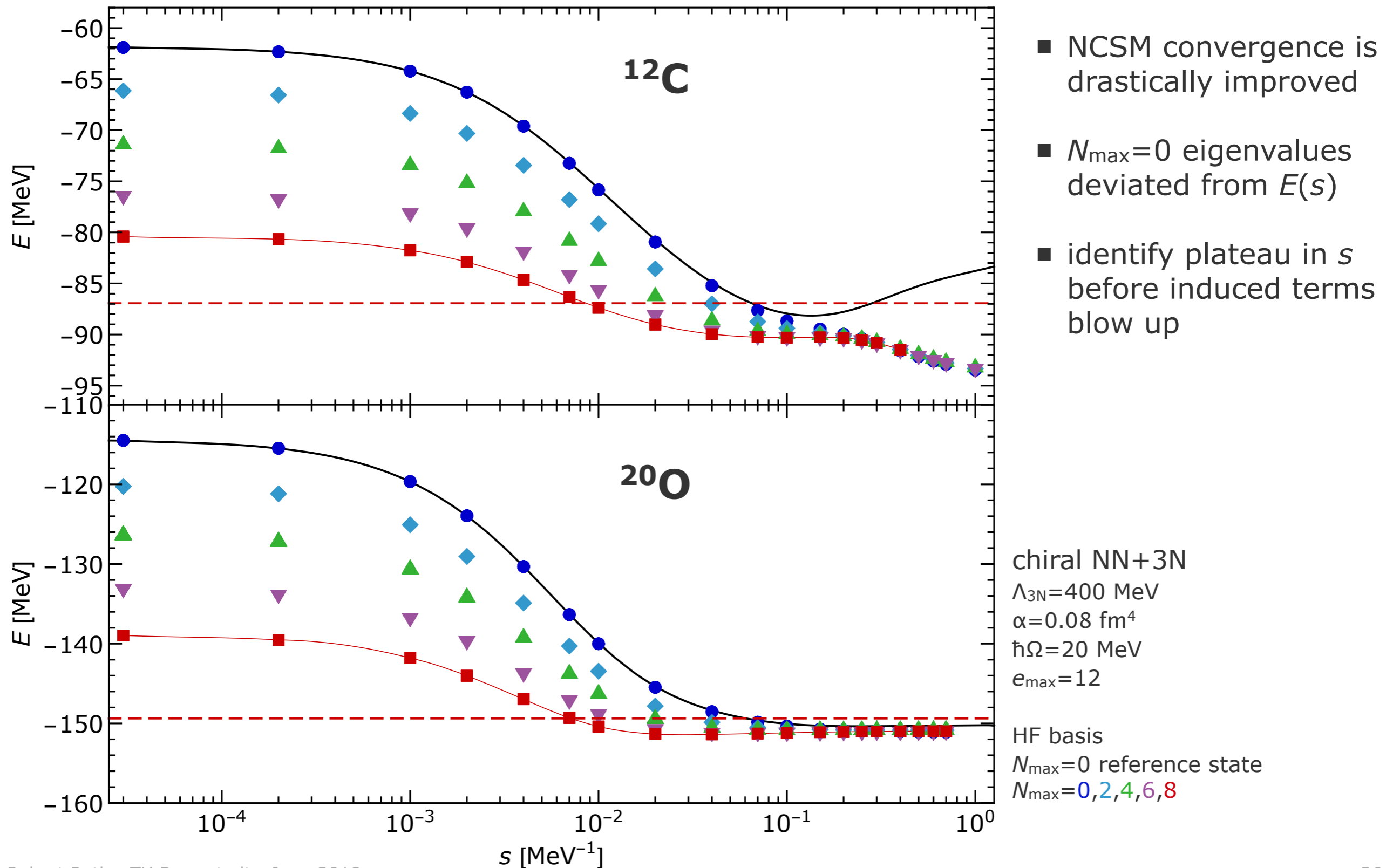
Gebrerufael, et al.; PRL 118, 152503 (2017)



Hamilton
 matrix in
 $N_{\text{max}}=2$
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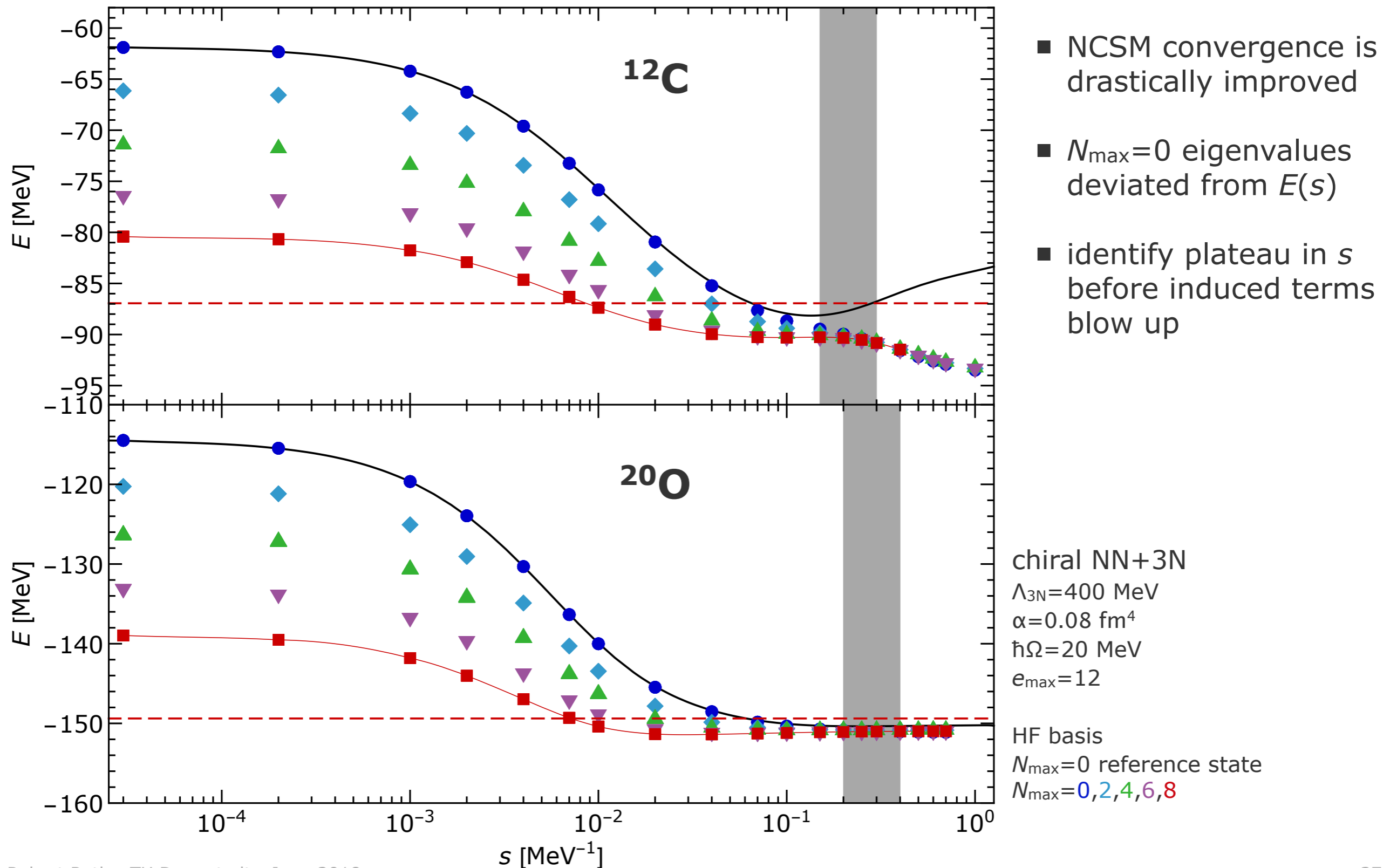
In-Medium NCSM

Gebrerufael, et al.; PRL 118, 152503 (2017)



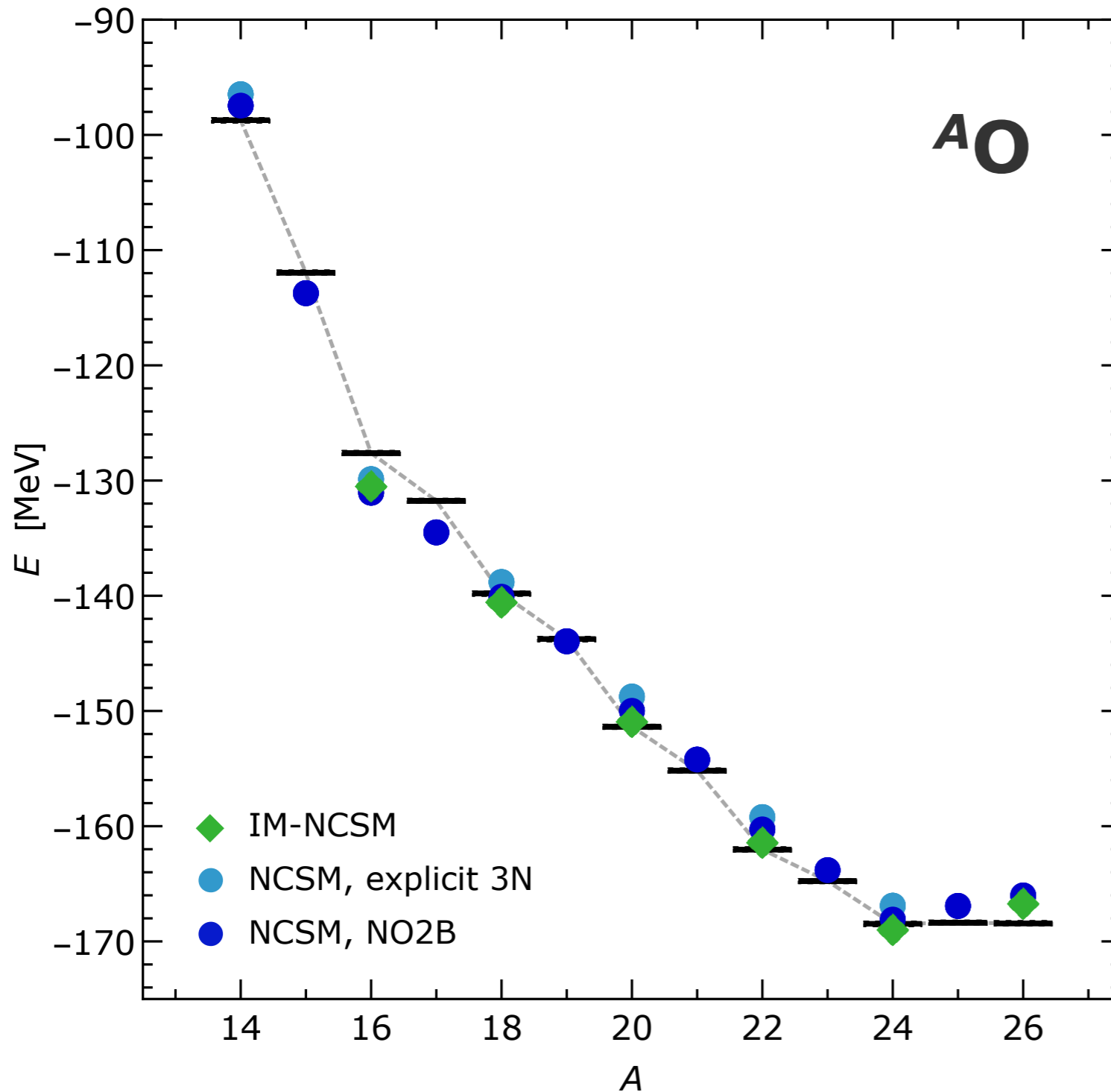
In-Medium NCSM

Gebrerufael, et al.; PRL 118, 152503 (2017)



IM-NCSM: Oxygen Isotopes

Gebrerufael, et al.; PRL 118, 152503 (2017)



- excellent agreement with direct NCSM
- IM-SRG evolution limited to $J=0$ reference states and thus even-mass isotopes

chiral NN+3N

$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

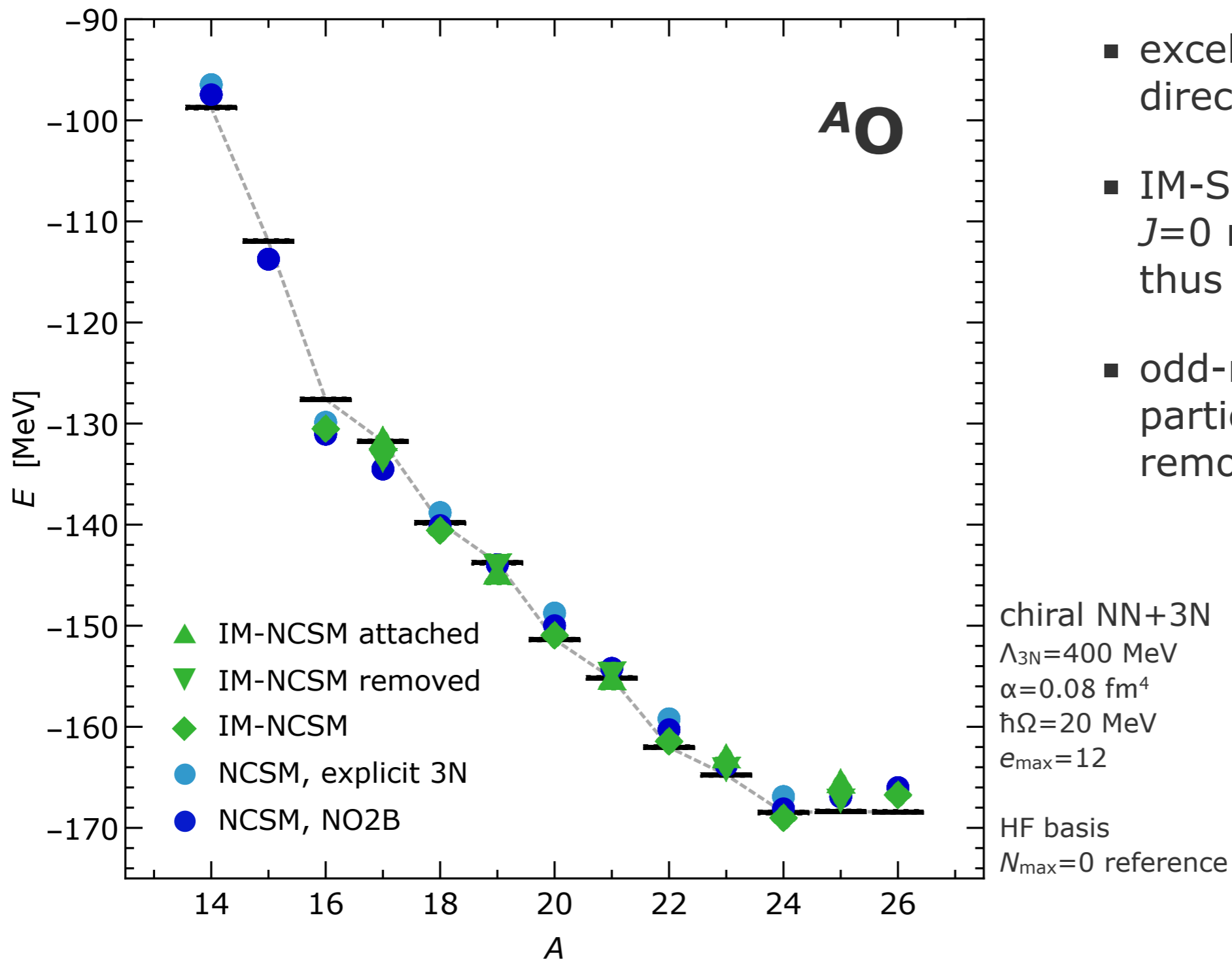
$e_{\max}=12$

HF basis

$N_{\max}=0$ reference

IM-NCSM: Oxygen Isotopes

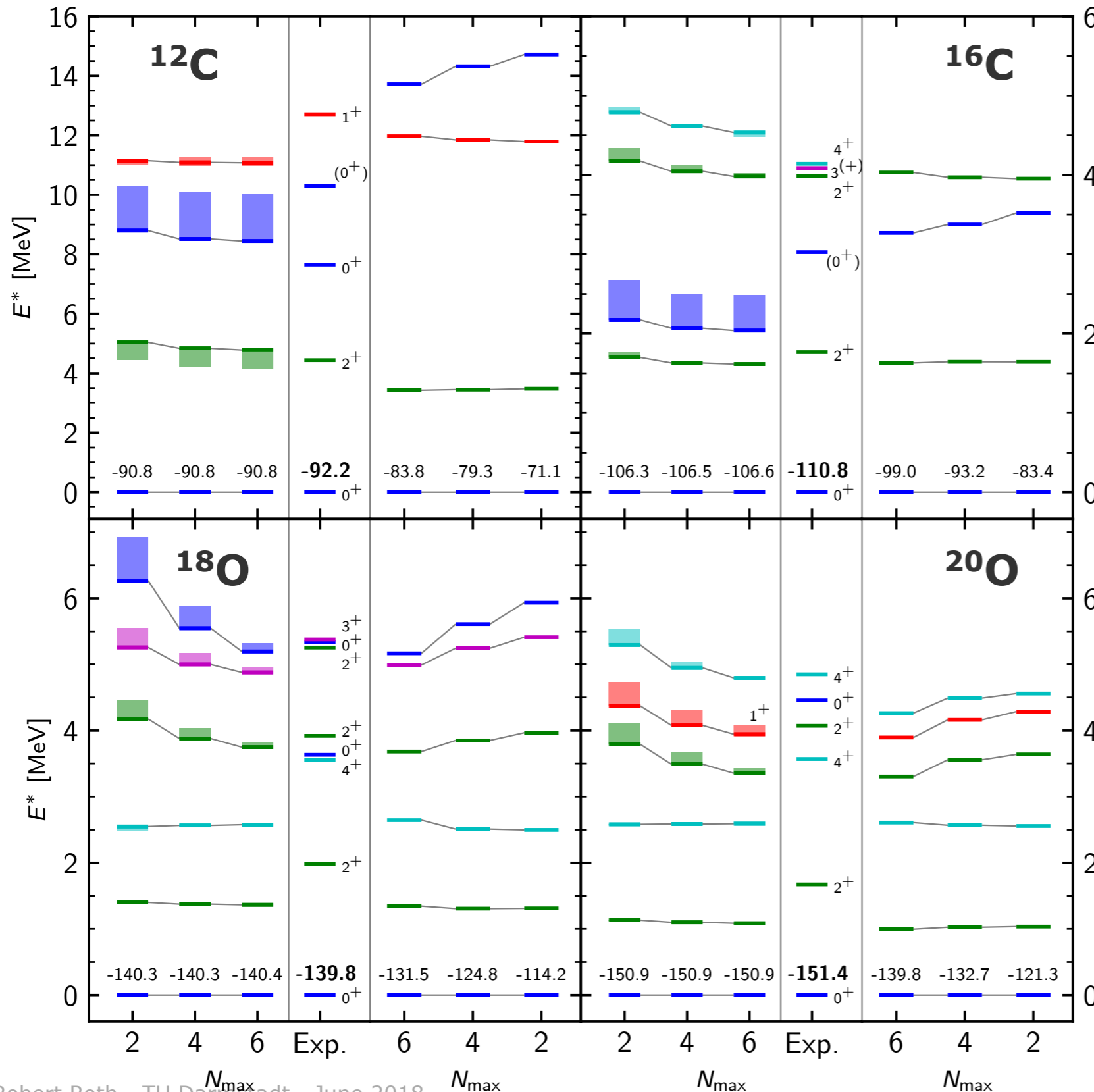
Vobig, Gebrerufael, Roth; in prep.



- excellent agreement with direct NCSM
- IM-SRG evolution limited to $J=0$ reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

IM-NCSM: Excitation Spectra

Gebrerufael, et al.; PRL 118, 152503 (2017)



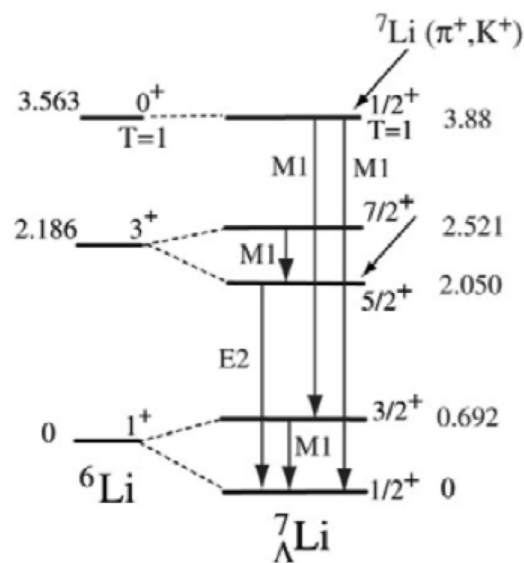
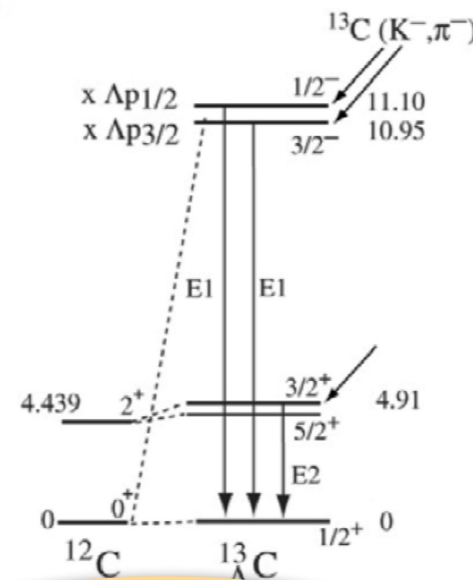
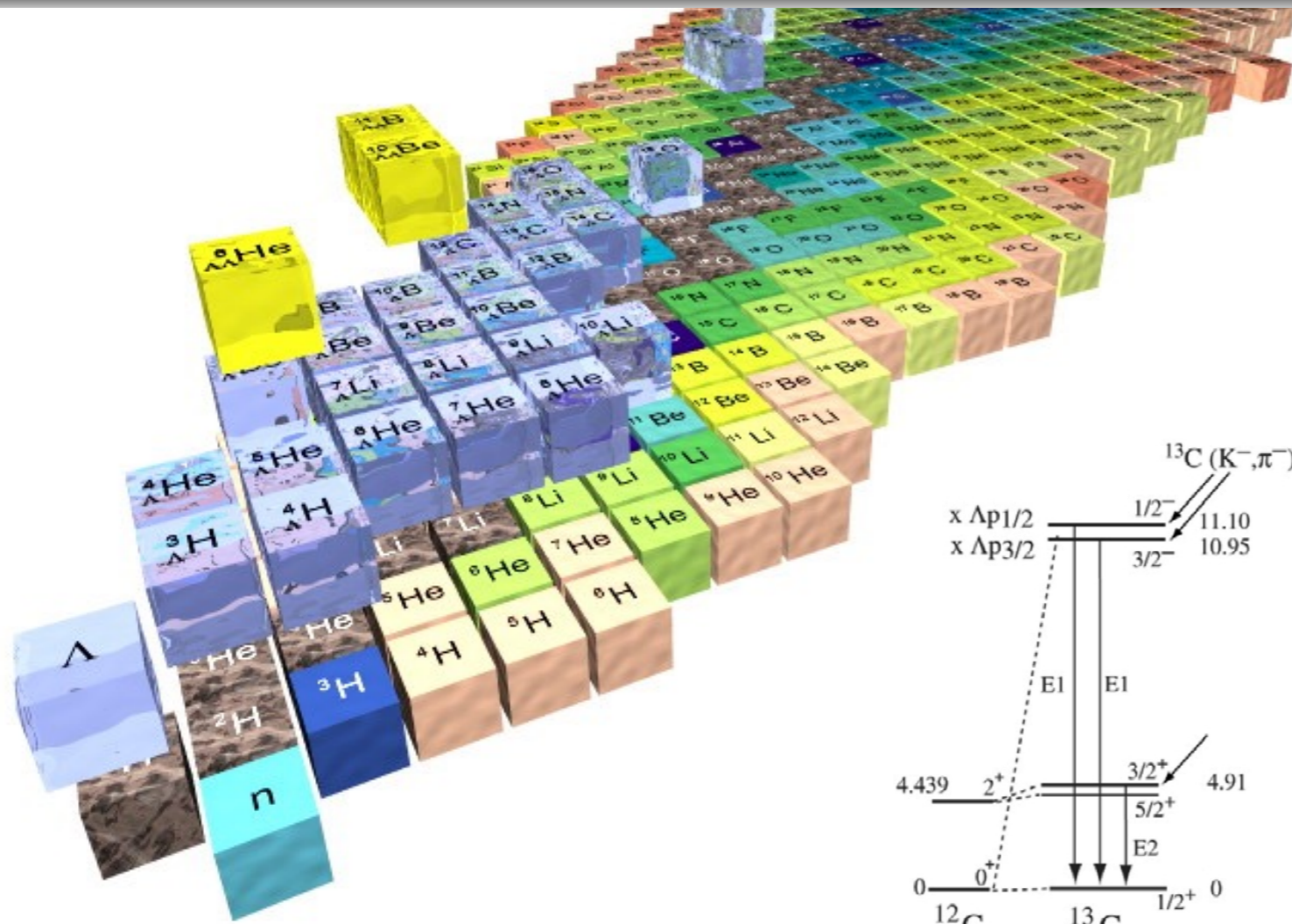
■ IM-NCSM and direct NCSM in excellent agreement for converged states

■ first excited 0^+ states in ^{12}C and ^{16}C differ

chiral NN+3N
 $\Lambda_{3N}=400$ MeV
 $\alpha=0.08$ fm⁴
 $\hbar\Omega=16$ MeV
 $e_{\text{max}}=12$
 HF basis

Hypernuclei

Ab Initio Hypernuclear Structure



constrain YN interactions with hypernuclear spectroscopy



- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body and phenomen. shell-model, mean-field or cluster-model calculations done so far
- chiral YN & YY interactions at (N)LO are available

time to transfer ab initio toolbox to hypernuclei

Ab Initio Toolbox for Hypernuclei

Wirth et al.; PRL 113, 192502 (2014); PRL 117, 182501 (2016)

■ Hamiltonian from chiral EFT

- NN+3N: standard chiral Hamiltonian (Entem&Machleidt, Navrátil)
- YN: LO chiral interaction (Haidenbauer et al.), NLO in progress

■ Similarity Renormalization Group

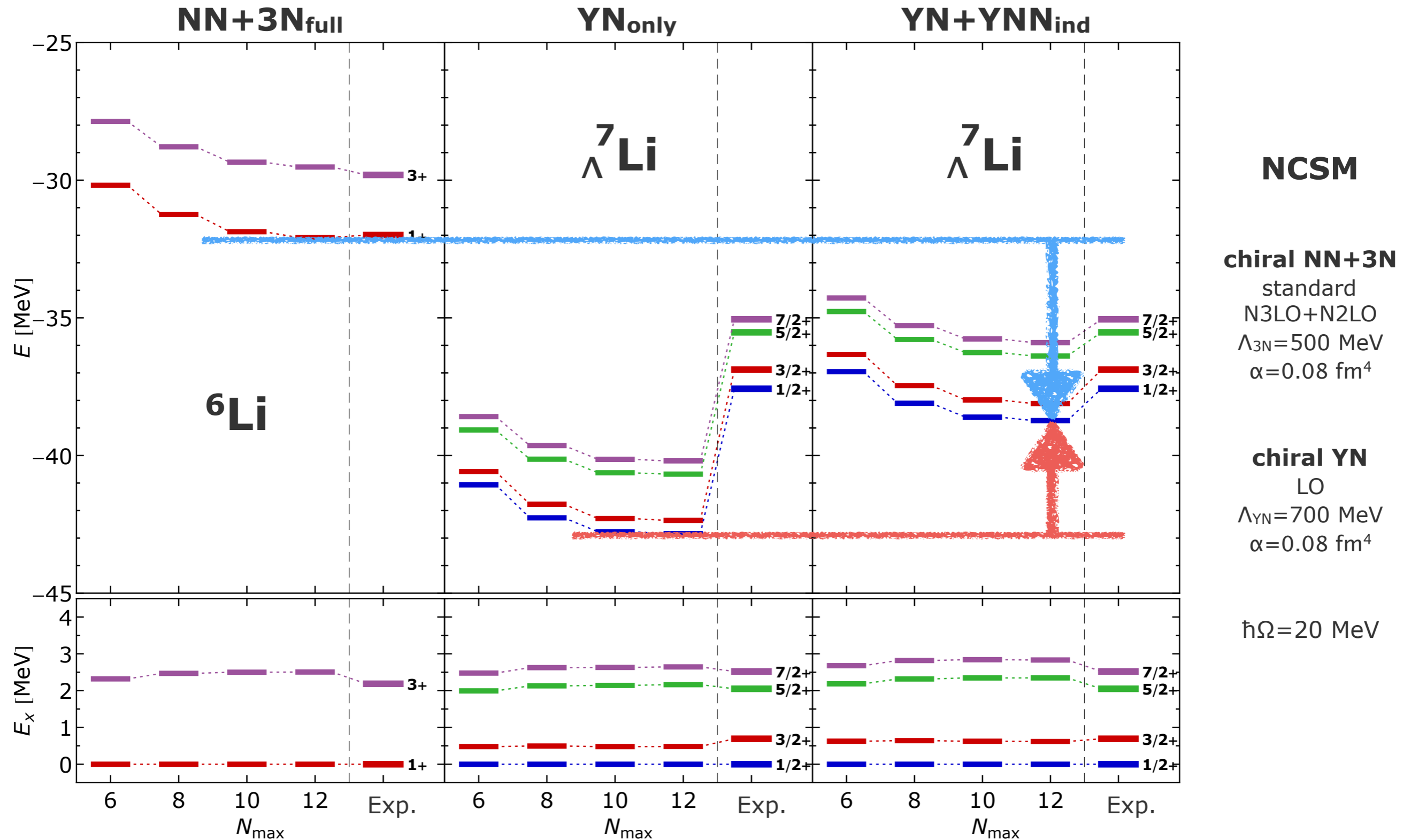
- consistent SRG-evolution of NN, 3N, YN interactions
- using particle basis and including $\Lambda\Sigma$ -coupling (larger matrices)
- Λ - Σ mass difference and $p\Sigma^\pm$ Coulomb included consistently

■ Importance Truncated No-Core Shell Model

- include explicit $(p, n, \Lambda, \Sigma^+, \Sigma^0, \Sigma^-)$ with physical masses
- larger model spaces easily tractable with importance truncation
- all p-shell single- Λ hypernuclei are accessible

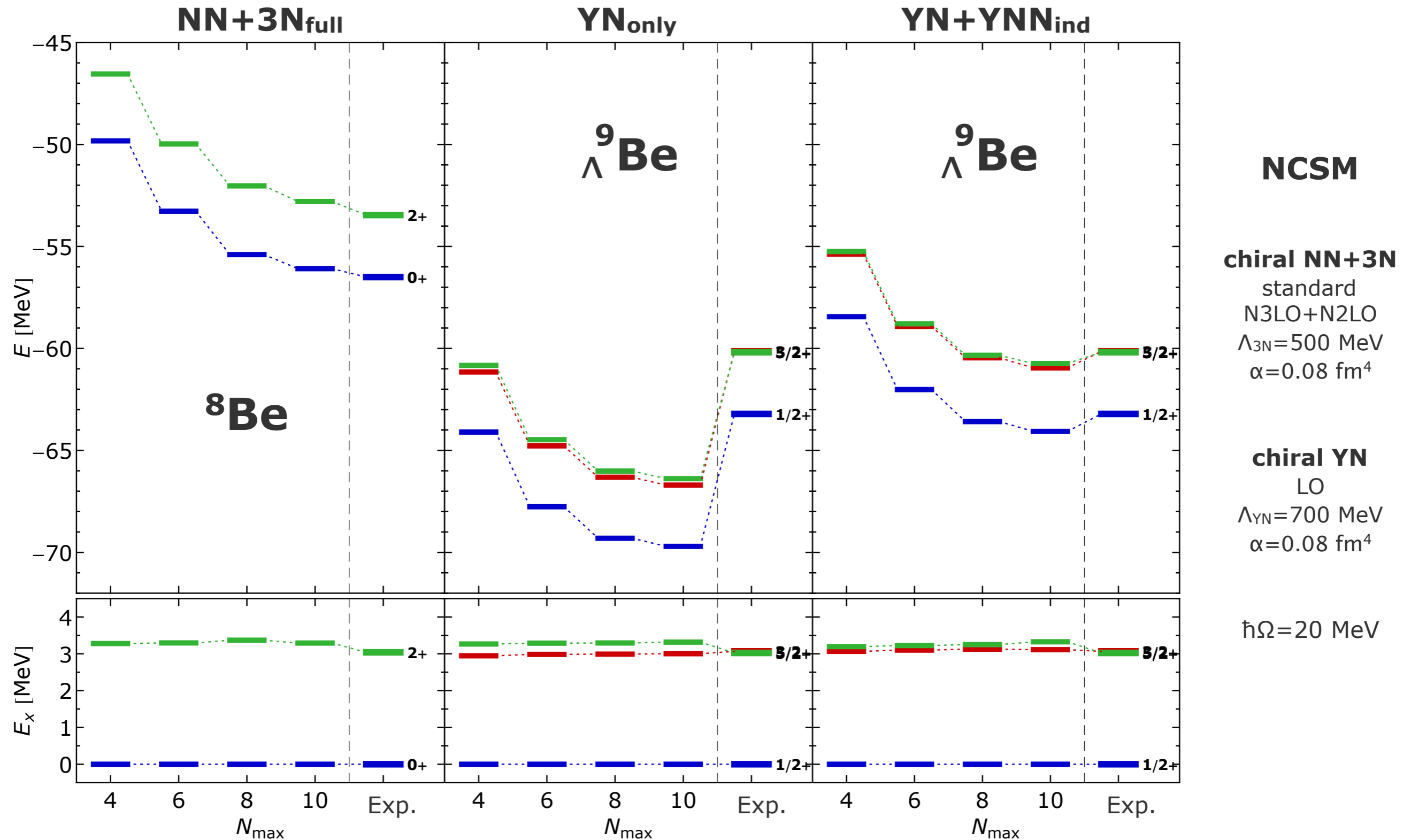
Application: $\Lambda^7\text{Li}$

Wirth et al.; PRL 113, 192502 (2014); PRL 117, 182501 (2016)



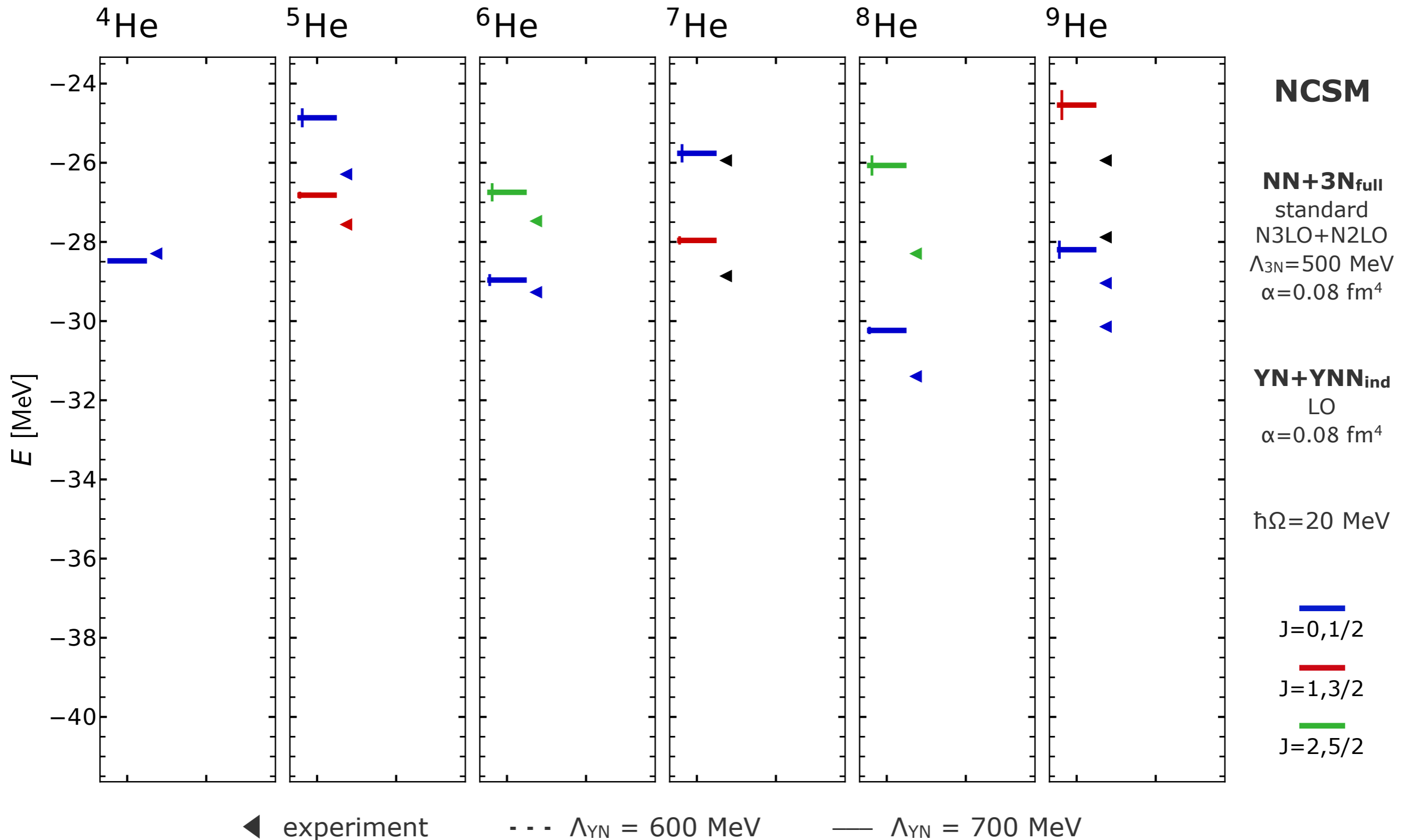
Application: $\Lambda^9\text{Be}$

Wirth et al.; PRL 113, 192502 (2014); PRL 117, 182501 (2016)



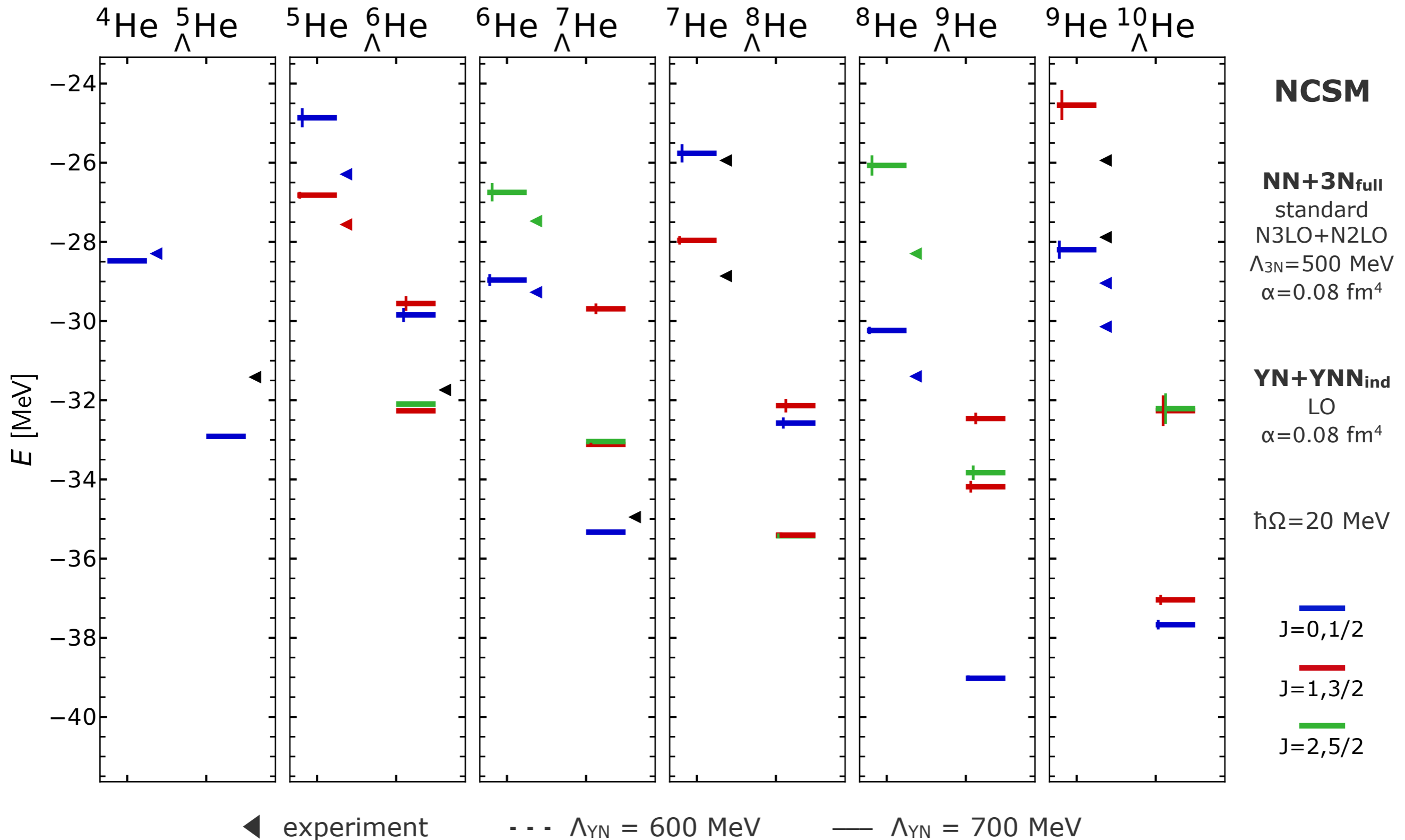
Light Neutron-Rich Hypernuclei

Wirth et al.; PLB 779, 336 (2018)



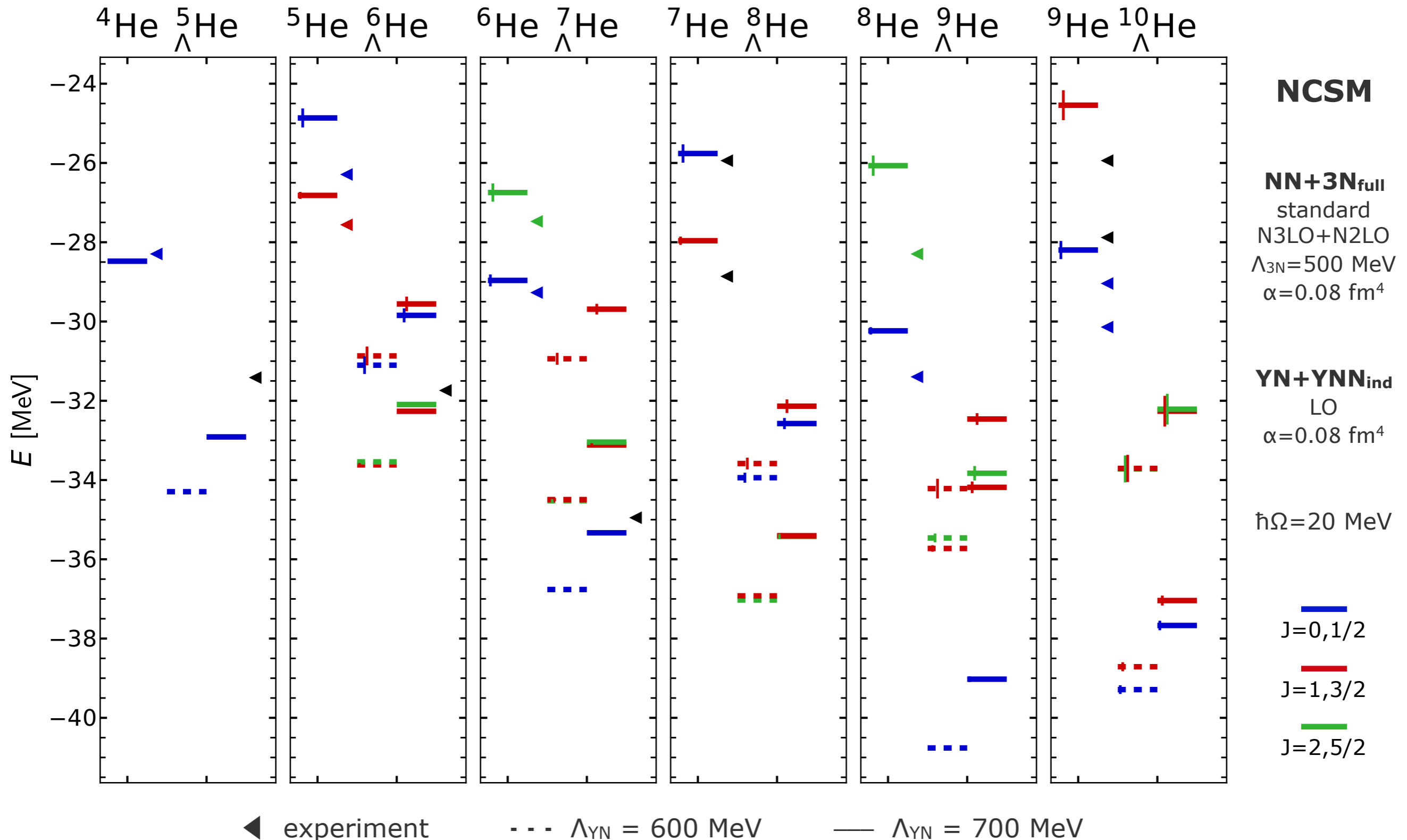
Light Neutron-Rich Hypernuclei

Wirth et al.; PLB 779, 336 (2018)



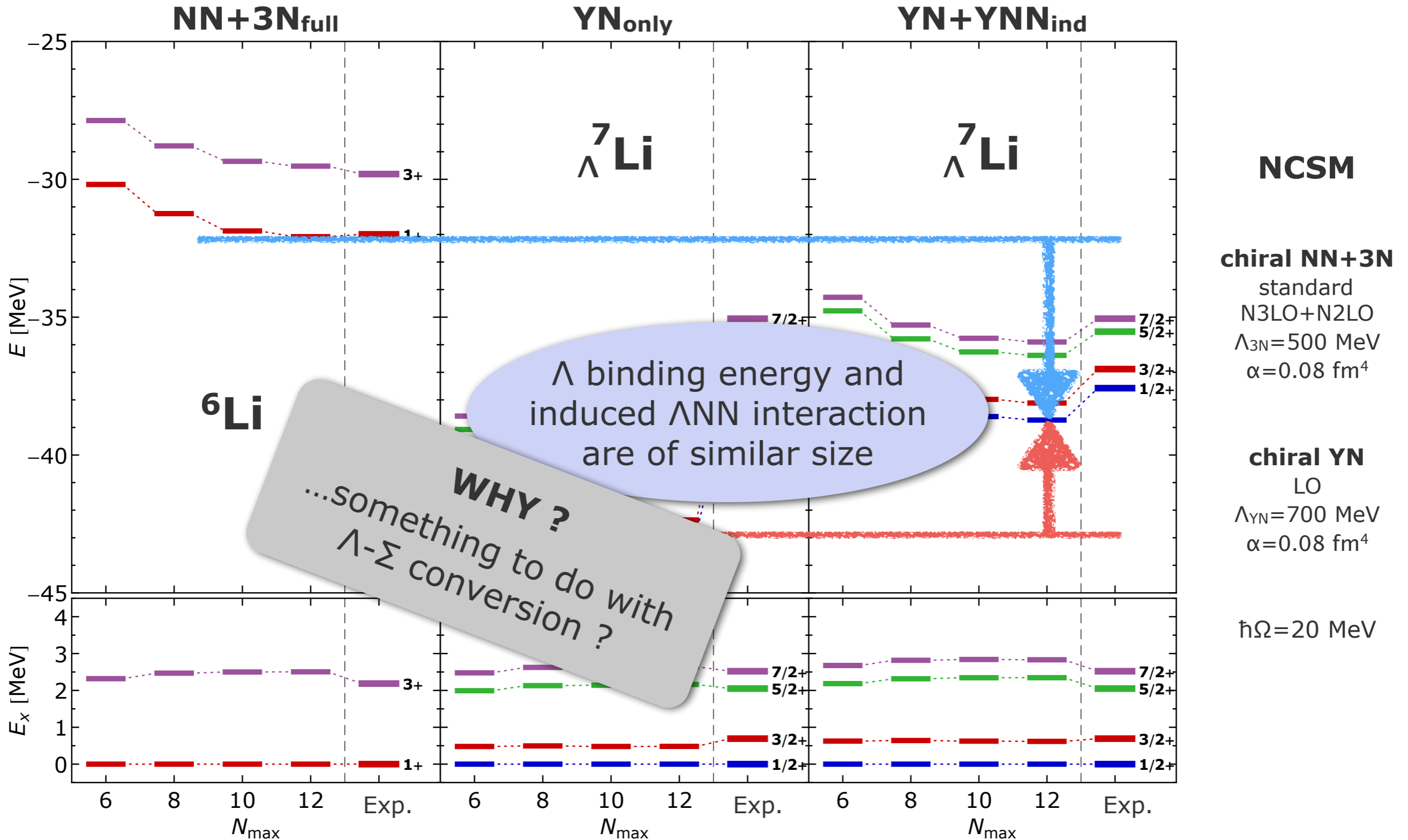
Light Neutron-Rich Hypernuclei

Wirth et al.; PLB 779, 336 (2018)



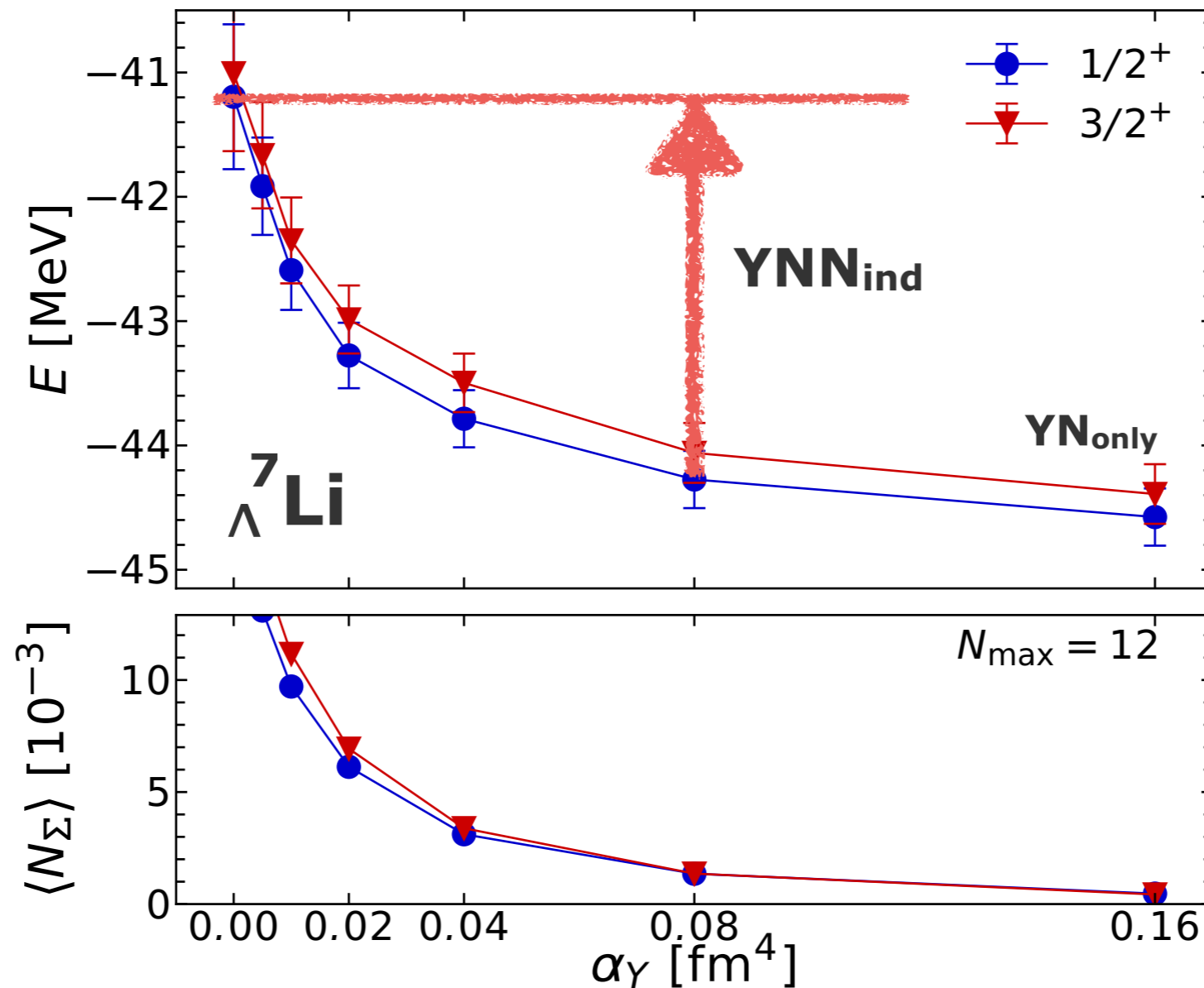
Application: $\Lambda^7\text{Li}$

Wirth et al.; PRL 113, 192502 (2014); PRL 117, 182501 (2016)



Suppression of Λ - Σ Conversion

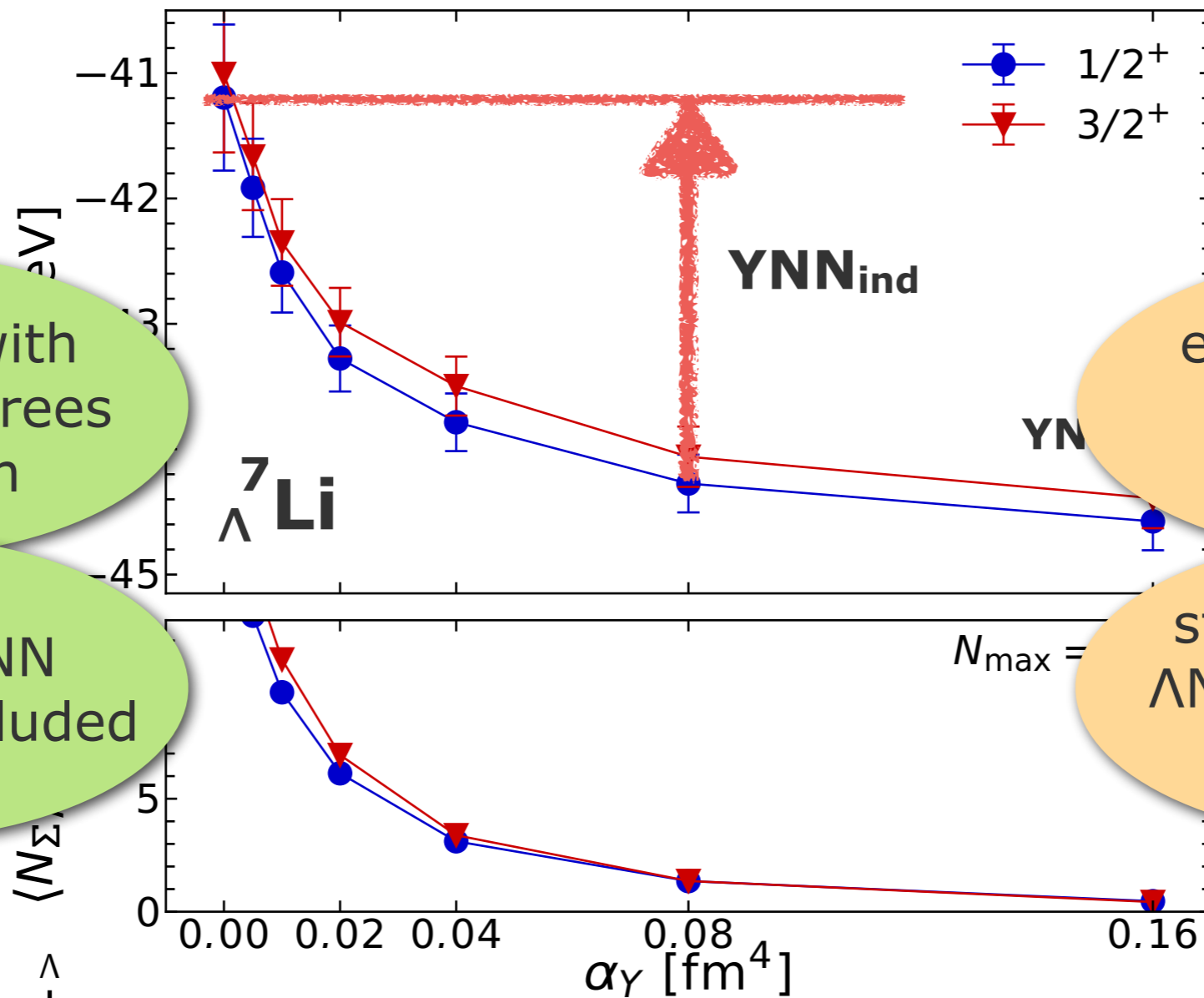
Wirth et al.; PRL 117, 182501 (2016)



- design SRG-generator that **suppresses the Λ - Σ conversion** exclusively
- Σ admixture in the wave functions eliminated or “integrated out”
- same large induced YNN interactions as in standard SRG

Suppression of Λ - Σ Conversion

Wirth et al.; PRL 117, 182501 (2016)

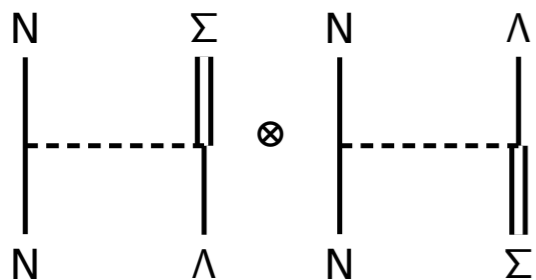


full theory with explicit Σ degrees of freedom

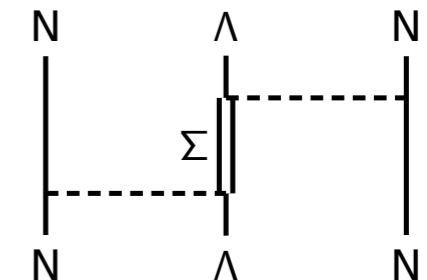
no initial YNN interaction included

effective Λ -only theory, Σ fully decoupled

strong repulsive Λ NN interaction is induced

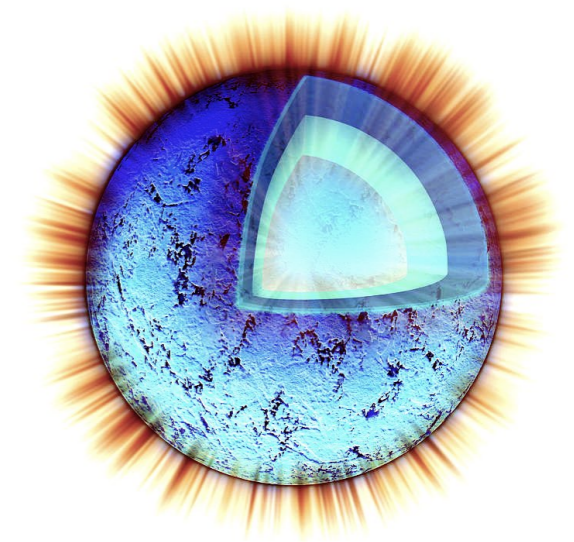


SRG evolves full coupled-channel theory to effective Λ -only theory

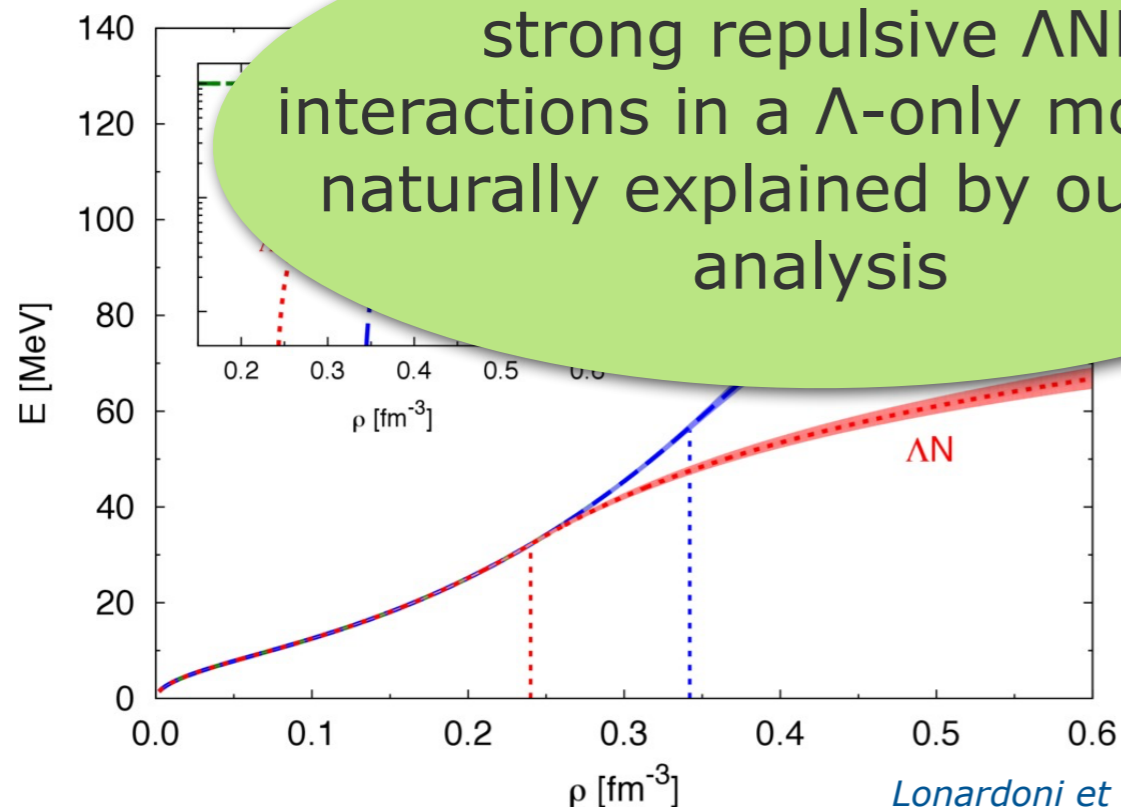


Implications for the Hyperon Puzzle

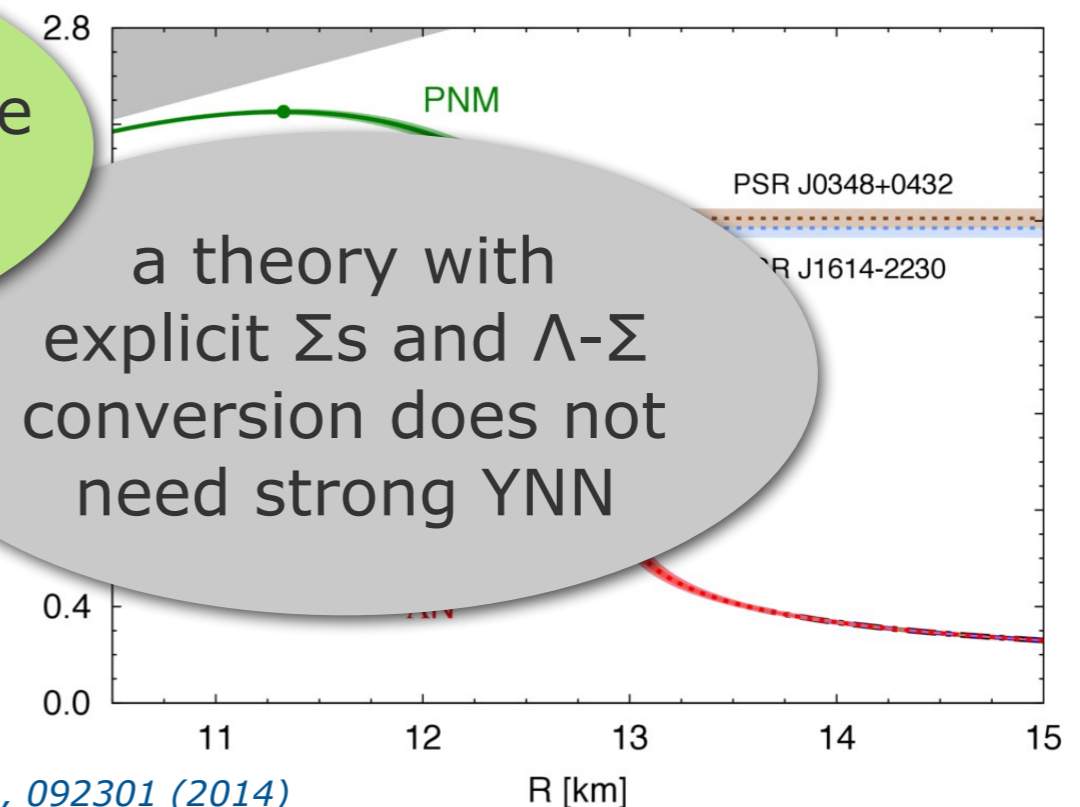
- neutron stars reach densities, where hyperon production should be energetically favorable
- including explicit Λ s with ΛN interaction softens EOS - does not support $2M_{\odot}$ neutron star
- phenomenological fix: introduce strongly repulsive ΛNN interaction



fineart
america



Lonardonì et al.; PRL 114, 092301 (2014)



Conclusions

A Look Back...

- past 20 years have seen dramatic progress in ab initio many-body methods for nuclear structure and reactions
 - ...extensions of NCSM, coupled-cluster theory, in-medium SRG, self-consistent Green's function, many-body perturbation theory
- a number of important developments are in progress
 - ...spectroscopy of open-shell nuclei, merging NCSM and IM-SRG, derivation of valence-space interactions, broad range of observables
- the reach of ab initio methods has grown tremendously
 - ...medium-mass and heavy nuclei, low-lying and collective excitations, continuum effects and reaction observables, resonances, hypernuclei

A Look Ahead...

- for the next few years the focus will move towards improvements of the chiral interactions
 - ...consistent higher orders, systematic study of order-by-order convergence, inclusion of consistent currents, improved fitting strategies
- rigorous quantification of theoretical uncertainties will play an important role
 - ...propagation of uncertainties from chiral EFT inputs to nuclear structure observables, full quantification of many-body uncertainties
- lots of relevant physics predictions...

All My Best Wishes to...



... and special thanks
for so many things

GSI Theory Excursion
2002

Epilogue

■ thanks to my group and my collaborators

- S. Alexa, T. Hüther, M. Knöll, L. Mertes, J. Müller, C. Stumpf, A. Tichai, K. Vobig, C. Walde, R. Wirth, T. Wolfgruber
Technische Universität Darmstadt
- P. Navrátil
TRIUMF, Vancouver
- A. Tichai, T. Duguet
CEA Saclay
- H. Hergert
NSCL / Michigan State University
- J. Vary, P. Maris
Iowa State University
- E. Epelbaum, H. Krebs & the LENPIC Collaboration
Universität Bochum, ...



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