SRG Transformed Chiral NN+3N Interactions For Nuclear Structure

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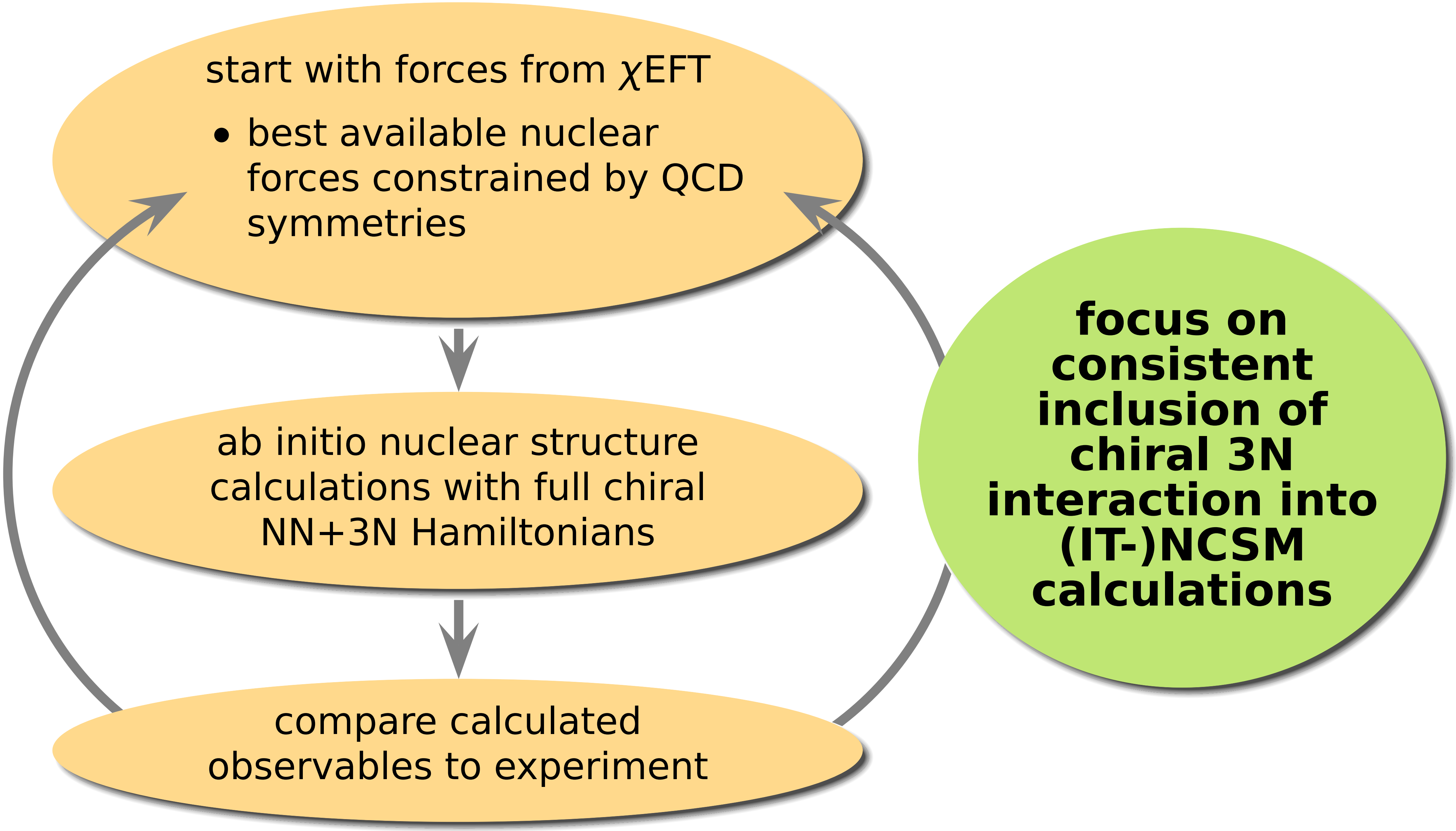
Round Trip: QCD and Nuclear Structure



Outline: From Diagrams to Observables

chiral forces
NN at N^{3}LO and 3N at N^{2}LO

↓

unitary transformation by
Similarity Renormalization Group

↓

trafo from Jacobi into
$\mathcal{J}T$-coupled matrix elements

↓

Importance-Truncated No-Core
Shell Model

↓

benchmark of SRG-transformed
chiral NN+3N Hamiltonians

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Similarity Renormalization Group (SRG)

evolution of the **Hamiltonian to band-diagonal form** with respect to uncorrelated many-body basis

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hamil

$$\tilde{H}_\alpha = U_\alpha{}^\dagger H U_\alpha$$

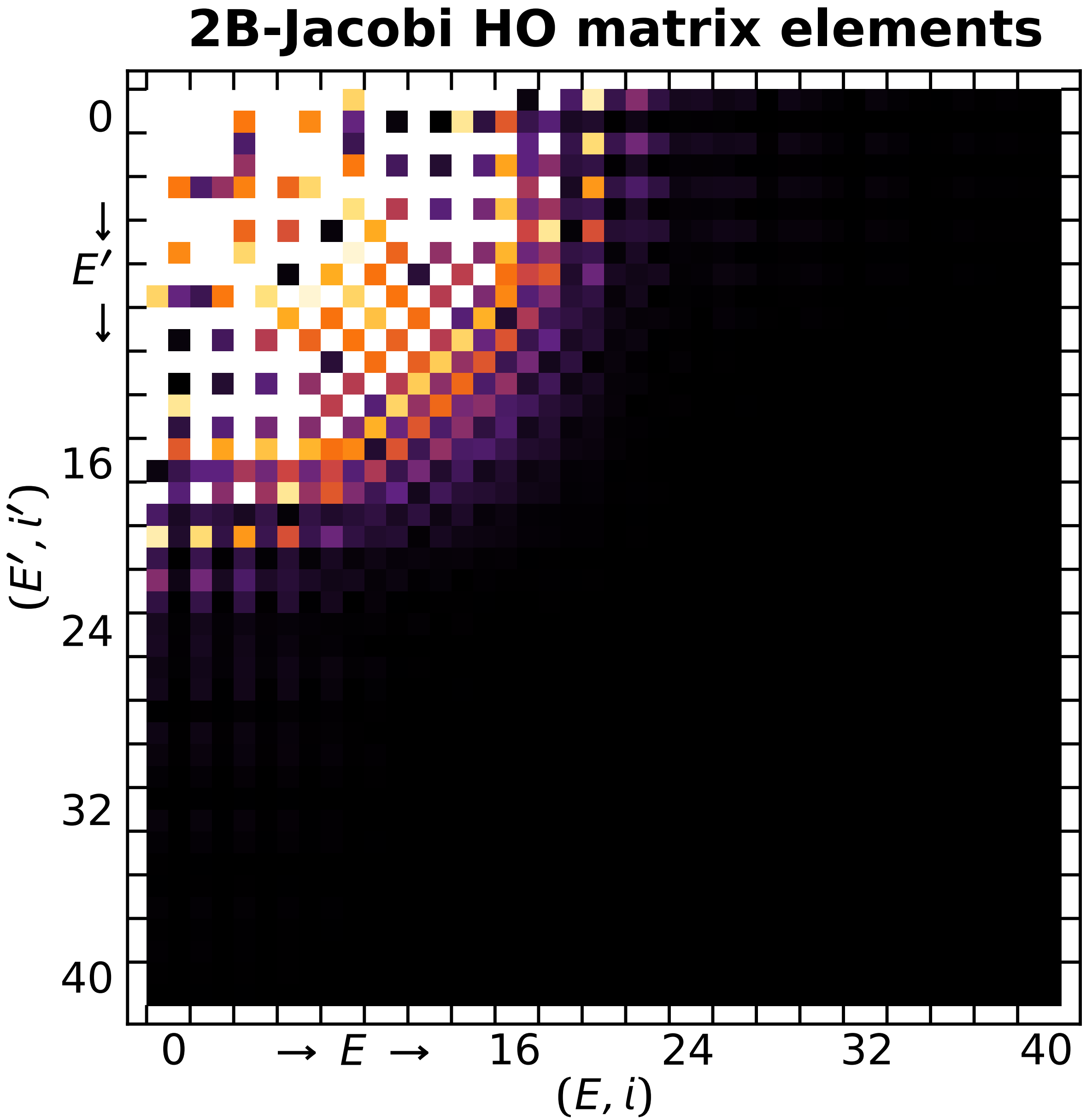
- **evolution equations** for $\tilde{H}_\alpha$ depending on generator η_α

$$\frac{d}{d\alpha}\tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \qquad \eta_\alpha^\dagger = -\eta_\alpha$$

- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta_\alpha = (2\mu)^2 [T_{int}, \tilde{H}_\alpha]$$

SRG Evolution in Two-Body Space

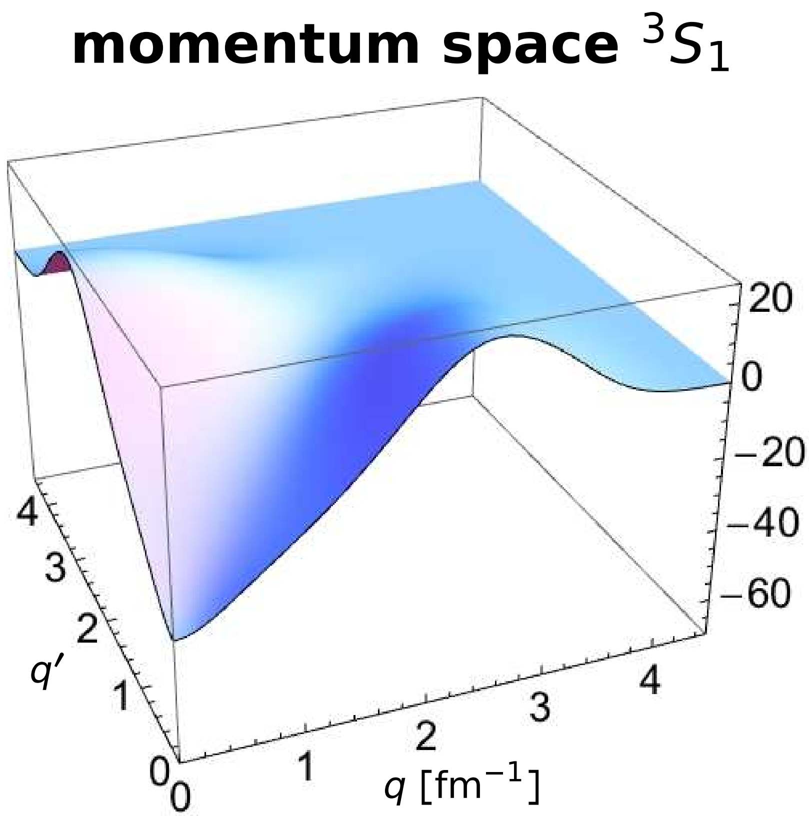


$\alpha = 0.00\,\mathrm{fm}^4$

$\Lambda = \infty\,\mathrm{fm}^{-1}$

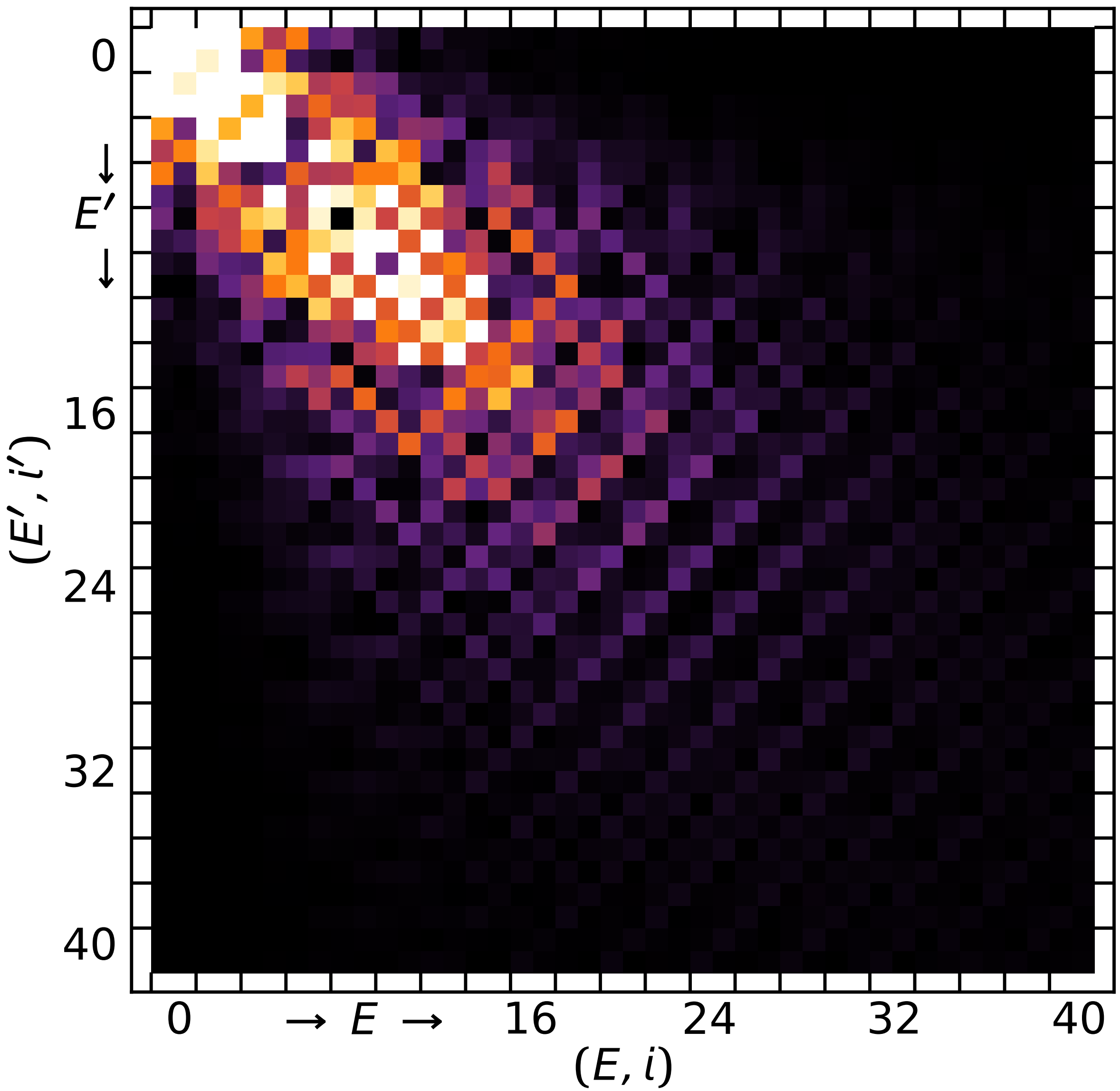
$\langle E'(L'S)J^\pi T |\, \widetilde{\mathrm{H}}_\alpha \,| E(LS)J^\pi T \rangle$

$J^\pi = 1^+, T = 0, \hbar\Omega = 28\,\mathrm{MeV}$



SRG Evolution in Two-Body Space

2B-Jacobi HO matrix elements



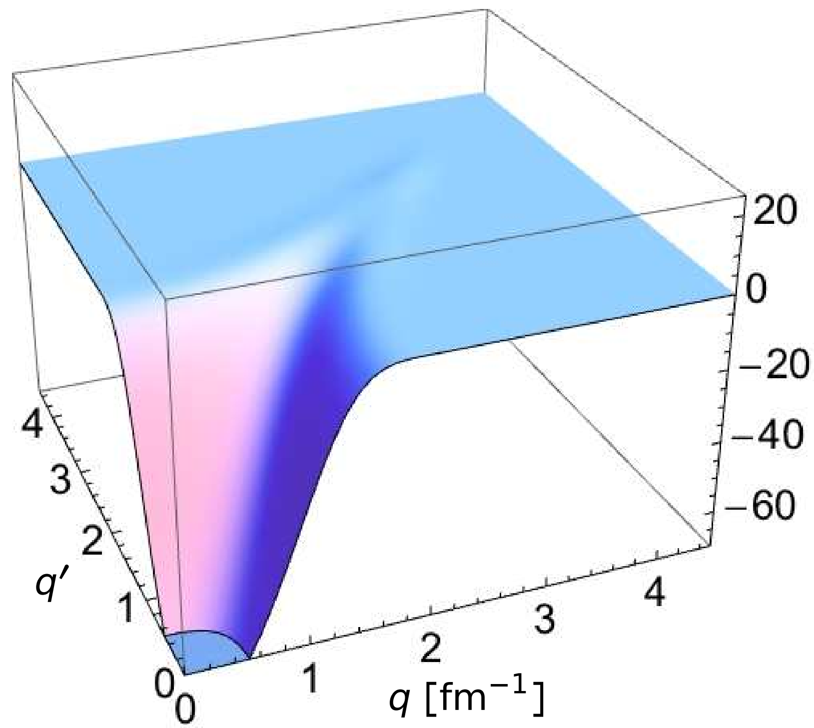
$\alpha = 0.32\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

$\langle E'(L'S)J^\pi T | \widetilde{\mathrm{H}}_\alpha | E(LS)J^\pi T \rangle$

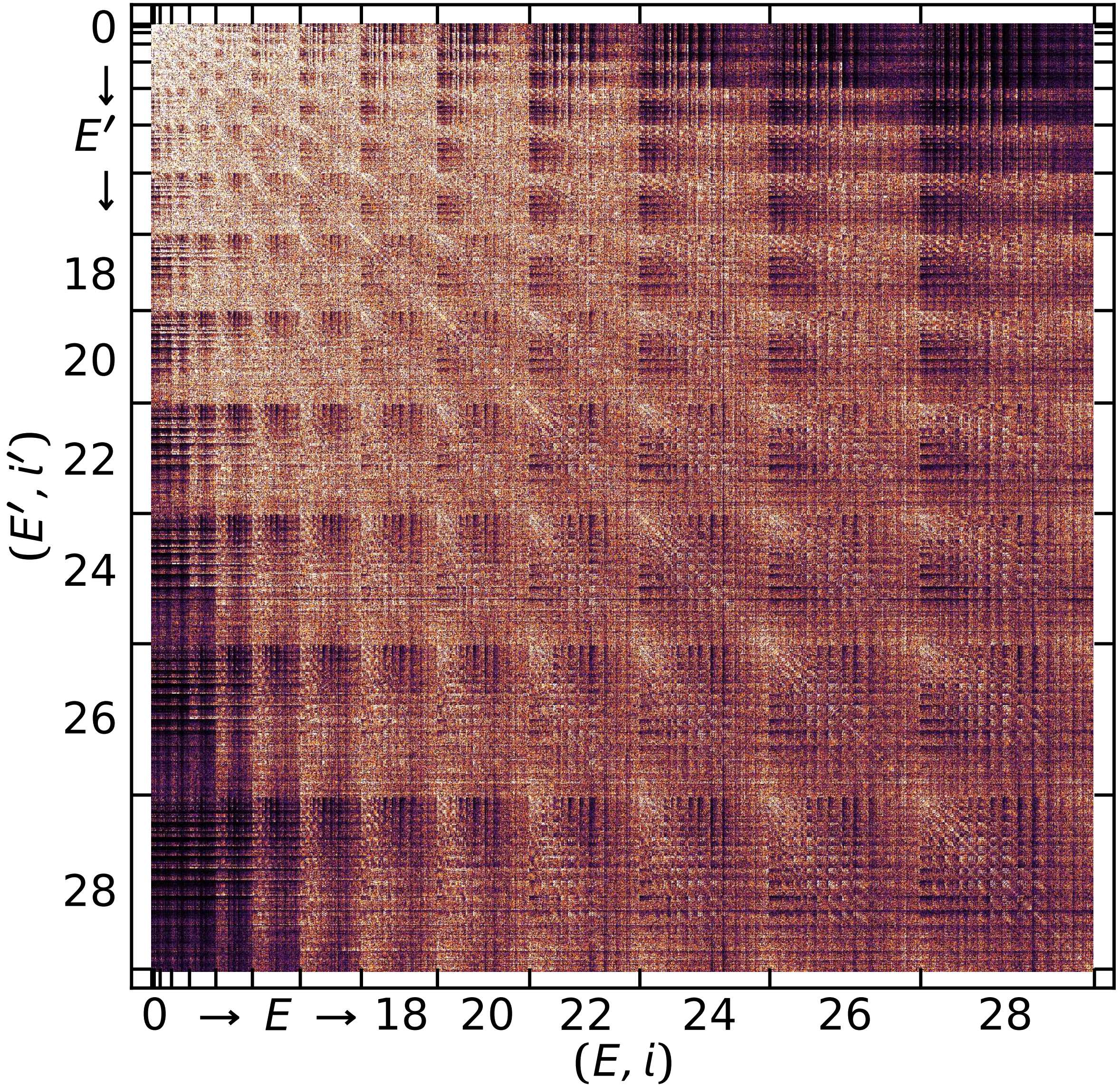
$J^\pi = 1^+, T = 0, \hbar\Omega = 28\,\mathrm{MeV}$

momentum space $^3S_1$



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



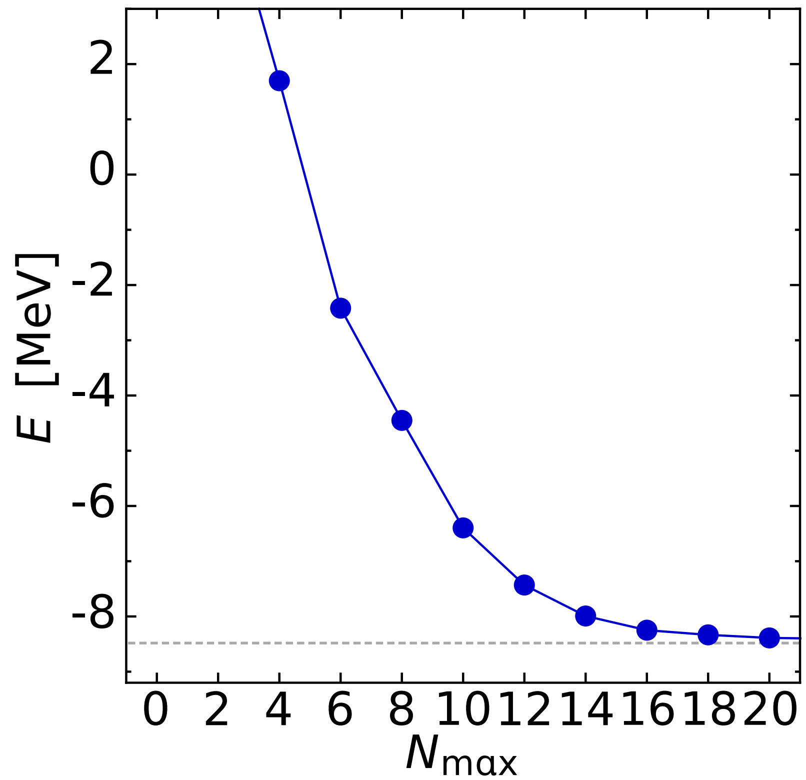
$$\alpha = 0.00\,\mathrm{fm}^4$$

$\Lambda = \infty\,\mathrm{fm}^{-1}$

$$\langle E' i' J T | \widetilde{\mathrm{H}}_\alpha | E i J T \rangle$$

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

NCSM ground state ^{3}H



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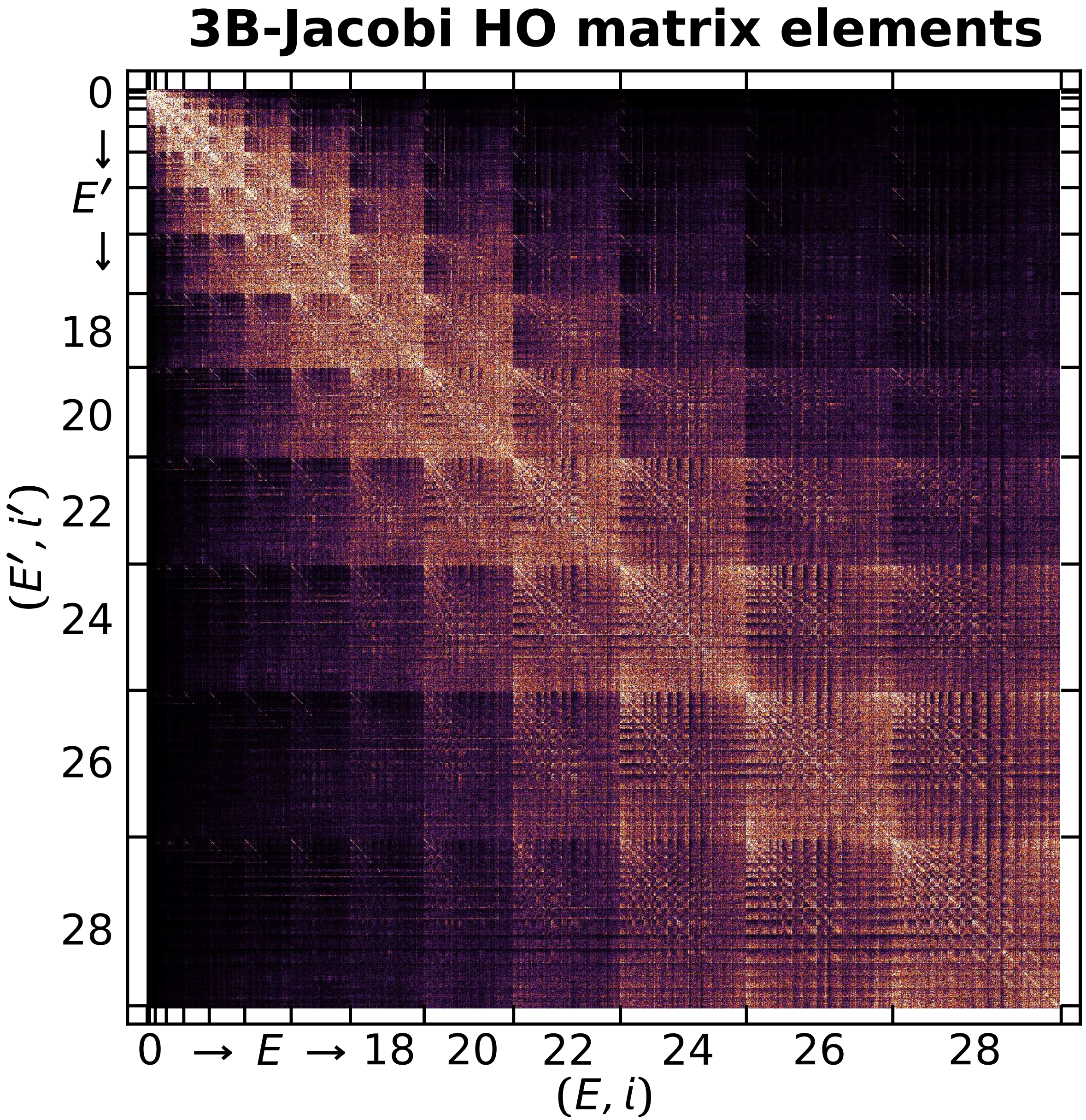

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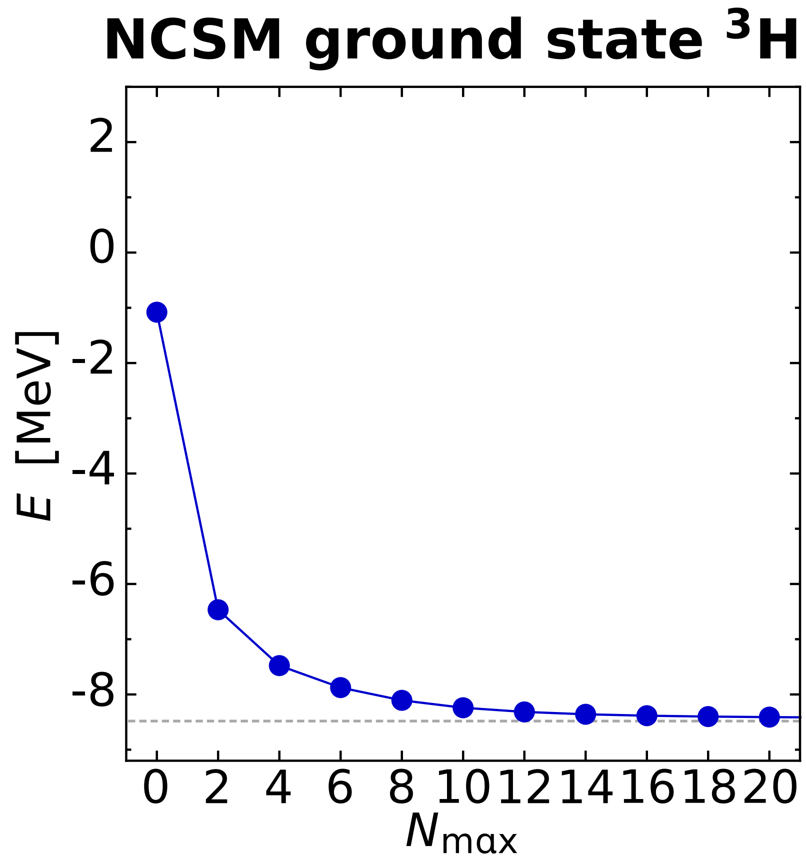

Calculations in *A*-Body Space

- **irreducible *n*-body contributions** $\widetilde{H}_\alpha^{[n]}$ induced by the SRG transformation

$$\widetilde{H}_\alpha = \widetilde{H}_\alpha^{[1]} + \widetilde{H}_\alpha^{[2]} + \widetilde{H}_\alpha^{[3]} + \dots$$

- **cluster truncation**: can construct cluster-orders up to $n = 3$ from evolution in 2B and 3B space, have to discard $n > 3$
  - only the **full evolution in *A*-body space** conserves *A*-body energy eigenvalues and, thus, independence of α
  - α-dependence of eigenvalue **milto-**
    nian measures impact of

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

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$\mathcal{J}T$-coupled matrix elements

m-scheme matrix elements needed
for many-body calculations

$$
{}_a\langle [(j_a, j_b)J_{ab}, j_c]\mathcal{J}, [(t_a, t_b)t_{ab}, t_c]T |\, \mathrm{H}\, | [(j'_a, j'_b)J'_{ab}, j'_c]\mathcal{J}, [(t_a, t_b)t'_{ab}, t_c]T \rangle_a
$$

$$
= 3! \sum_{l_{cm}} \times \sum_{\alpha} \tilde{T} \begin{pmatrix} a & b & c & J_{ab} & J & \mathcal{J} \\ n_{cm} & l_{cm} & n_{12} & l_{12} & n_3 & l_3 \\ s_{ab} & j_{12} & j_3 & & & \end{pmatrix} \times \sum_{\alpha'} \tilde{T} \begin{pmatrix} a' & b' & c' & J'_{ab} & J & \mathcal{J} \\ n_{cm} & l_{cm} & n'_{12} & l'_{12} & n'_3 & l'_3 \\ s'_{ab} & j'_{12} & j'_3 & & & \end{pmatrix} \times \sum_{i,i'} c_{\alpha,i}\, c_{\alpha',i'} \left\langle EJTi \right| \mathrm{H} \left| E'JTi' \right\rangle
$$

- *m*-scheme matrix elements very memory consuming
- transformation directly into $\mathcal{J}T$**-coupled** *m*-scheme
  - key for efficient application up to $E_{3\text{max}}=16$
  - computational demanding
- developed optimized storage scheme for **fast on-the-fly decoupling**

$\tilde{T}$ coefficients...

$$\tilde{T}\begin{pmatrix} a & b & c & J_{ab} & J & \mathcal{J} \\ n_{cm} & l_{cm} & n_{12} & l_{12} & n_3 & l_3 \\ s_{ab} & j_{12} & j_3 & & & \end{pmatrix}$$
$$= \sum_{L_{ab}}\sum_{\mathcal{L}_{12}}\sum_{\mathcal{L}}\sum_{S_3}\sum_{\Lambda}$$
$$\times\, \delta_{2n_a+l_a+2n_b+l_b+2n_c+l_c,2n_{cm}+l_{cm}+2n_3+l_3+2n_{12}+l_{12}}$$
$$\times\, \langle\langle \mathcal{N}_{12}\mathcal{L}_{12}, n_{12}l_{12}; L_{ab} | n_b l_b, n_a l_a \rangle\rangle_1$$
$$\times\, \langle\langle n_{cm}l_{cm}, n_3 l_3; \Lambda | \mathcal{N}_{12}\mathcal{L}_{12}, n_c l_c \rangle\rangle_2$$
$$\times \begin{Bmatrix} l_a & l_b & L_{ab} \\ s_a & s_b & s_{ab} \\ j_a & j_b & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{ab} & l_c & \mathcal{L} \\ s_{ab} & s_c & S_3 \\ J_{ab} & j_c & \mathcal{J} \end{Bmatrix} \begin{Bmatrix} l_{12} & l_3 & L_3 \\ s_{ab} & s_c & S_3 \\ j_{12} & j_3 & J \end{Bmatrix}$$
$$\times \begin{Bmatrix} l_c & \mathcal{L}_{12} & \Lambda \\ l_{12} & \mathcal{L} & L_{ab} \end{Bmatrix} \begin{Bmatrix} l_{cm} & l_3 & \Lambda \\ l_{12} & \mathcal{L} & L_3 \end{Bmatrix} \begin{Bmatrix} l_{cm} & L_3 & \mathcal{L} \\ S_3 & \mathcal{J} & J \end{Bmatrix}$$
$$\times\, \hat{j}_a \hat{j}_b \hat{j}_c \hat{J}_{ab} \hat{j}_{12} \hat{j}_3 \hat{s}_{ab} \hat{J} \hat{S}_3^2 \hat{\mathcal{L}}^2 \hat{\Lambda}^2 \hat{L}_3^2 \hat{L}_{ab}^2 (-1)^{l_c+\Lambda+L_{ab}+\mathcal{L}+S_3+l_{12}+\mathcal{J}}$$

scalar product of harmonic oscillator states of the two representations

- **harmonic oscillator brackets** $\langle\langle \ldots | \ldots \rangle\rangle$ & various **angular momentum recouplings** neccessary for coordinate transformation
- precaching indispensable

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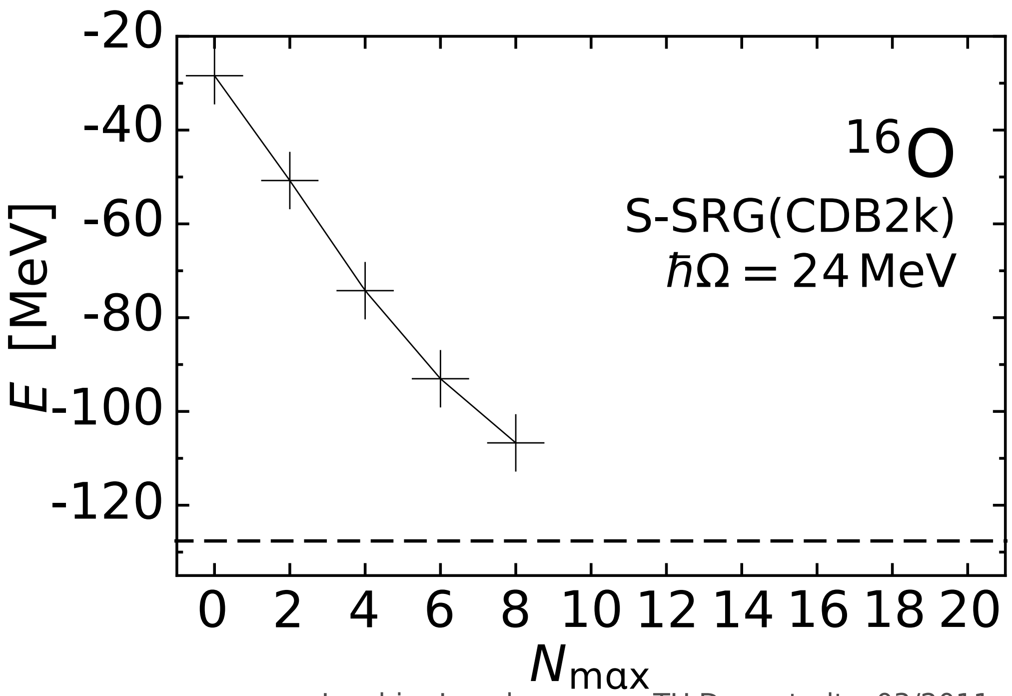
No-Core Shell Model (NCSM)

NCSM is one of the most powerful and universal exact ab initio methods

- compute low-lying eigenvalues of the Hamiltonian in a **model space of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\mathrm{max}}\hbar\Omega$
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of Slater-determinant basis with N_{max} and A



Importance Truncation: Basic Idea

- given a initial approximation $|\Psi_{\text{ref}}\rangle$ for the **target state** within a limited **reference space $\mathcal{M}_{\text{ref}}$**

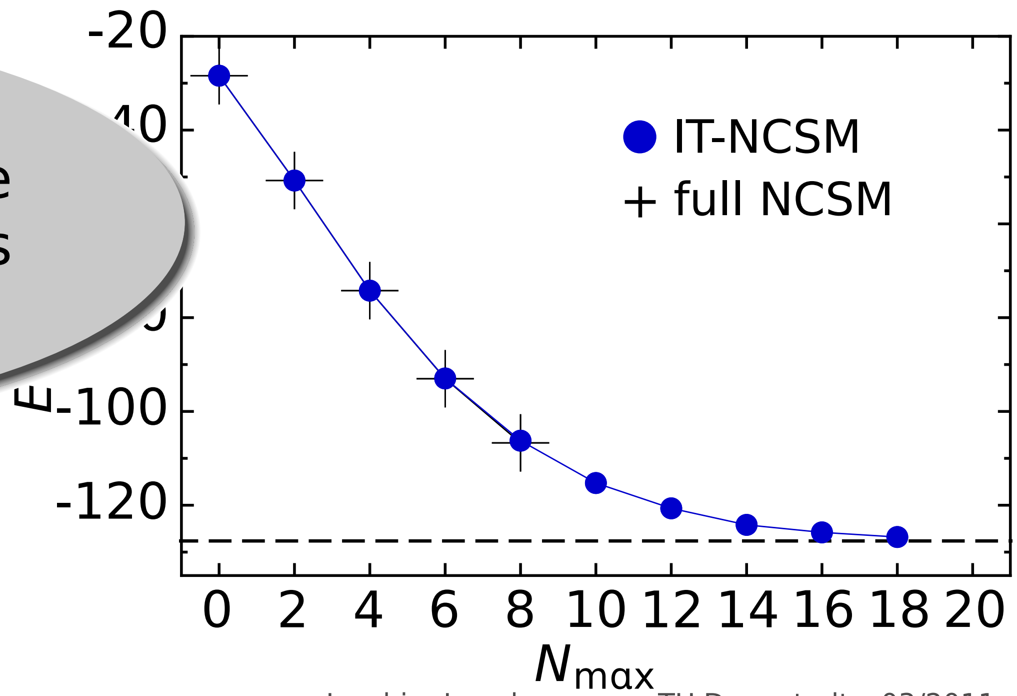
$$|\Psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_{\nu}^{(\text{ref})} |\Phi_{\nu}\rangle$$

- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

$\kappa_{\nu} =$ $\langle \Phi_{\nu} | H$ …

we have developed an parallelized IT-NCSM code that can handle 3N forces up to $E_{3\text{max}}$=16

- c…
  tru…
  spanned …
  with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$
  and solve eigenvalue problem



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A Tale of Three Hamiltonians

- **NN only**: start with NN-only initial Hamiltonian and evolve in two-body space

$$\tilde{H}_{\alpha}^{\text{NN-only}} = T_{\text{int}} + \tilde{T}_{\text{int},\alpha}^{[2]} + \tilde{V}_{\text{NN},\alpha}^{[2]}$$

- **NN+3N-induced**: start with NN-only initial Hamiltonian and evolve in three-body space

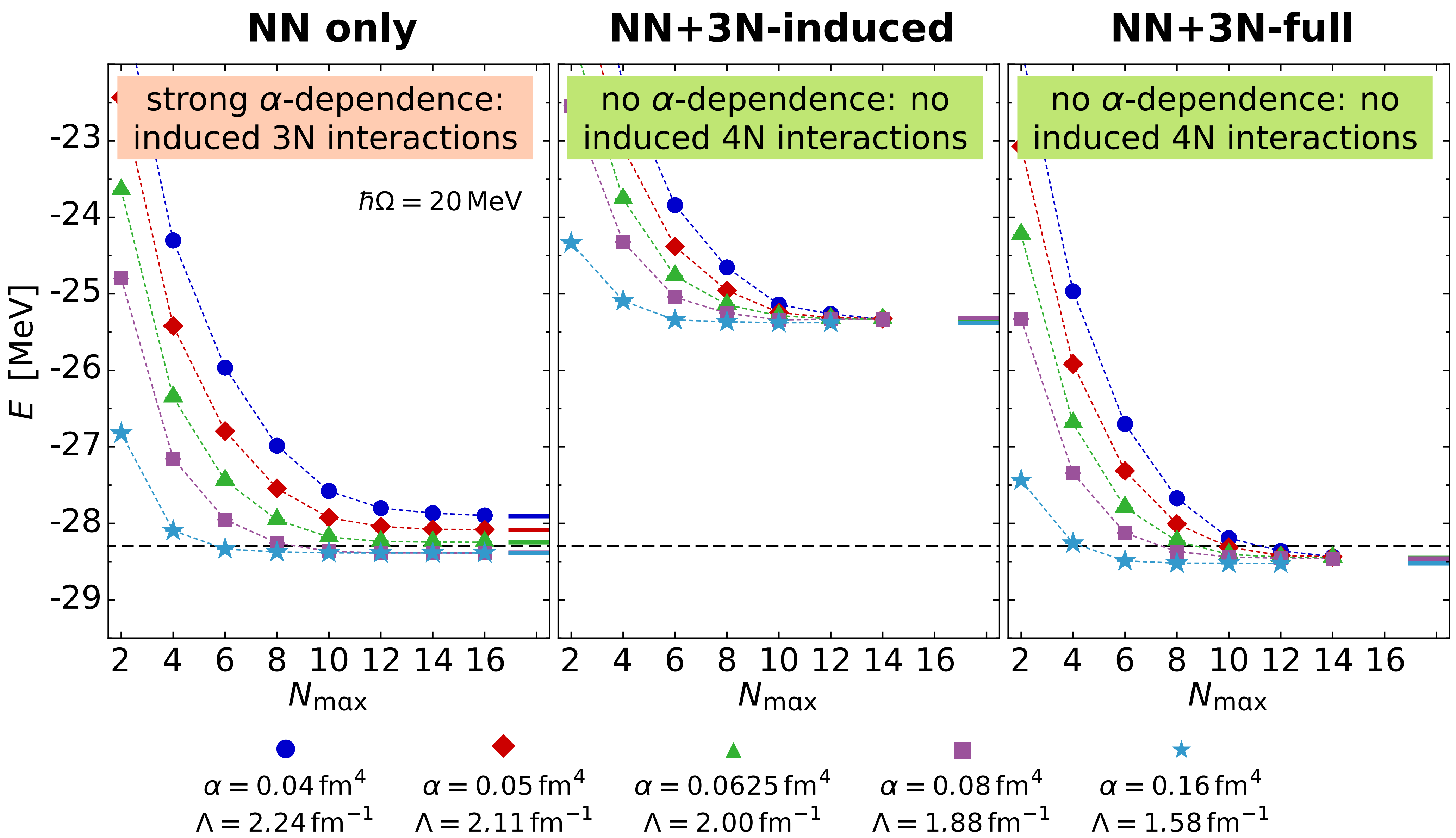
$$\tilde{H}_{\alpha}^{\text{NN+3N-induced}} = T_{\text{int}} + \tilde{T}_{\text{int},\alpha}^{[2]} + \tilde{V}_{\text{NN},\alpha}^{[2]} + \tilde{T}_{\text{int},\alpha}^{[3]} + \tilde{V}_{\text{NN},\alpha}^{[3]}$$

- **NN+3N-full**: start with NN+ … in three-body space

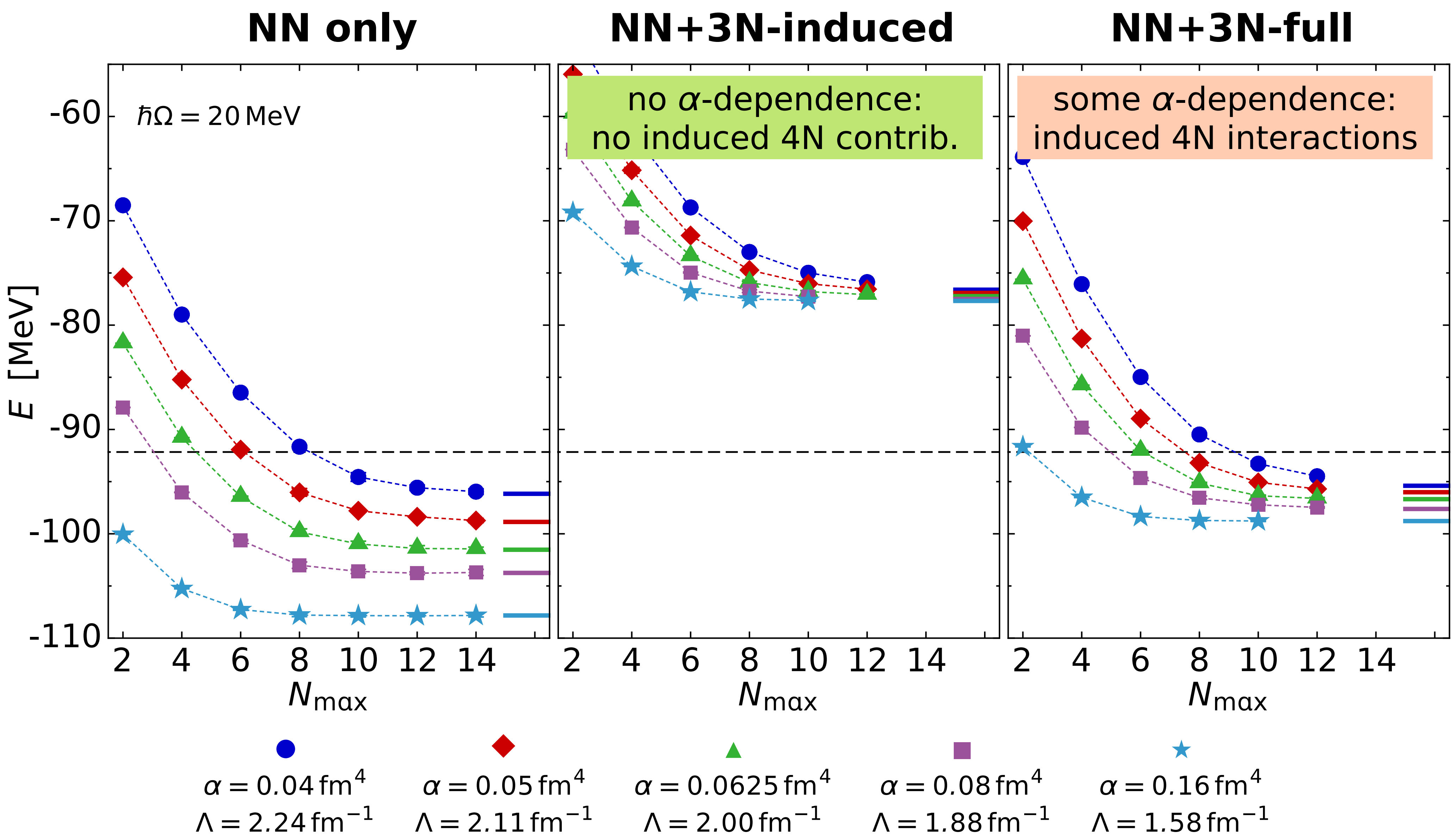
$$\tilde{H}_{\alpha}^{\text{NN+3N-full}} = T_{\text{int}} + \tilde{T}_{\text{int},\alpha}^{[\ldots]} \ldots$$

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

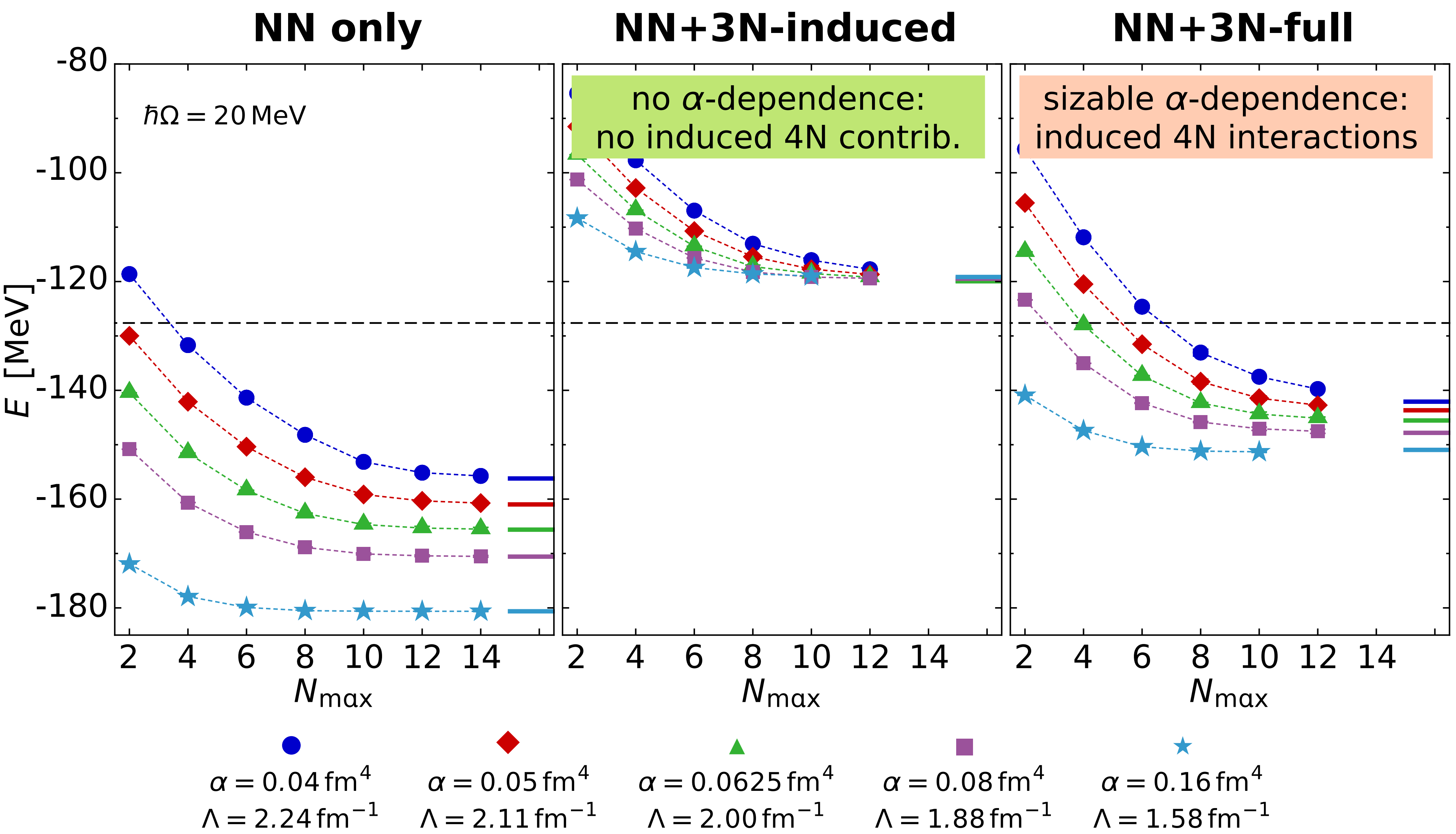
^{4}He: Ground-State Energies



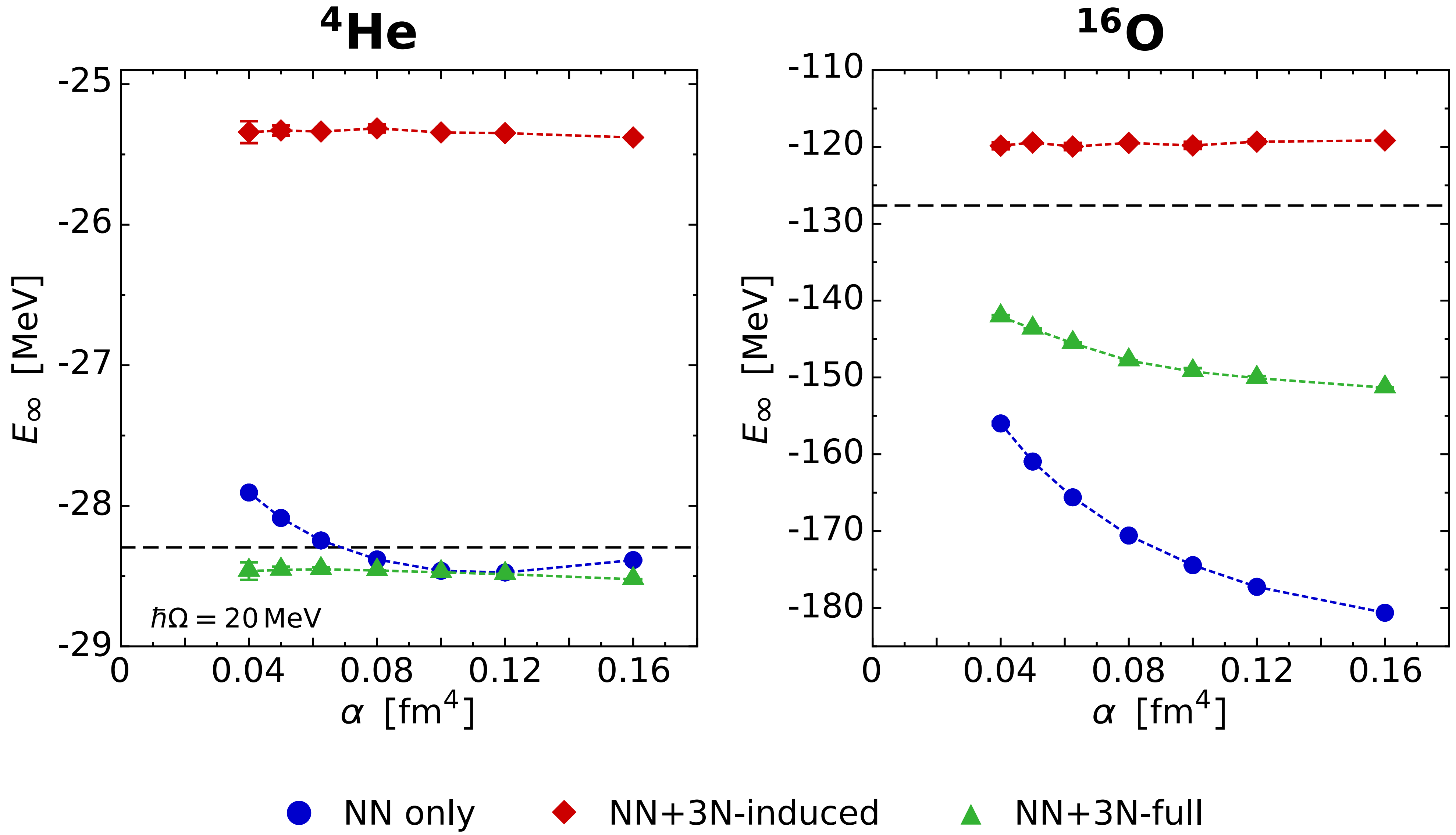
^{12}C: Ground-State Energies



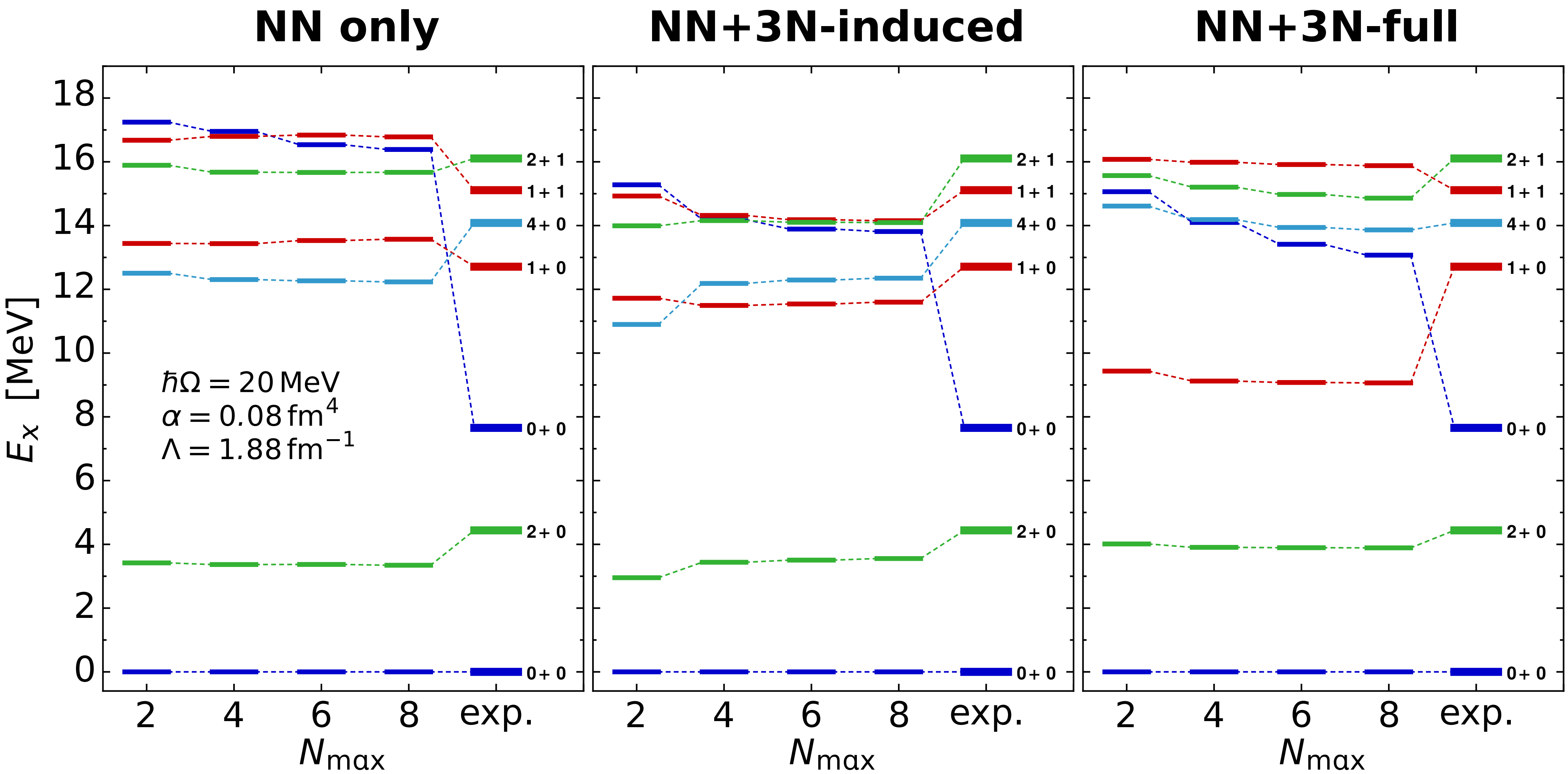
^{16}O: Ground-State Energies



^{16}O & ^{4}He: Energy vs. Flow Parameter



^{12}C: Spectroscopy



Conclusions

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- ab initio nuclear structure calculations with consistently SRG-evolved chiral NN+3N interactions
  - consistent SRG evolution up to the 3N level
  - efficient transformation and management of $\mathcal{J}T$-coupled 3N matrix elements
  - IT-NCSM with full 3N interactions up to $N_{\max} = 12$ (14) for all p-shell nuclei (and lower sd-shell)
- indications that induced 4N contributions resulting from initial 3N interaction become significant beyond mid-p-shell
- use modified SRG generators to suppress induced 4N contributions from the outset
- many exciting applications ahead...

Epilogue

- **thanks to our group & collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, A. Günther, M. Hild, H. Krutsch, P. Papakonstantinou, S. Reinhardt, **R. Roth**, F. Schmitt, C. Stumpf, R. Wirth

    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**

    TRIUMF Vancouver, Canada
- we thank Jülich Supercomputing Centre (JSC) & LOEWE-CSC for computing time

Thank you for your attention!

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