Ab Initio Spectroscopy and Sensitivity to Chiral 3N Interactions

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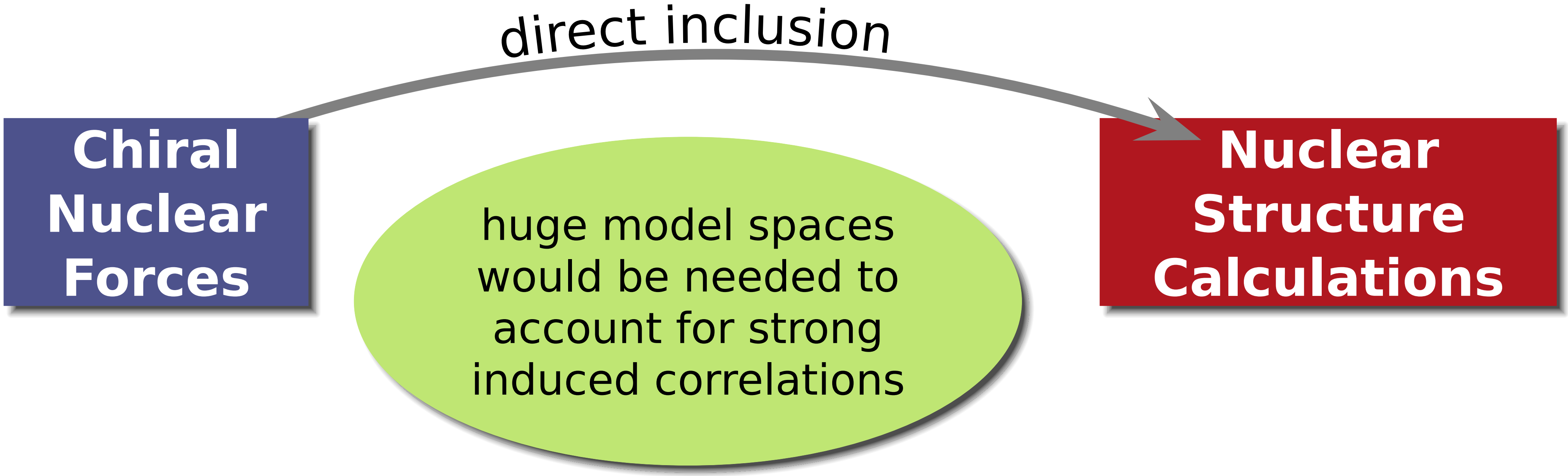
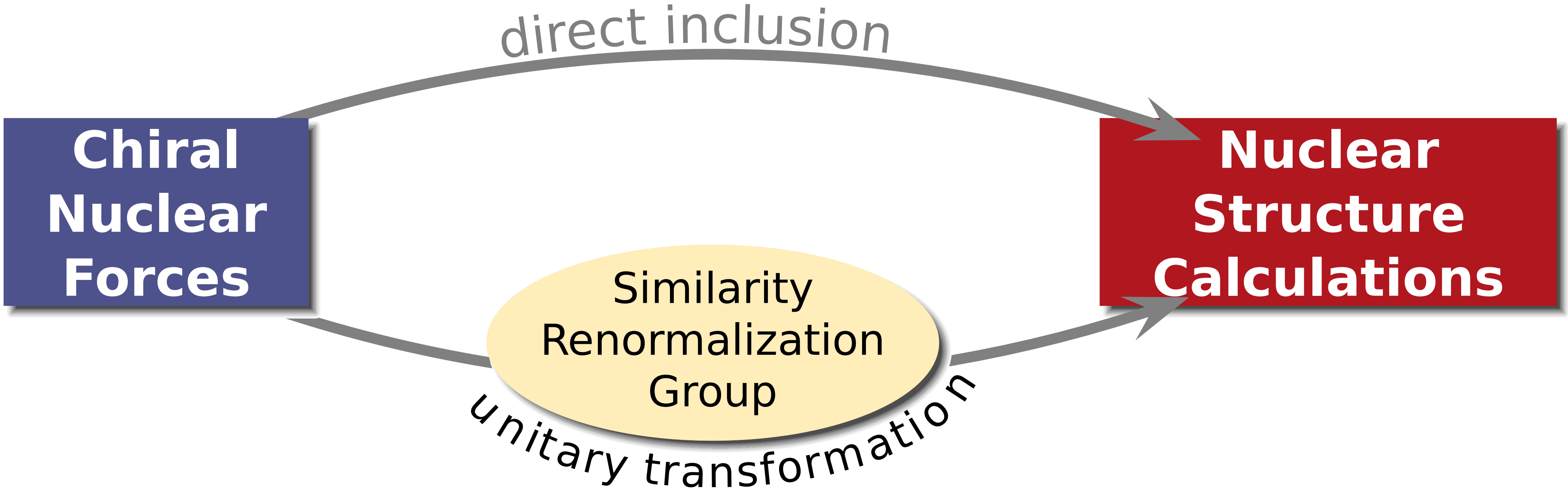
Chiral Hamiltonian



Chiral Hamiltonian



- NN interaction @ N^3LO [Entem, Machleidt, Phys.Rev C68, 041001(R) (2003)]
- 3N interaction @ N^2LO

- c_D & c_E fixed by binding energy and β-decay halflife of triton

  [Gazit et.al., Phys.Rev.Lett. 103, 102502 (2009)]

Technology: From Diagrams to Observables

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

↓

unitary transformation by Similarity Renormalization Group

benchmark of SRG-transformed chiral NN+3N Hamiltonians

Similarity Renormalization Group (SRG)

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

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hamil

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

- **evolution equation** for $\widetilde{H}_\alpha$ depending on generator η_α

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

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

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

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

benchmark of SRG-transformed
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$\mathcal{J}T$-coupled vs. m-scheme Matrix Elements

- m-scheme state

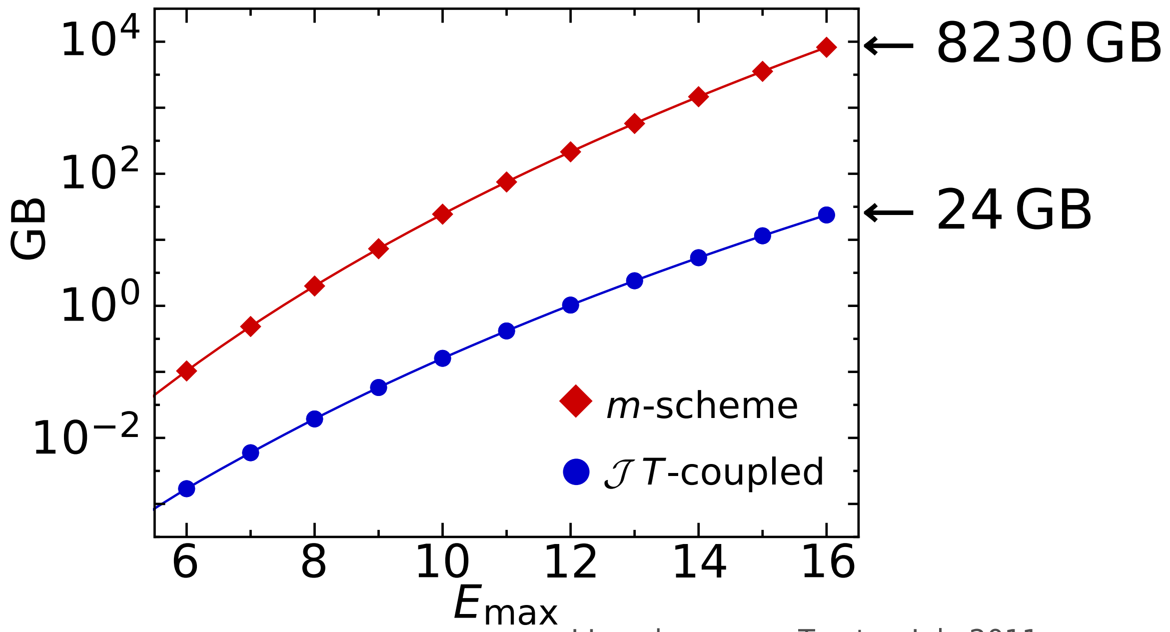
$$|(n_a l_a, s_a) j_a m_a, (n_b l_b, s_b) j_b m_b, (n_c l_c, s_c) j_c m_c, t_a m_{t_a}, t_a m_{t_b}, t_c m_{t_c}\rangle_a$$

- $\mathcal{J}$ T-coupled state

$$|\{[(n_a l_a, s_a) j_a, (n_b l_b, s_b) j_b] J_{ab}, (n_c l_c, s_c) j_c\} \mathcal{J}, [(t_a, t_b) t_{ab}, t_c] T\rangle_a$$

⇒ basic symmetries of the Hamiltonian can only be used in the $\mathcal{J}T$-coupled scheme

more than two orders of magnitude reduced memory needs



$\mathcal{J}T$-coupled Matrix Elements

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

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

- transformation directly into $\mathcal{J}T$**-coupled** scheme
  - key for efficient application up to $E_{3\max}$=16
  - computationally demanding
- invented optimized storage scheme for **fast on-the-fly decoupling**
- optimal for many-body approaches that rely on *m*-scheme matrix elements

$\tilde{T}$ 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

Technology: 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

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Importance-Truncated No-Core Shell Model

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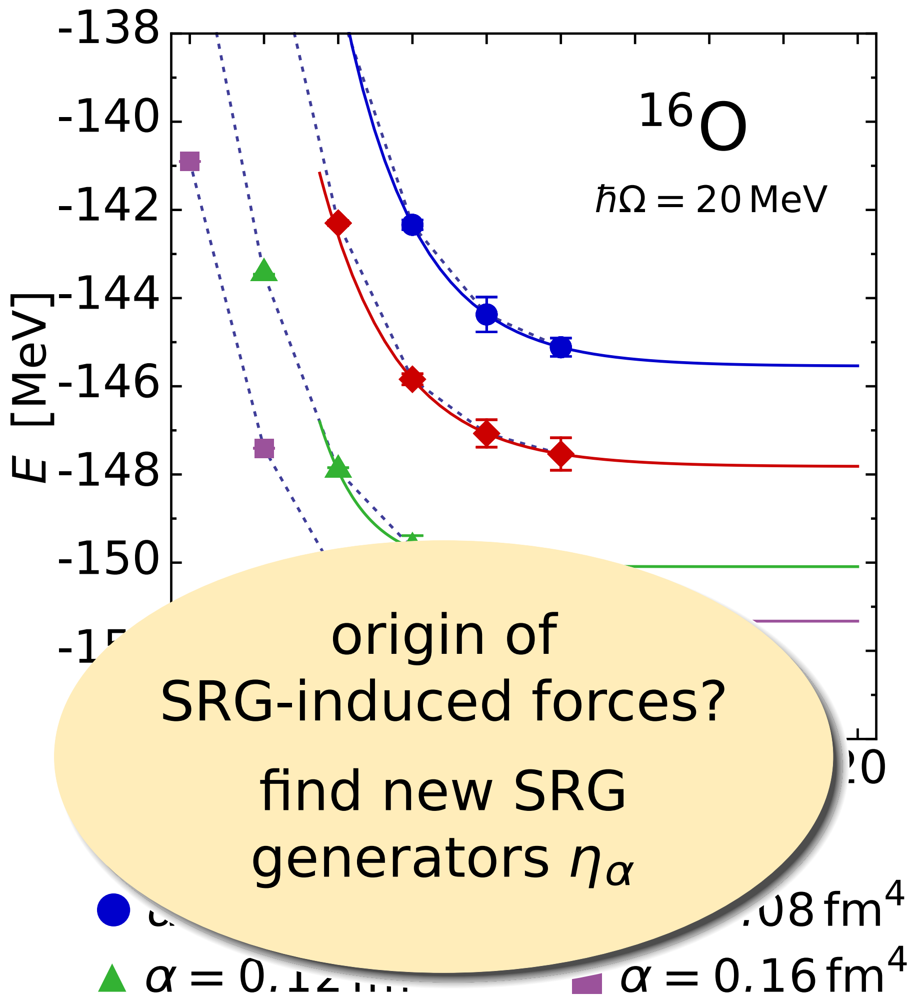
benchmark of SRG-transformed chiral NN+3N Hamiltonians

Reminder: Results in upper p-Shell

- sizable α-dependence of absolute energies



origin of SRG-induced forces?

find new SRG generators η_α

[Roth, Langhammer, Calci, Binder, Navrátil arXiv1105.3173]

Alternative SRG Generators
– First Results –

Modified SRG Generator

Find SRG generator that...

- preserves pre-diagonalization, i.e. improved convergence during many-body calculation
- suppresses induced four- and higher-body interactions from the outset

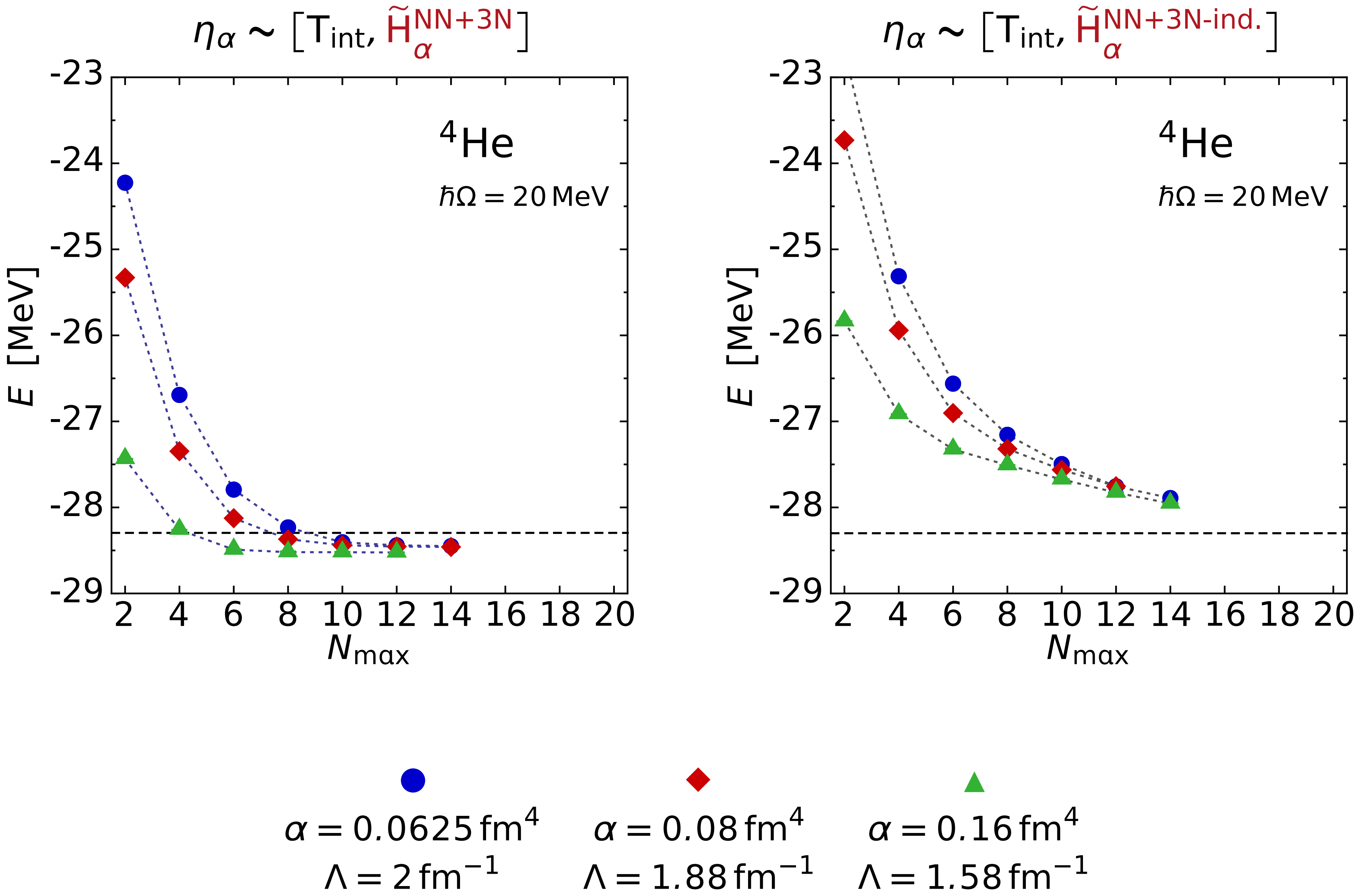
- α-dependence induced by initial 3N interaction (N^2LO)

  $\Rightarrow$ idea: leave out initial 3N force in the generator

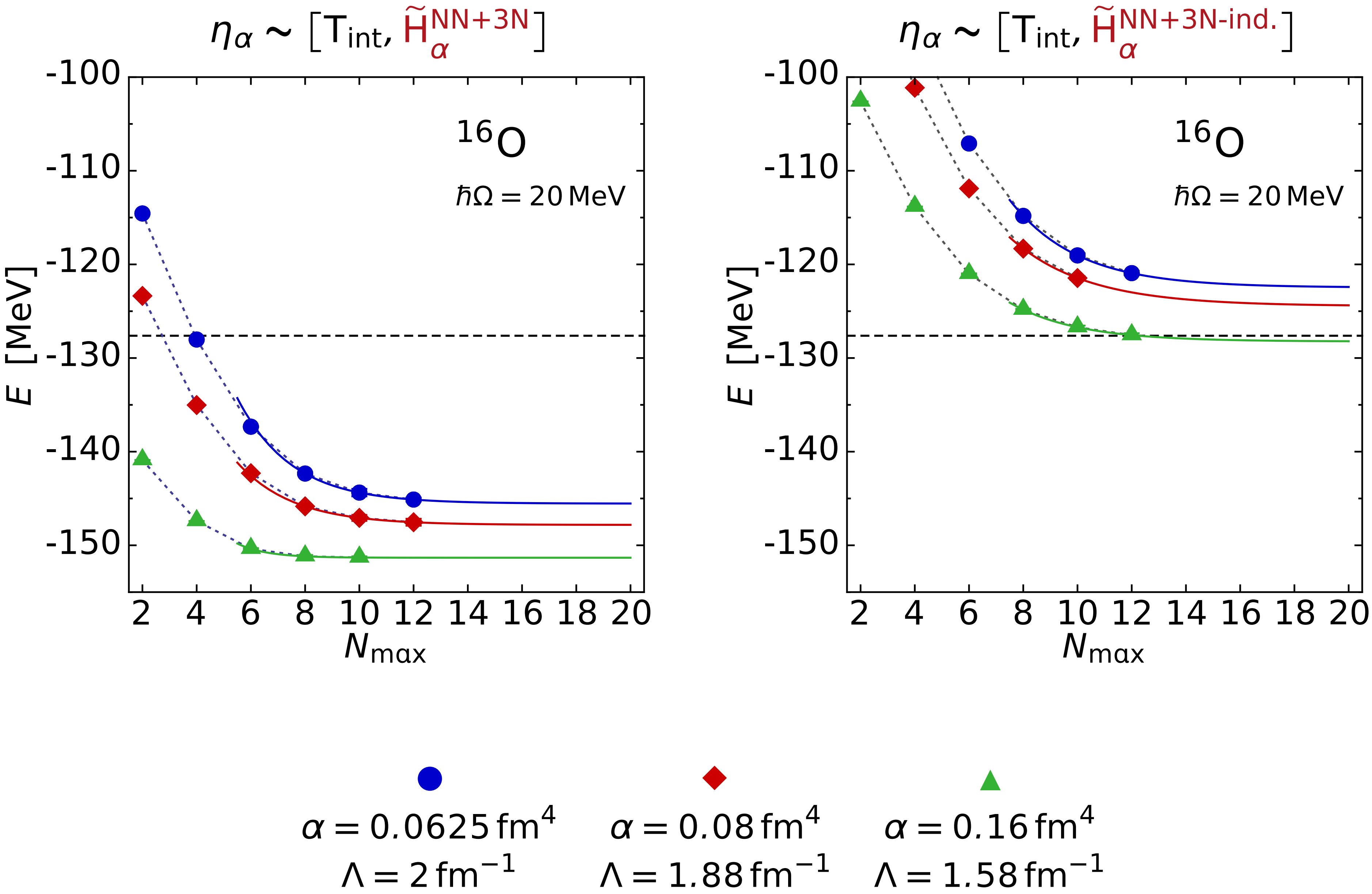
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}_\alpha^{\mathrm{NN+3N}} = \Big[\underbrace{(2\mu)^2\left[\mathrm{T}_{\mathrm{int}}, \widetilde{\mathrm{H}}_\alpha^{\mathrm{NN+3N\text{-}ind.}}\right]}_{\eta_\alpha}, \widetilde{\mathrm{H}}_\alpha^{\mathrm{NN+3N}}\Big]$$

- simultaneous evolution of the NN+3N and NN+3N-induced Hamiltonian needed

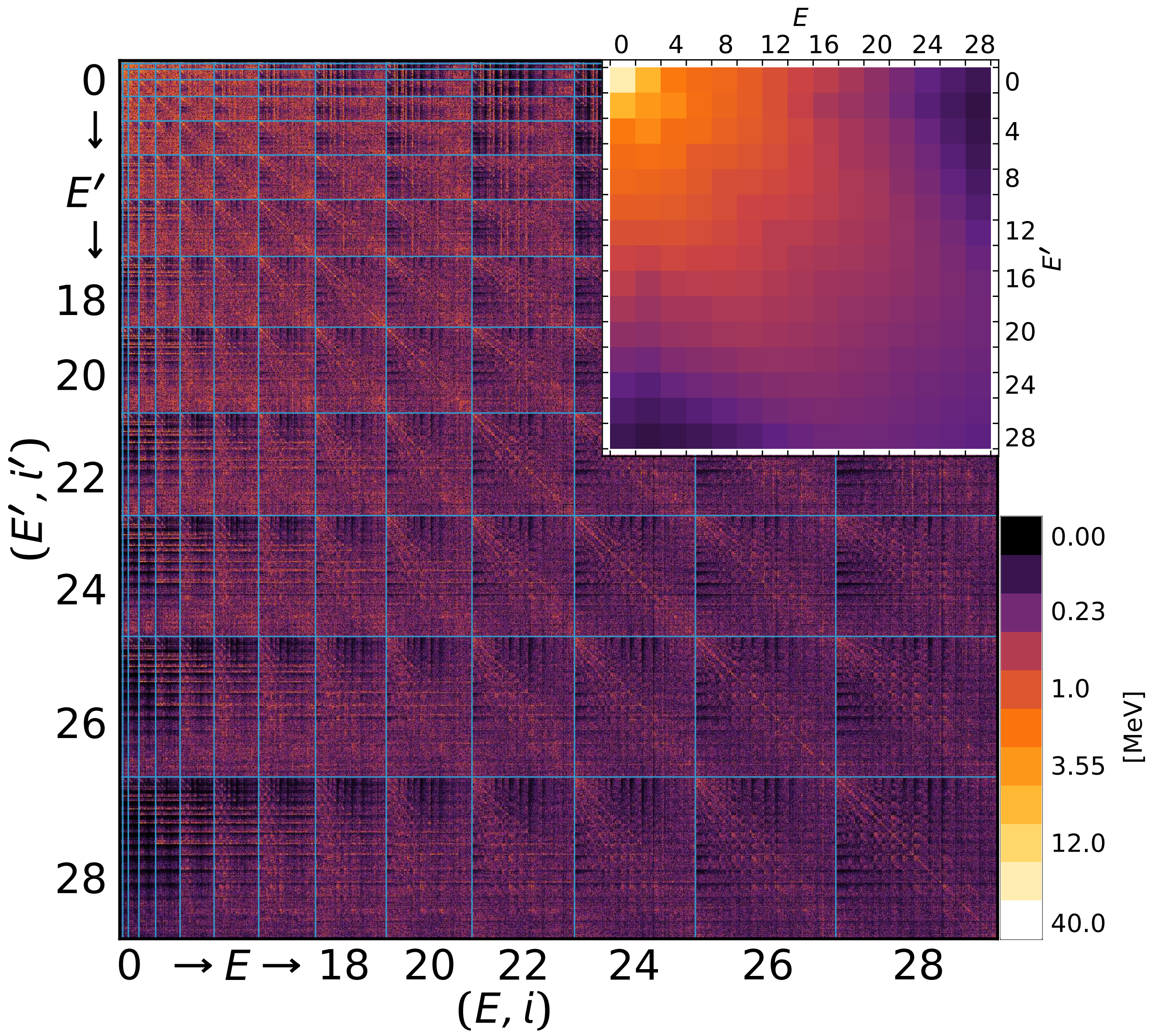
^{4}He - Standard vs. Modified SRG



^{16}O - Standard vs. Modified SRG



Matrix Element Analysis

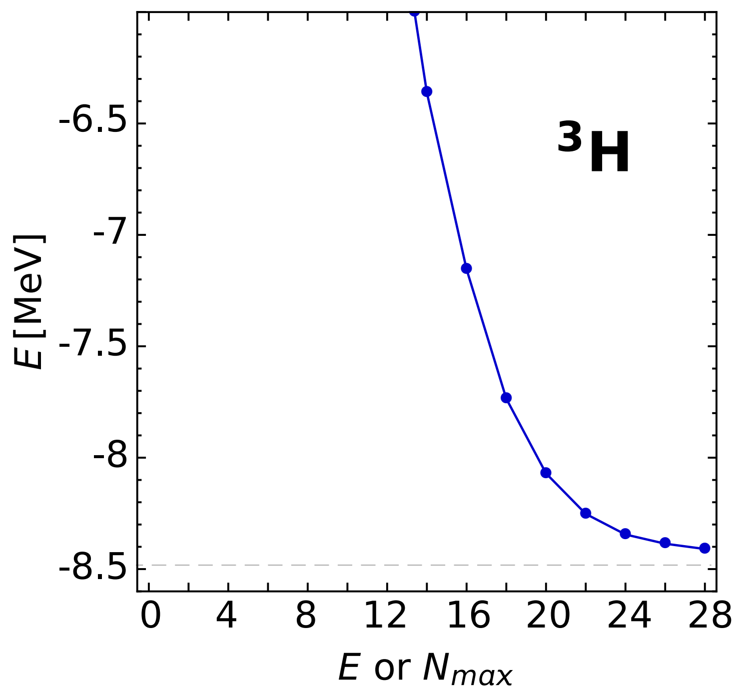


$$\alpha = 0.00\,\mathrm{fm}^4$$

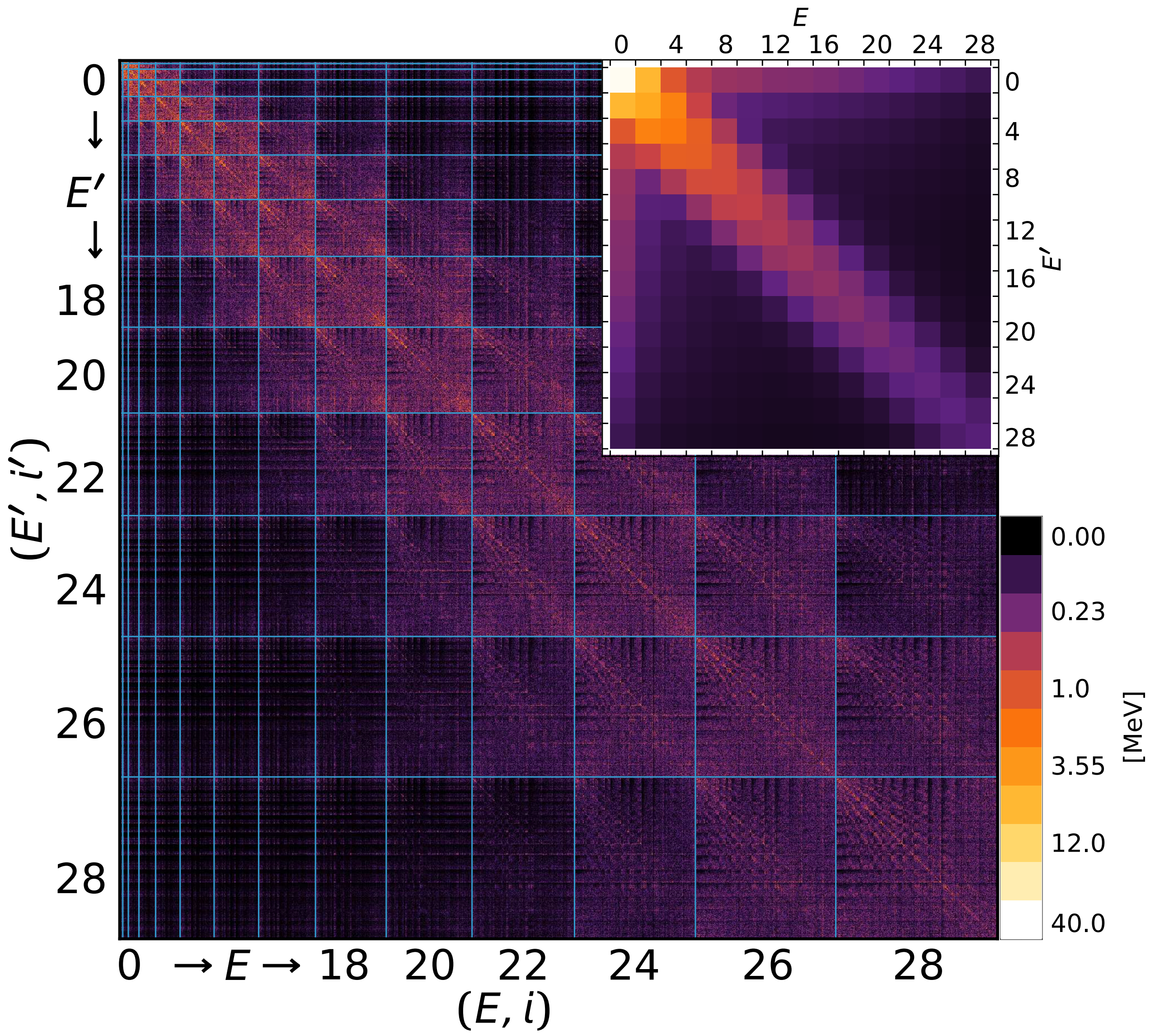
$\Lambda = \infty\,\mathrm{fm}^{-1}$

$$\langle EJTi \,|\, (\mathrm{H}^{\mathrm{NN+3N}} - \mathrm{T}_{int}) \,|\, E'JTi' \rangle$$

$$T = \tfrac{1}{2} \quad J^\pi = \tfrac{1}{2}^+ \quad \hbar\Omega = 20\,\mathrm{MeV}$$



Matrix Element Analysis

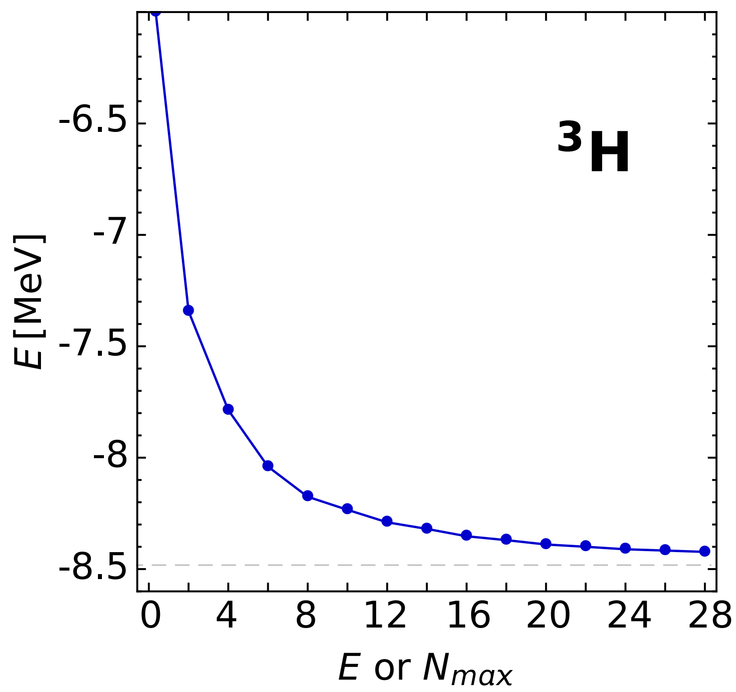


$\alpha = 0.32\,\mathrm{fm}^4$

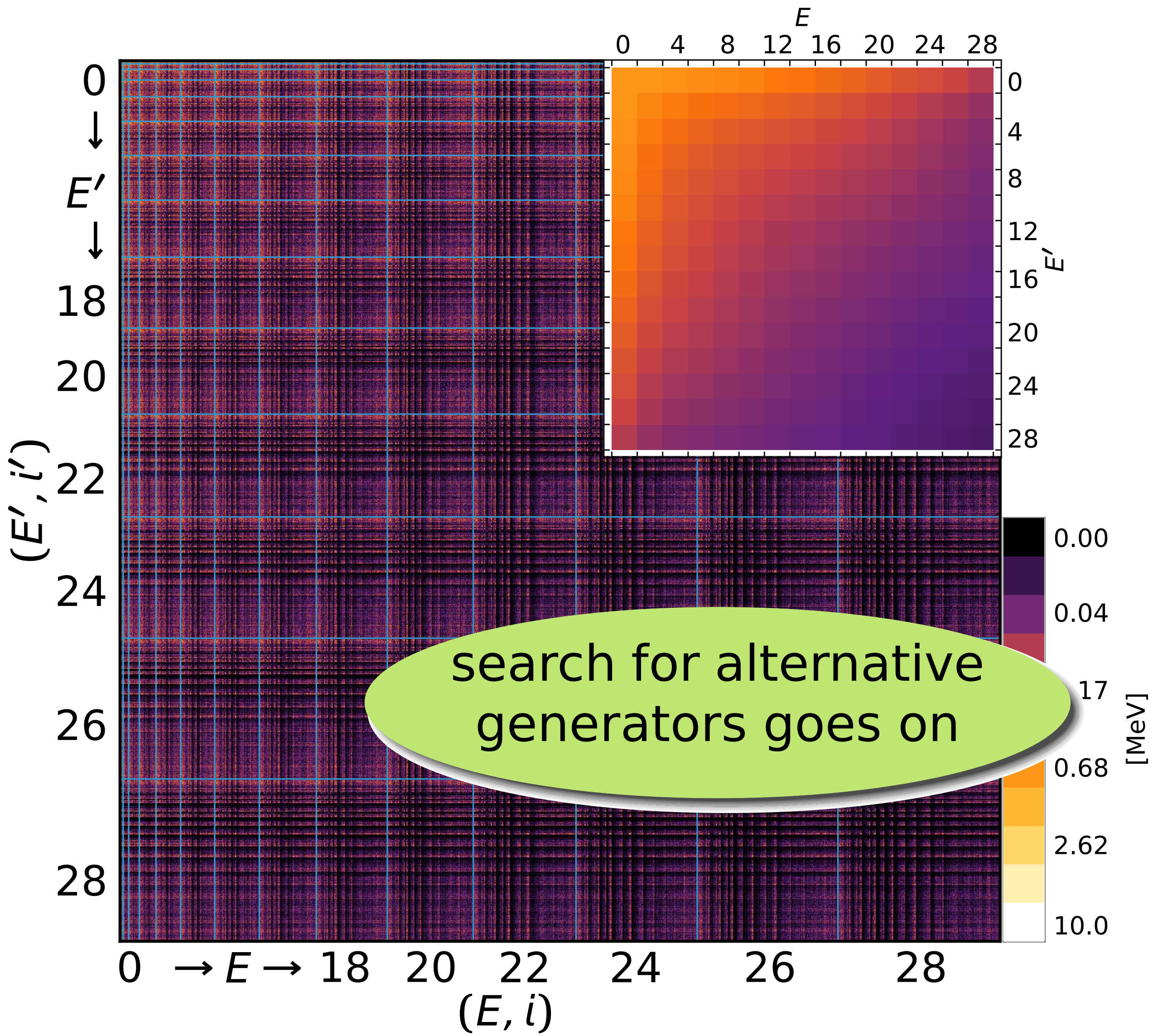
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

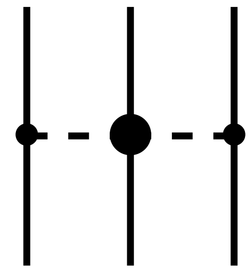
$$\langle EJTi | (\mathrm{H}^{\mathrm{NN+3N}} - \mathrm{T}_{int}) | E'JTi' \rangle$$

$T = \frac{1}{2} \quad J^\pi = \frac{1}{2}^+ \; \hbar\Omega = 20\,\mathrm{MeV}$



Matrix Element Analysis of TPE Contribution





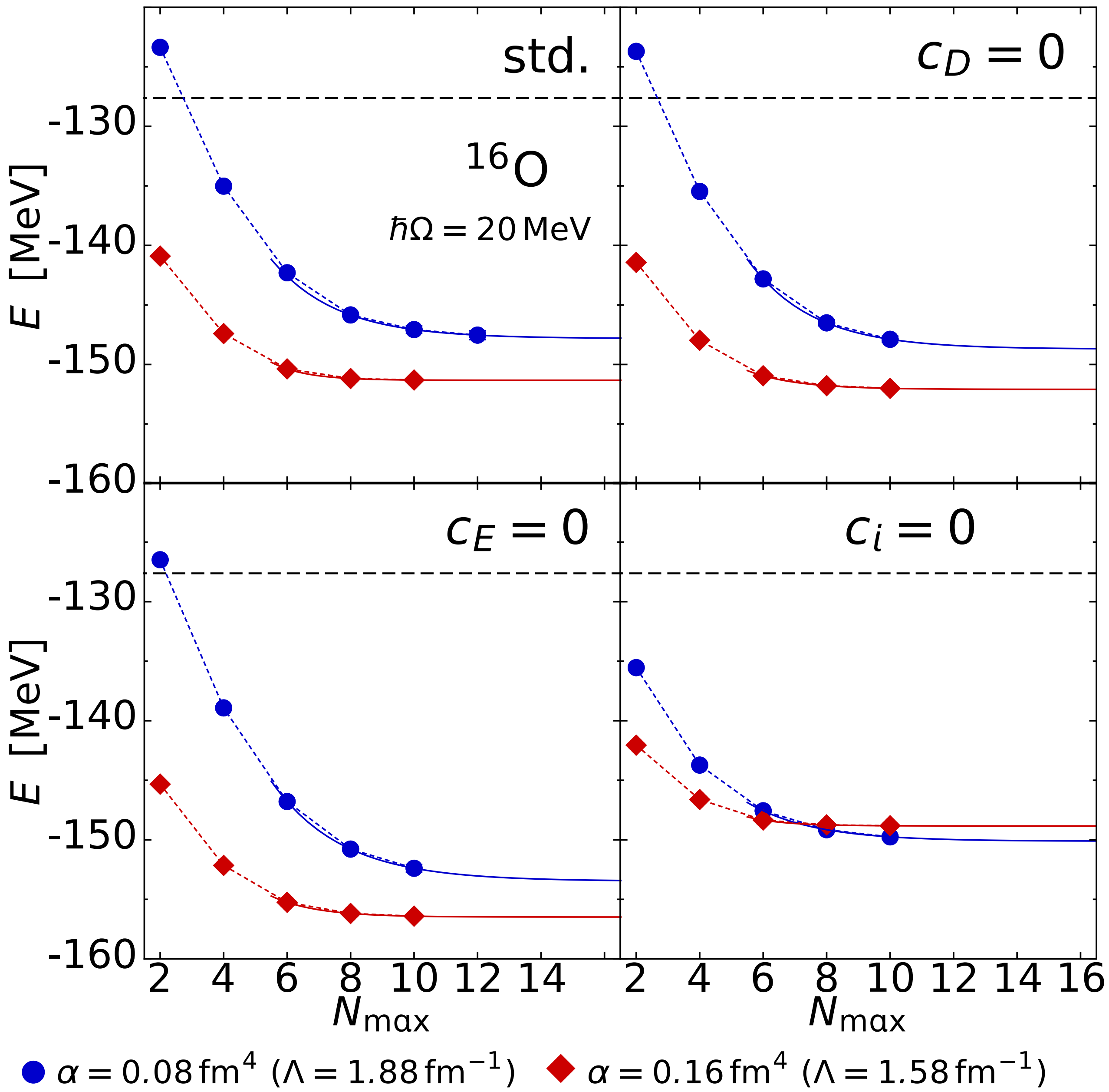
$$\langle EJTi \big| (\mathrm{V}^{\mathrm{TPE}} - \mathrm{T}_{int}) \big| E'JTi' \rangle$$

$$T = \tfrac{1}{2} \quad J^\pi = \tfrac{1}{2}^+ \quad \hbar\Omega = 20\,\mathrm{MeV}$$

- far off-diagonal matrix elements not affected due to modified generator

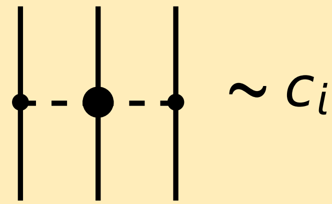
⇒ slow convergence

Origin of SRG Induced 4-body Forces



- set individual LECs of 3N force to zero
- refit the remaining to ^3H binding energy
- $c_D = 0$ or $c_E = 0$: α-dependence unchanged

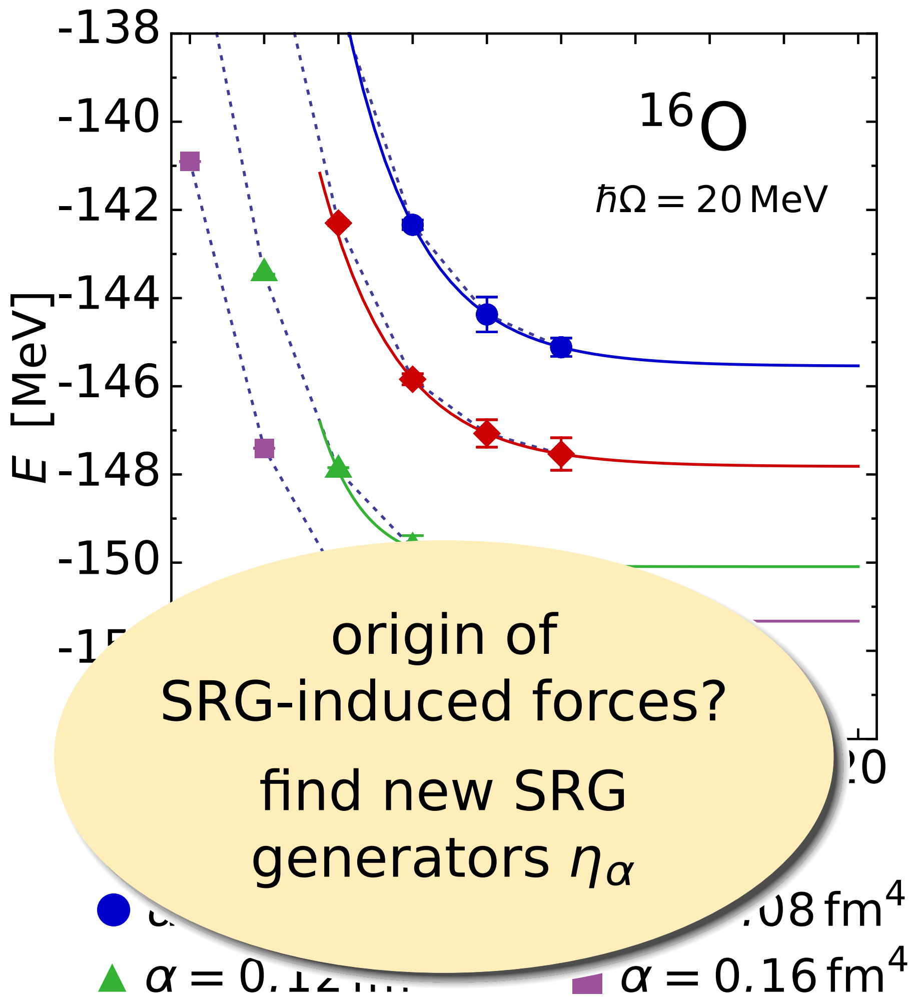
- **two-pion exchange**



induces many-body forces during SRG

Reminder: Results in upper p-shell

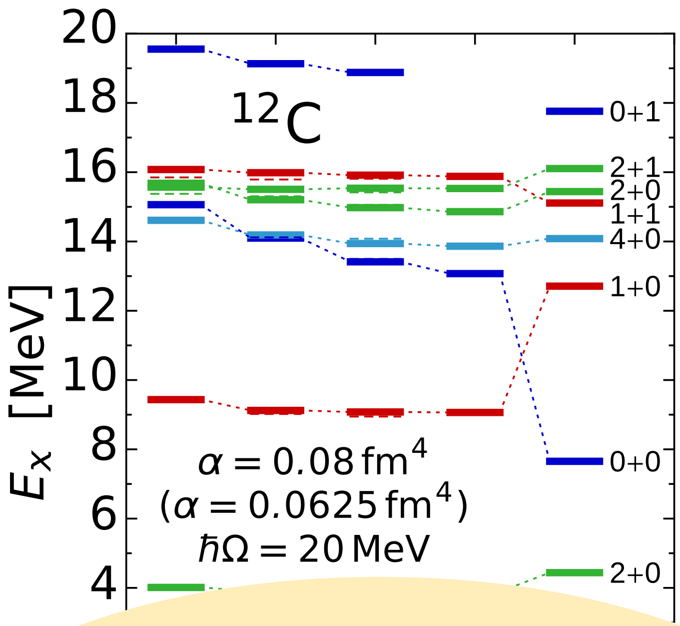
- sizable α-dependence of absolute energies



origin of
SRG-induced forces?

find new SRG
generators η_α

- α-dependence of relative energies negligible

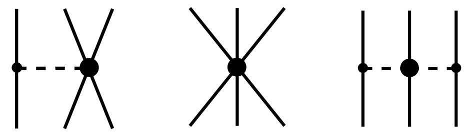


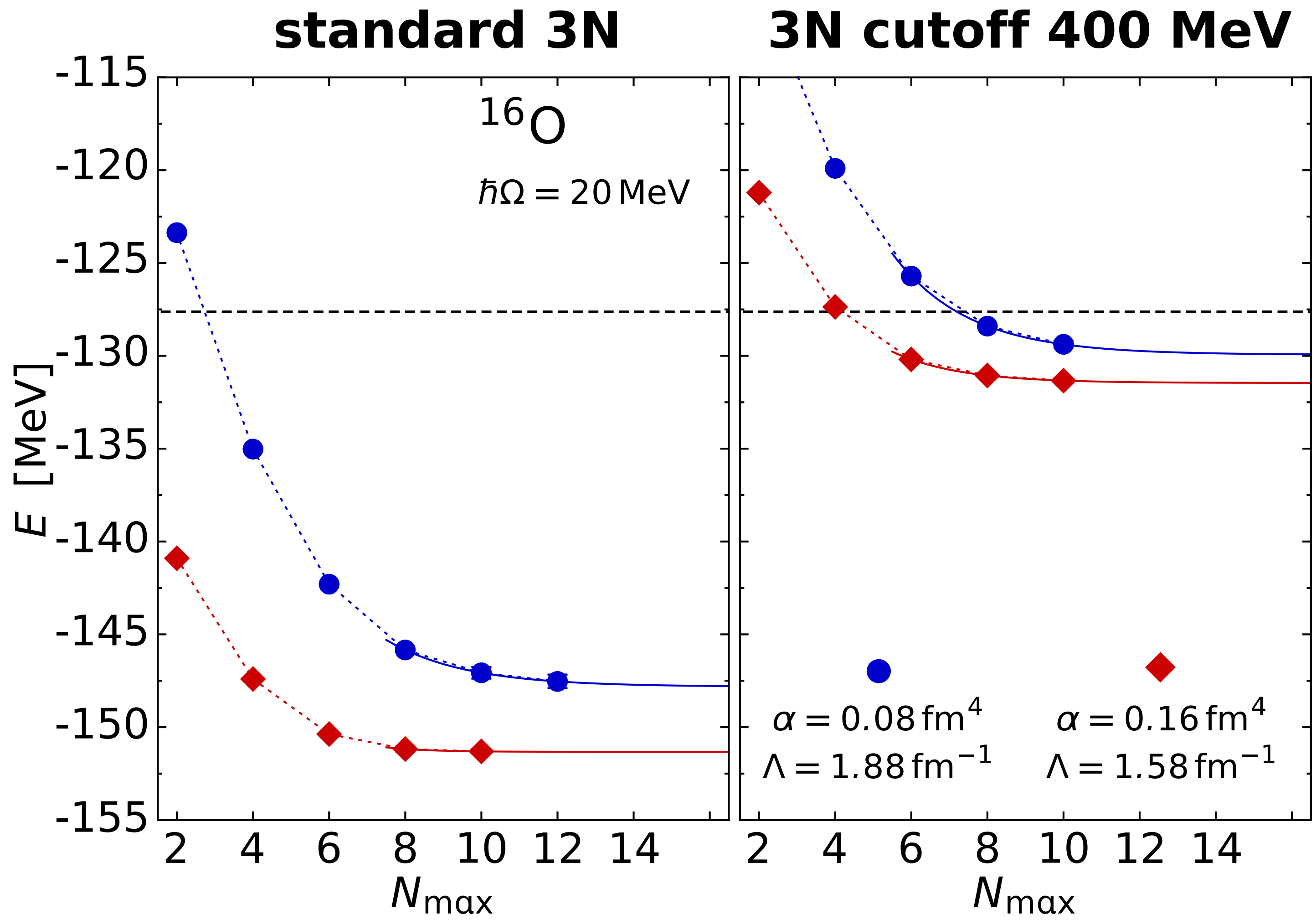
sensitivity studies
of chiral interactions on
LEC or cutoff variation
possible

[Roth, L
arXiv1105.31

Benchmark of chiral forces
– Sensitivity on 3N Cutoff –

Cutoff Sensitivity of Chiral 3N Force

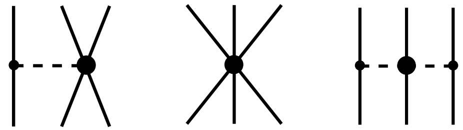
- reduce cutoff to $\Lambda = 400\,\mathrm{MeV}$ for 
- refit c_E to ^{4}He binding energy, $c_D = -0.2$

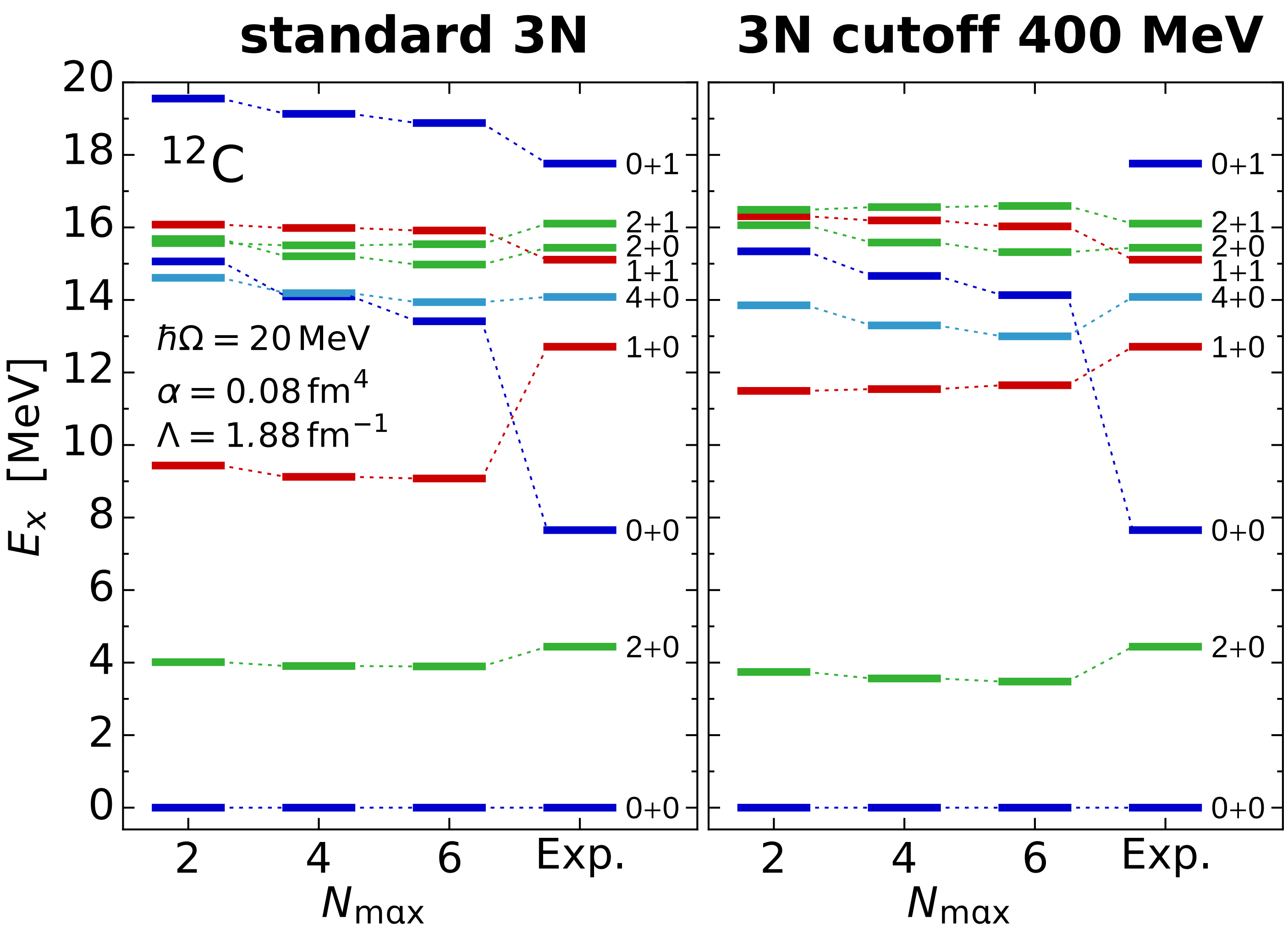


Sensitivities

- sizable reduction of α-dependence
- shift towards experiment

Cutoff Sensitivity of Chiral 3N Force

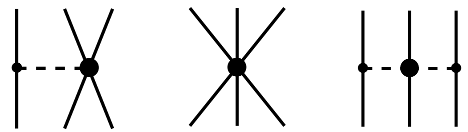
- reduce cutoff to $\Lambda = 400\,\text{MeV}$ for 
- refit c_E to ^{4}He binding energy, $c_D = -0.2$

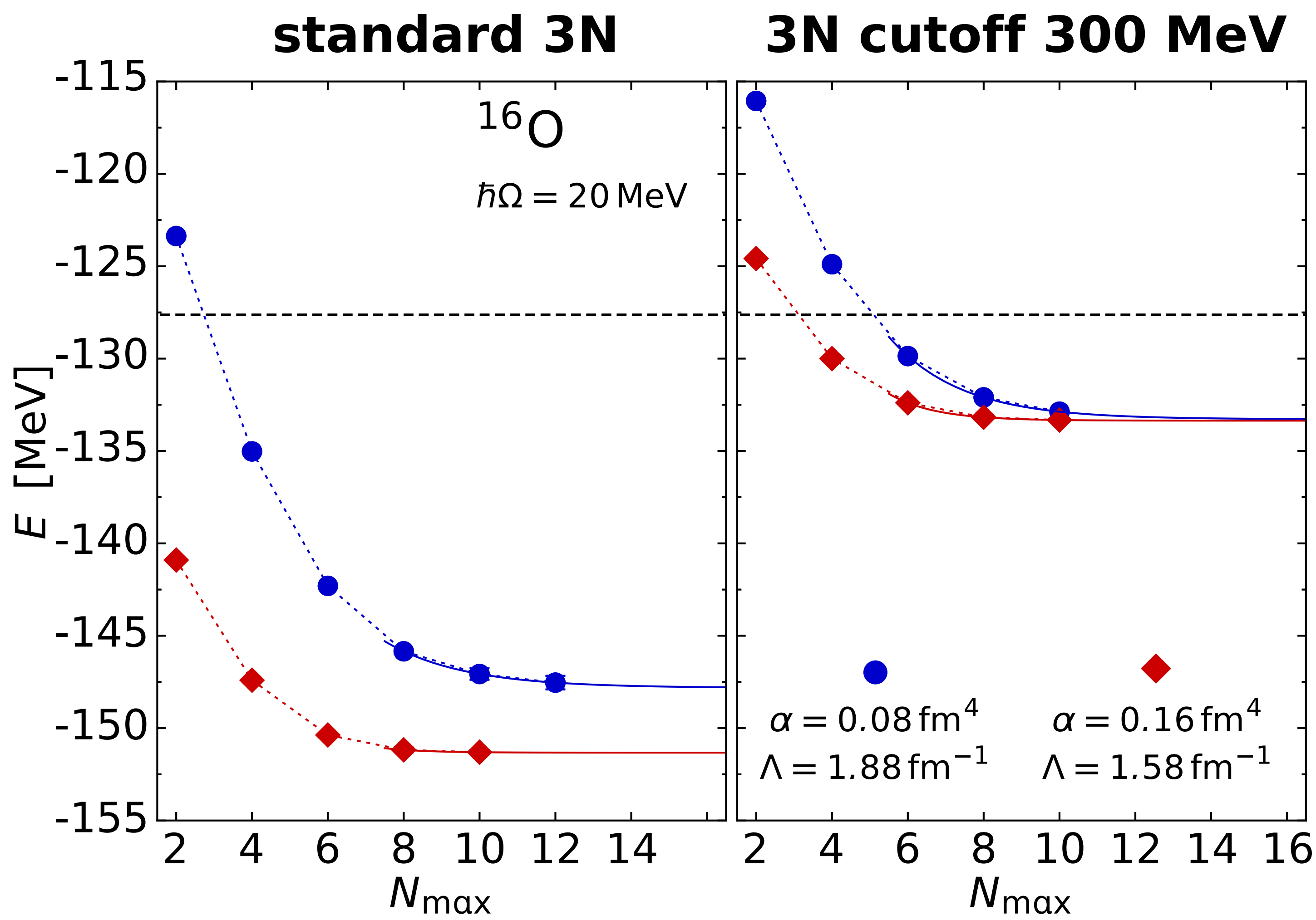


Sensitivities

- significant shift of 1^+0 state
- much smaller effects for other states

Cutoff Sensitivity of Chiral 3N Force

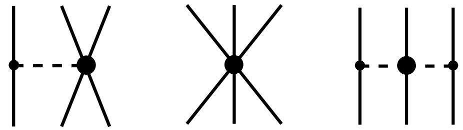
- reduce cutoff to $\Lambda = 300\,\text{MeV}$ for 
- refit c_E to ^{4}He binding energy, $c_D = -0.2$



Sensitivities

- α-dependence vanishes
- shift towards experiment

Cutoff Sensitivity of Chiral 3N Force

- reduce cutoff to $\Lambda = 300\,\mathrm{MeV}$ for 
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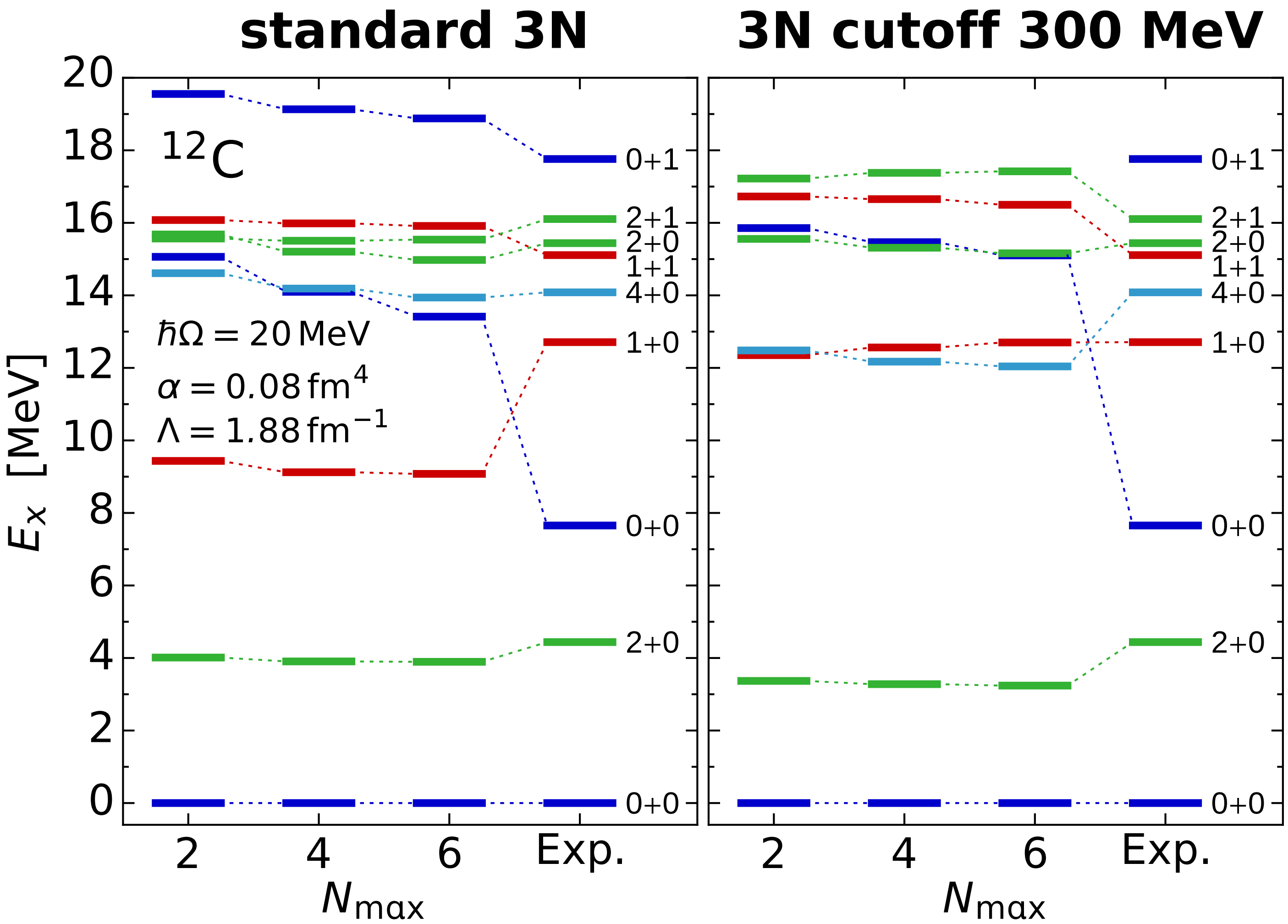


Sensitivities

- again shift of 1^+0 state
- strong effect on almost all other states

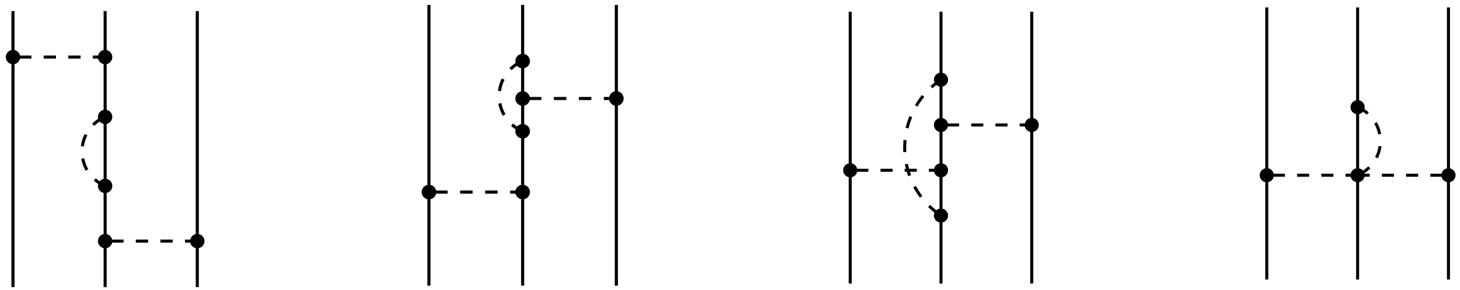
Benchmark of Chiral Forces
– LEC Variations –

Shifted c_i's...

- shift the NN data based c_i's

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

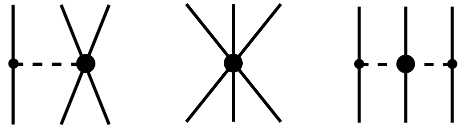
- equivalent to inclusion of the following TPE diagrams at N^3LO
  Bernard, Epelbaum, Krebs and Meißner [Phys.Rev. C77, 064004]

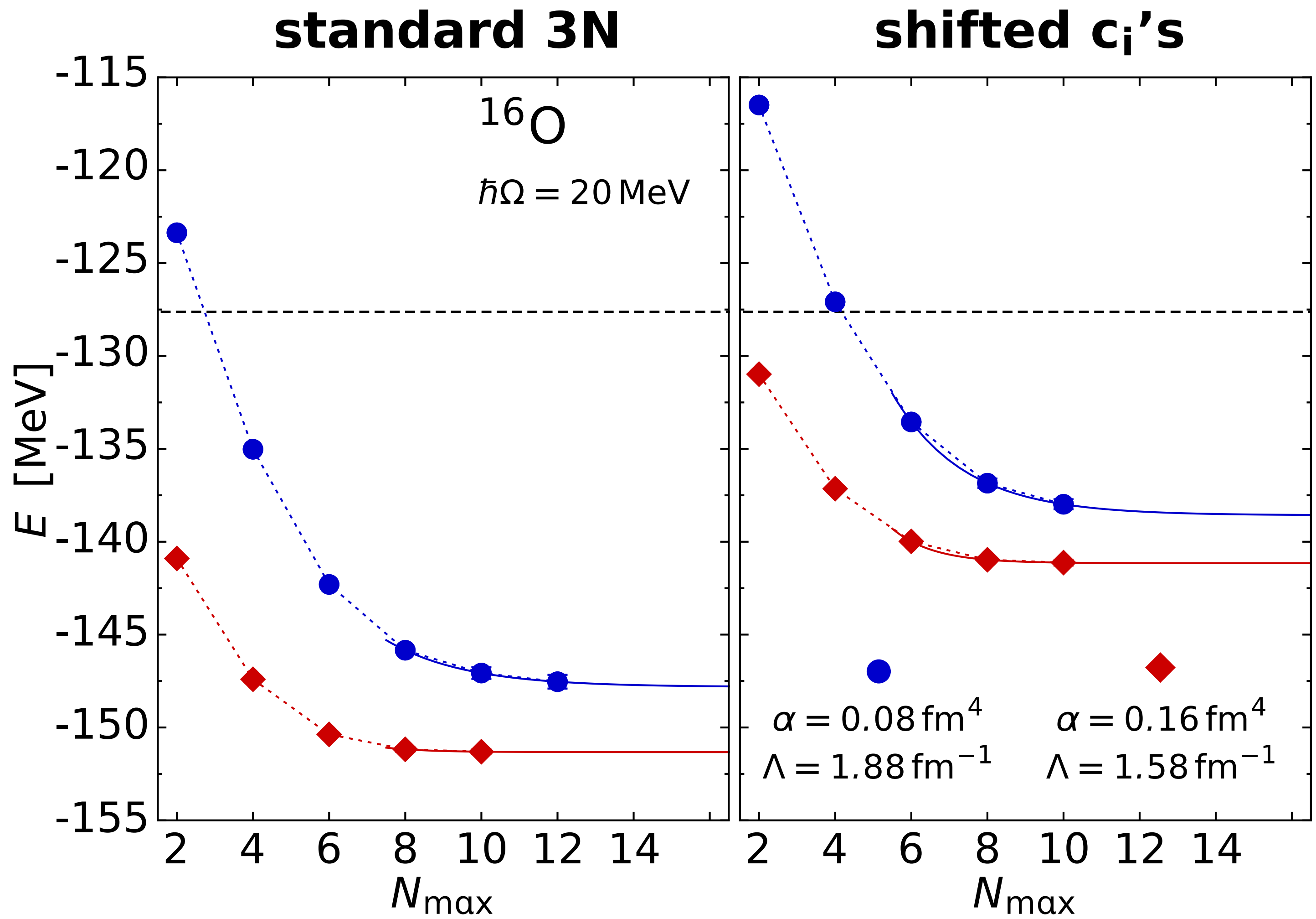


- changes of c_i's at the order of $20\% - 30\%$

$\Rightarrow$ **might have significant impact on spectra**

LEC Sensitivity of Chiral 3N Force

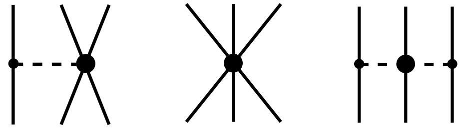
- shift c_i's used in 
- refit c_E to ^{4}He binding energy



Sensitivities

- α-dependence slightly reduced
- slight shift towards experiment

LEC Sensitivity of Chiral 3N Force

- shift c_i's used in 
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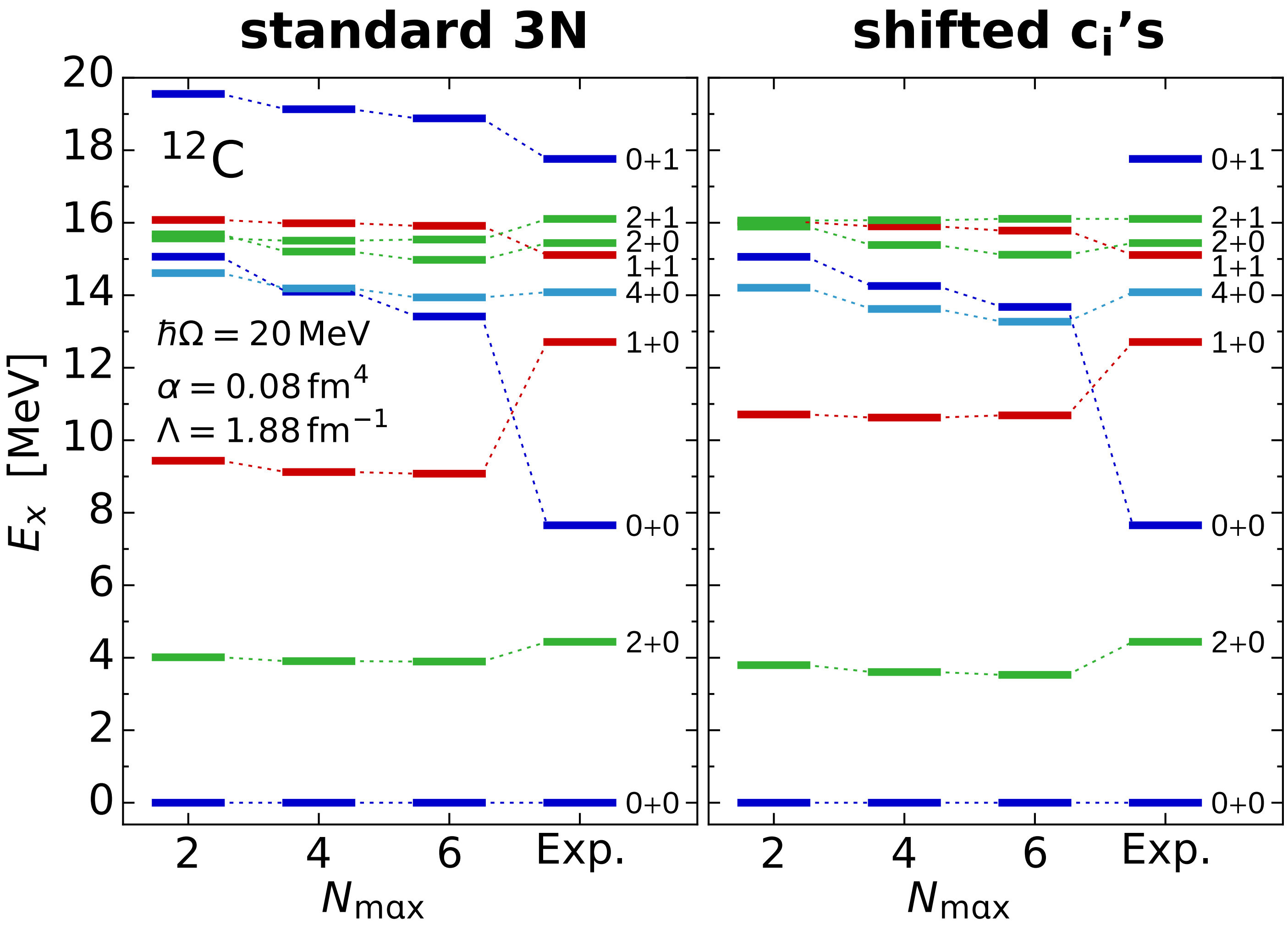


Sensitivities

- again 1^+ state affected
- minor effects on the other states

Sensitivity on weakly constrained c_3 & c_4

- LECs from πN vertices are quite loosely constraint

- some possible c_i combinations

	c_1 [GeV^{-1}]	c_3 [GeV^{-1}]	c_4 [GeV^{-1}]
Rentmeester et al. PRC 67, 044001	-0.76	-4.78	3.96
Büttiker et al. NPA 668, 97	-0.81	**-4.70**	**3.40**
Fettes [illegible]	[illegible]	[illegible]	3.47
Entem et al. [illegible]	[illegible]	[illegible]	3.40
Entem et al. PRC 68,041001(R)	-0.81	**-3.20**	**5.40**

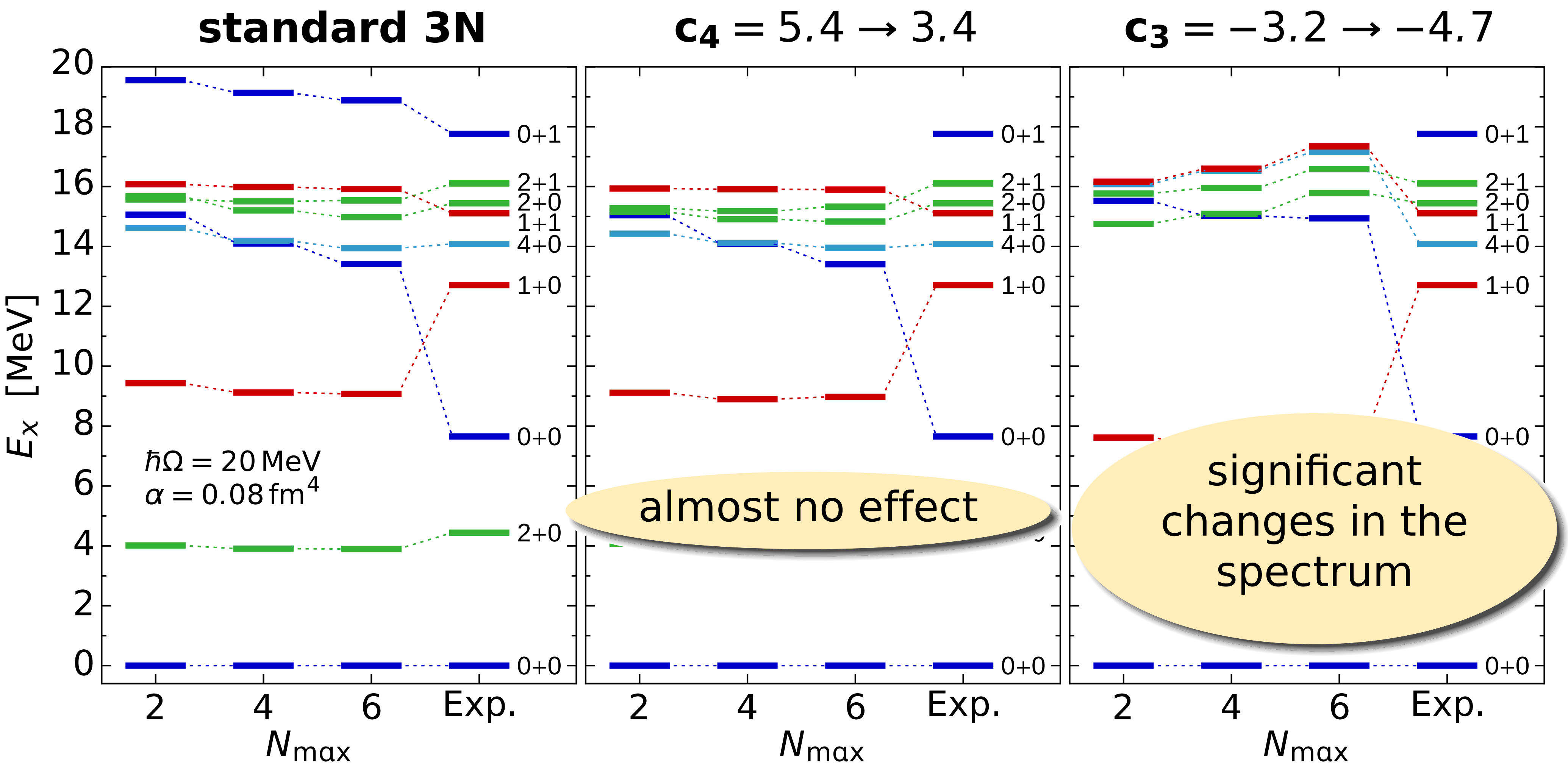
Let's study the changes on the ^{12}C spectrum...

- What happens if we start varying the c_i's within or even beyond these bounds?

- Is one LEC more **important for spectra** than the other?

Sensitivity on c_3 & c_4: ^{12}C

- refit c_E to ^{4}He binding energy, $c_D = -0.2$



- **c_3 seems to be very important for spectra**

Conclusions

- breakthrough in handling of three-body matrix elements
  - consistent similarity transformation including **full 3N forces** and inclusion into (IT-)NCSM calculations
  - **investigations of the whole p-shell** (even beyond) possible at moderate computational cost

- sensitivity studies of p-shell nuclei spectra on cutoff or LEC variation
  - especially 1^+0 **state in ^{12}C very sensitive** to cutoff variation
  - ^{12}C spectrum rather insensitive to variations of c_4, **but sensitive to variation of** c_3
  - ready to adopt matrix elements of N^{3}LO three-body force

- modified SRG generator

Epilogue

- **thanks to our group & collaborators**
  - **S. Binder**, A. Blum, **A. Calci**, B. Erler, A. Günther, M. Hild, H. Krutsch, D. Kulawiak, P. Papakonstantinou, S. Reinhardt, **R. Roth**, F. Schmitt, R. Trippel, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada

COMPUTING TIME

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