Similarity Renormalization Group for Chiral NN+3N Interactions: Physics & Technology

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Road Map

Nuclear Structure & Reaction Observables

Importance Truncated NCSM
ab initio studies in the p- & sd-shell

Applications to Nuclear Spectra
spectroscopy and sensitivity on 3N

Coupled Cluster Approach
systematic extension to heavy nuclei

...

Similarity Renormalization Group

pre-diagonalization of Hamiltonian by unitary transformation
computational technology for 3N matrix elements

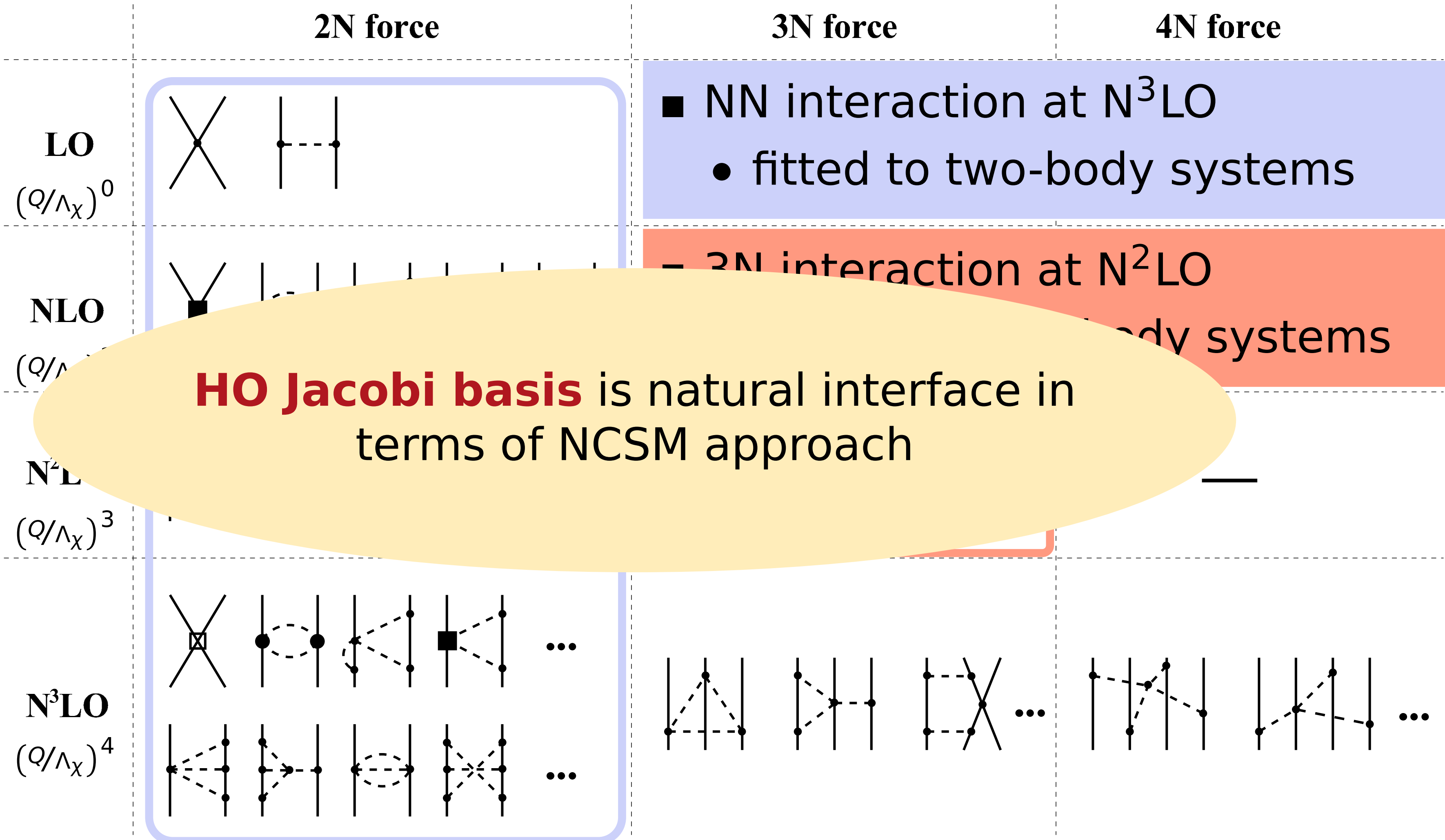
Chiral Effective Field Theory

systematic low-energy effective theory of QCD
consistent & improvable NN, 3N,... interactions

Low-Energy Quantum Chromodynamics

Chiral Effective Field Theory

- using **pions** and **nucleons** as degrees of freedom



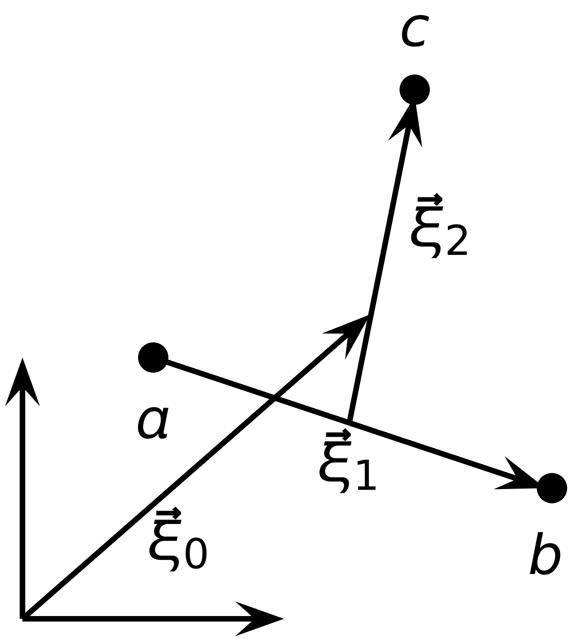
- NN interaction at N^{3}LO
  - fitted to two-body systems
- 3N interaction at N^{2}LO
  - …dy systems

HO Jacobi basis is natural interface in terms of NCSM approach

- provides **NN** and **3N interactions** in a **consistent** manner

Jacobi Coordinates

- "**relative coordinates**" for 3-body system



$$\vec{\xi}_0 = \sqrt{\frac{1}{3}}\ [\vec{r}_a + \vec{r}_b + \vec{r}_c]$$

$$\vec{\xi}_1 = \sqrt{\frac{1}{2}}\ [\vec{r}_a - \vec{r}_b]$$

$$\vec{\xi}_2 = \sqrt{\frac{2}{3}}\ \left[\frac{1}{2}(\vec{r}_a + \vec{r}_b) - \vec{r}_c\right]$$

- allow for separation in center-of-mass and relative part
- nuclei characterized by relative motion

concentrate on **relative part**

HO Jacobi Basis

- 2-body basis
  - antisymmetric:

$$|EiJM_J TM_T\rangle = |(NL,S)JM_J, TM_T\rangle$$

- 3-body basis
  - antisymmetric under $1 \longleftrightarrow 2$:

$$|\alpha\rangle = |[(n_{12}l_{12}, s_{12})j_{12}, (n_3 l_3, s_3)j_3]JM_J, (t_{12}, t_3)TM_T\rangle$$

  - antisymmetric:

$$|EiJM_J TM_T\rangle = \sum_\alpha c_{\alpha,i}\,|\alpha\rangle$$

- interaction is M_J-independent
- average over M_T for 3B matrix elements

Antisymmetrization of 3B Jacobi Basis

$$|EiJM_JTM_T\rangle = \sum_{\alpha} c_{\alpha,i}\,|\alpha\rangle$$

- **diagonalize antisymmetrizer** in α-basis (P. Navrátil)
  - for each EJT-block separately
- use coefficients $c_{\alpha,i}$ to eigenvalue 1
  - **coefficients of fractional parentage** (CFPs)

$$\langle\alpha|\mathcal{A}|\alpha'\rangle = \begin{pmatrix} \boxed{EJT} & & & \\ & \boxed{E'J'T'} & & \\ & & \boxed{E''J''T''} & \\ & & & \ddots \end{pmatrix}$$

Similarity Renormalization Group

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

Similarity Renormalization Group (SRG)

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

- continuous **unitary transformation** of the Hamiltonian

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

- leads to **evolution equation**

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = \left[\eta_\alpha, \widetilde{H}_\alpha\right] \quad \text{with} \quad \eta_\alpha = -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} = -\eta_\alpha^\dagger$$

initial value problem with $\widetilde{H}_{\alpha=0} = H$

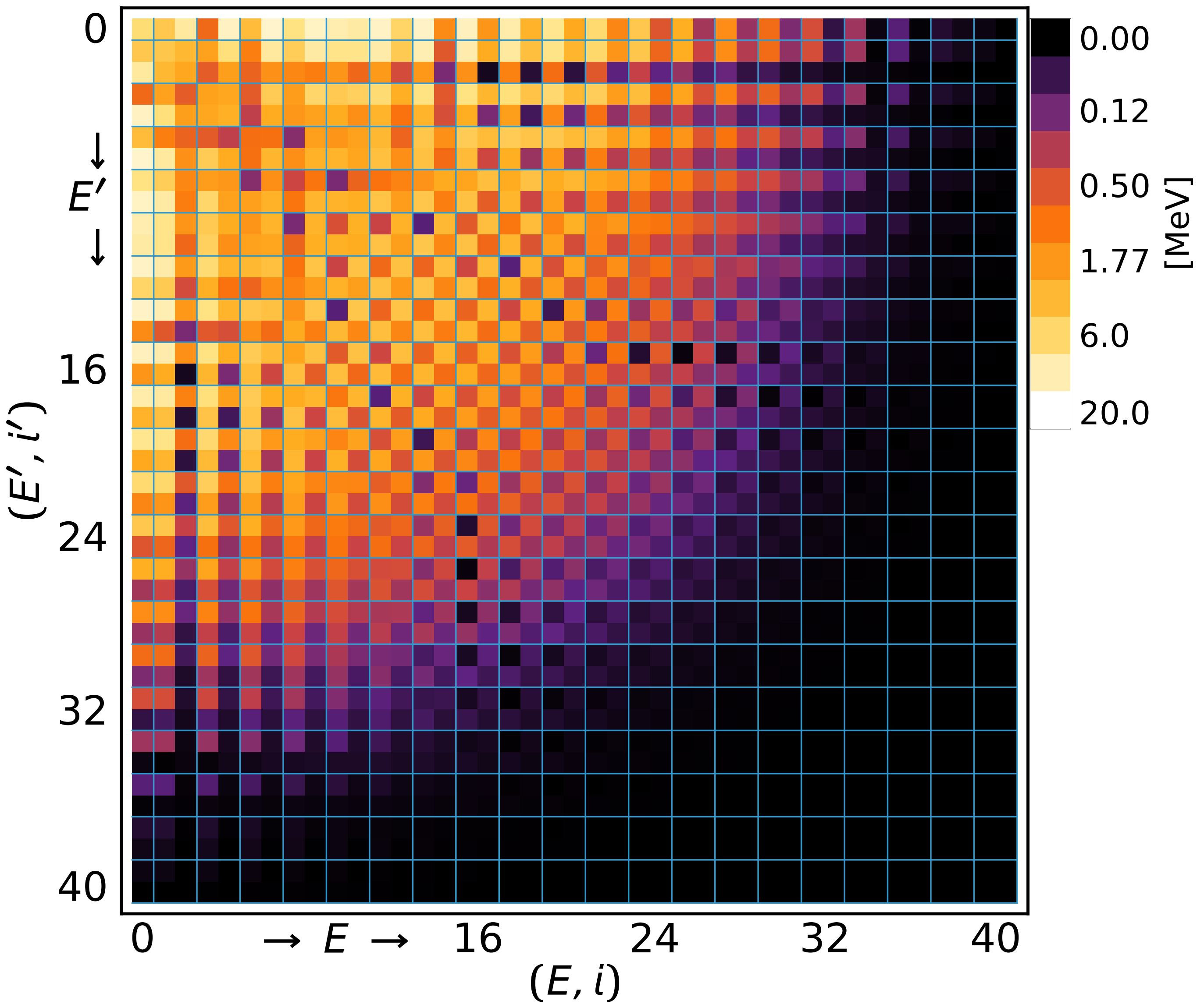
- choose **dynamic generator**

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

advantages of SRG:
simplicity and **flexibility**

SRG Evolution in Two-Body Space

2B-Jacobi HO matrix elements



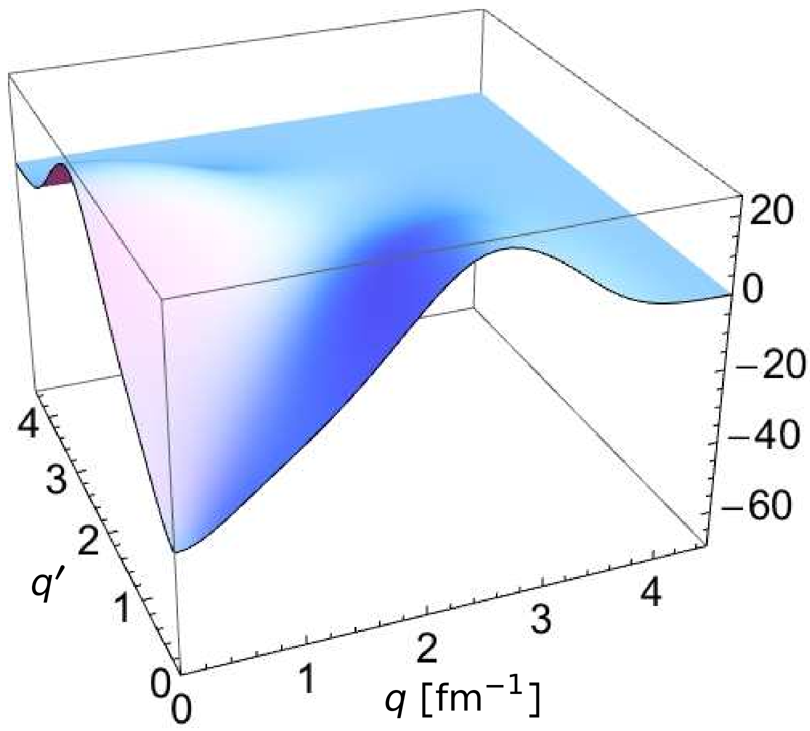
$\alpha = 0.00\,\mathrm{fm}^4$

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

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

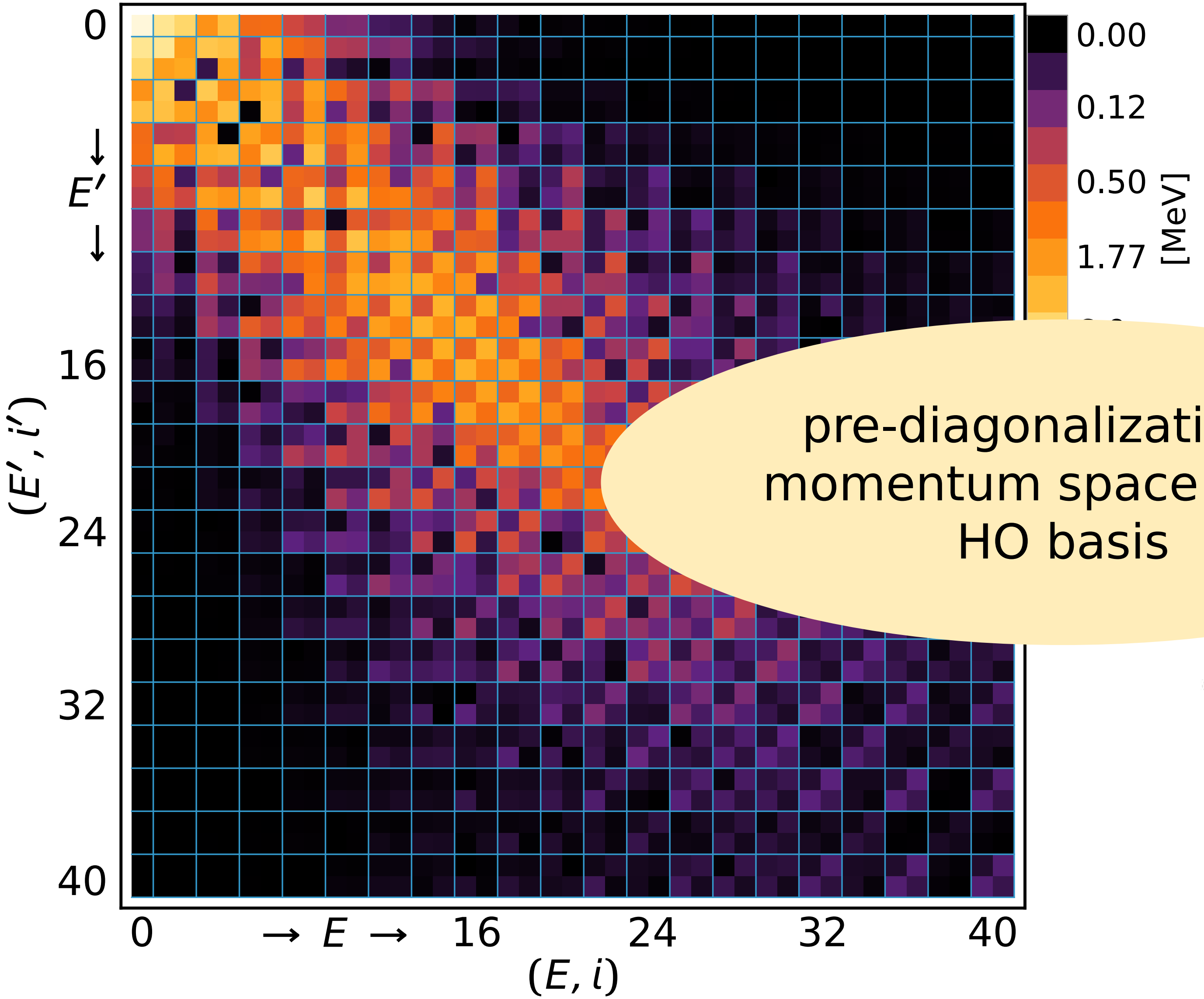
$J^\pi = 1^+, T = 0, \hbar\Omega = 20\,\mathrm{MeV}$

momentum space $^3S_1$



SRG Evolution in Two-Body Space

2B-Jacobi HO matrix elements



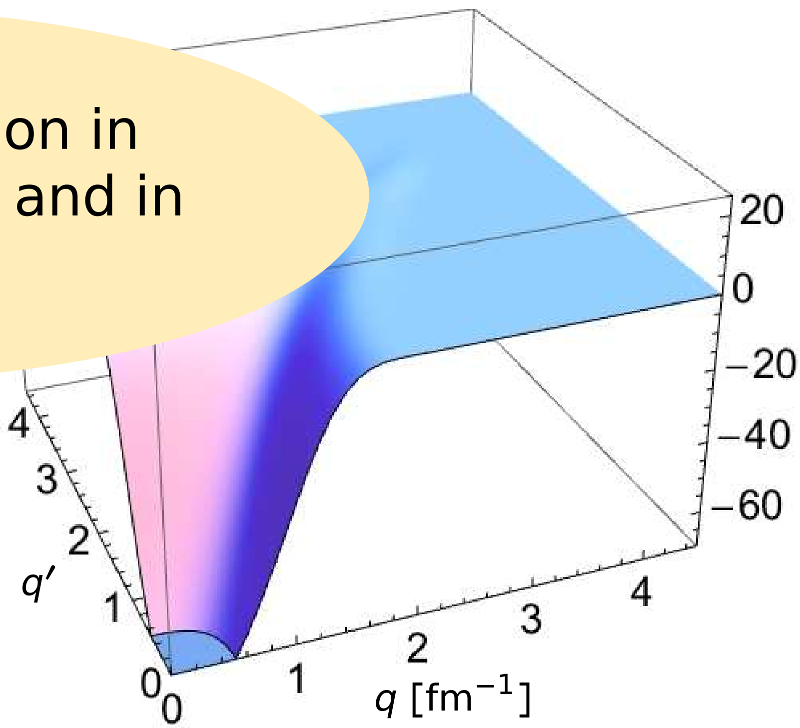
$\alpha = 0.32\,\mathrm{fm}^4$

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

$\langle E'i'JT | \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | EiJT \rangle$

$J^\pi = 1^+, T = 0, \hbar\Omega = 20\,\mathrm{MeV}$

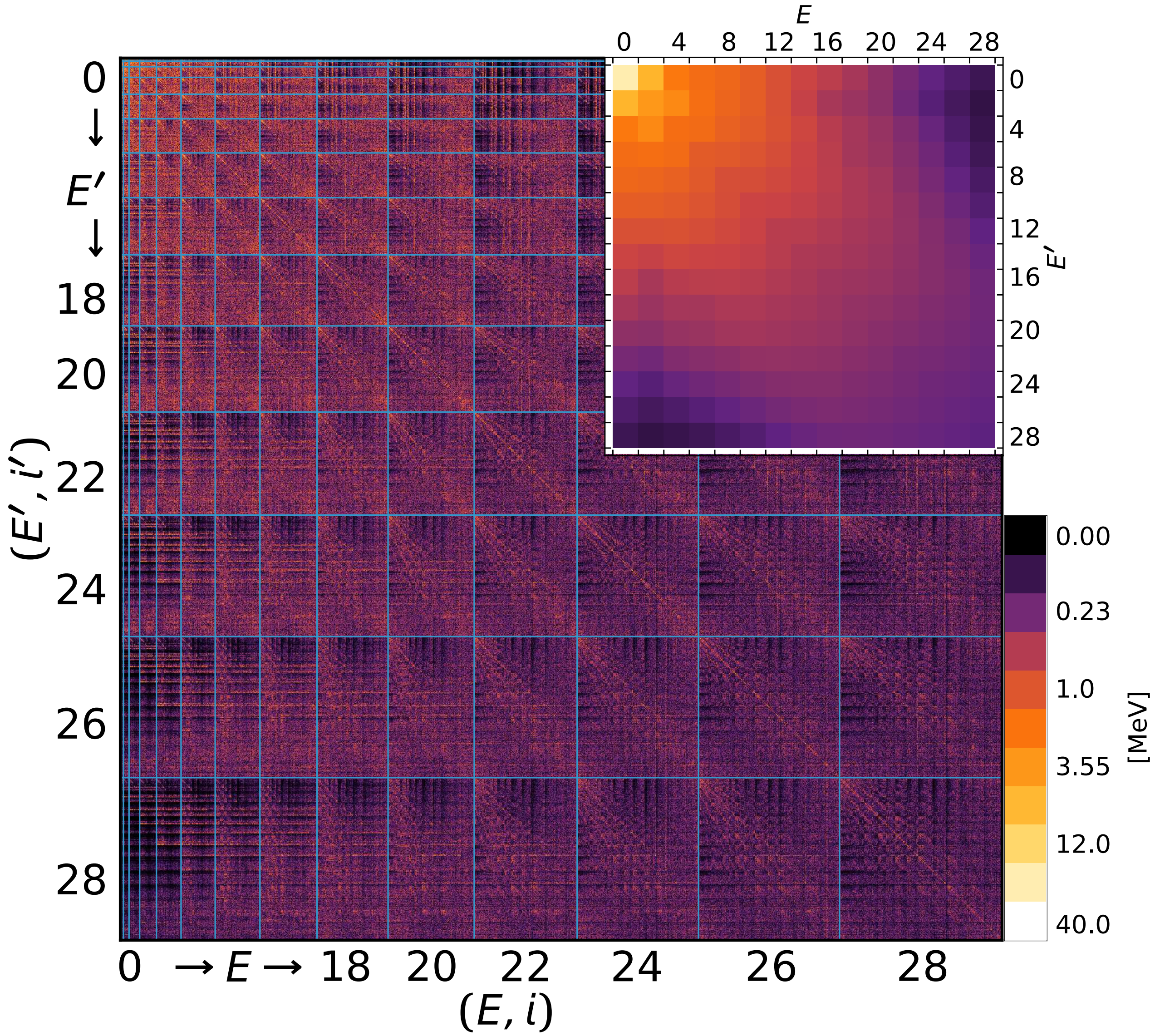
momentum space $^3S_1$



pre-diagonalization in momentum space and in HO basis

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



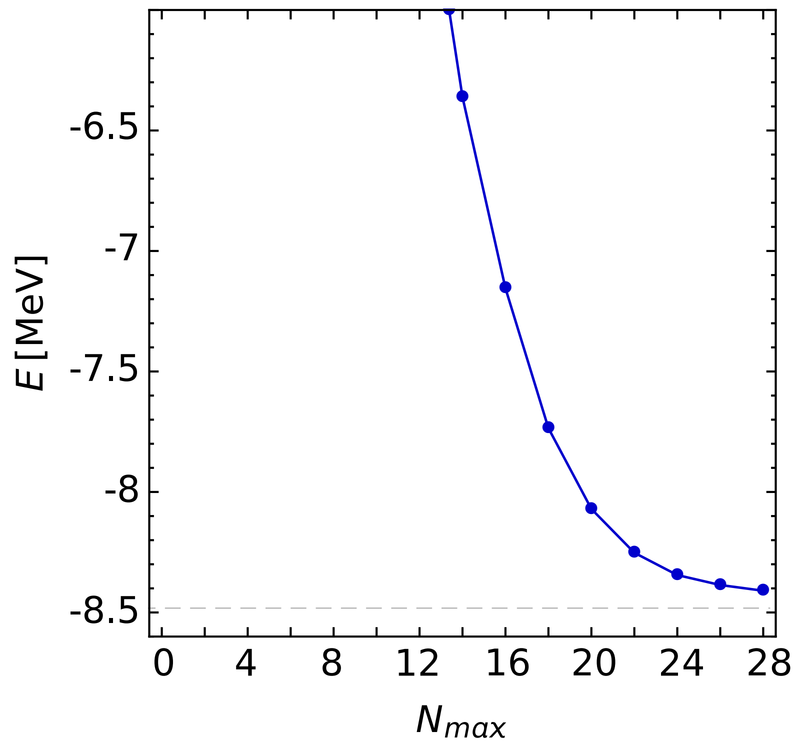
$$\alpha = 0.00\,\mathrm{fm}^4$$

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

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

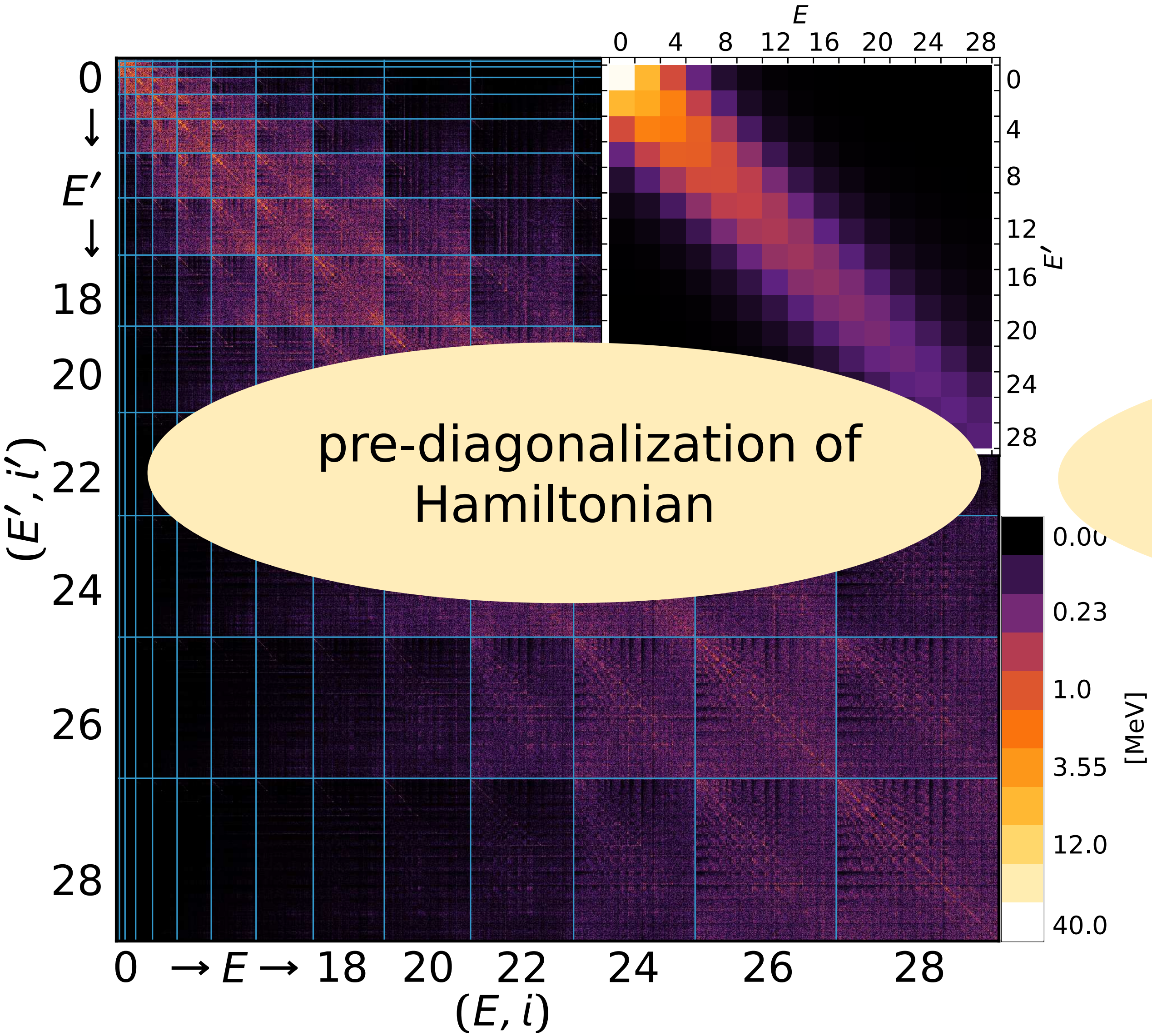
$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 20\,\mathrm{MeV}$$

NCSM ground state ^{3}H



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



pre-diagonalization of Hamiltonian

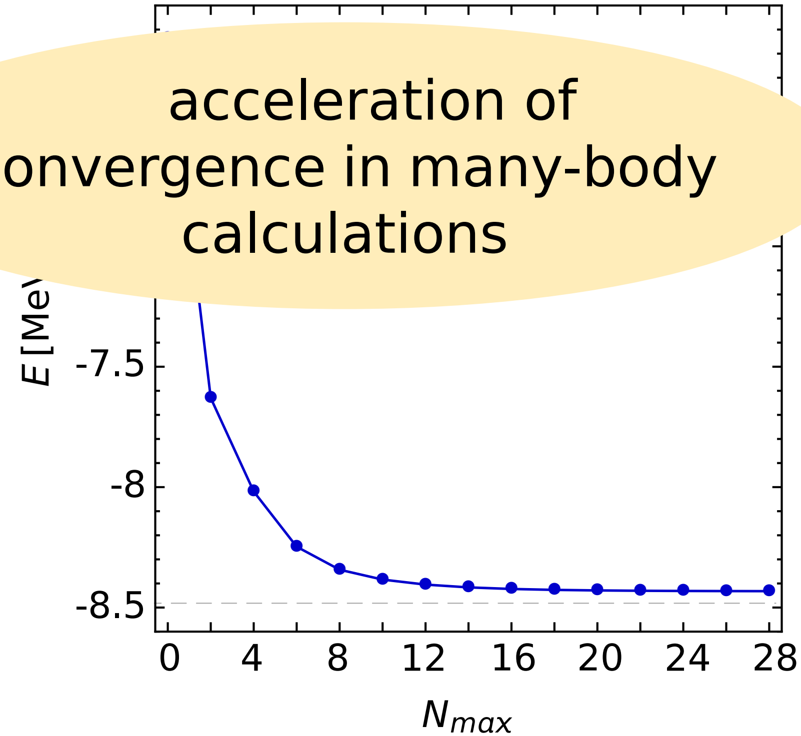
$$\alpha = 0.32\,\mathrm{fm}^4$$

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

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

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

NCSM ground state ^{3}H

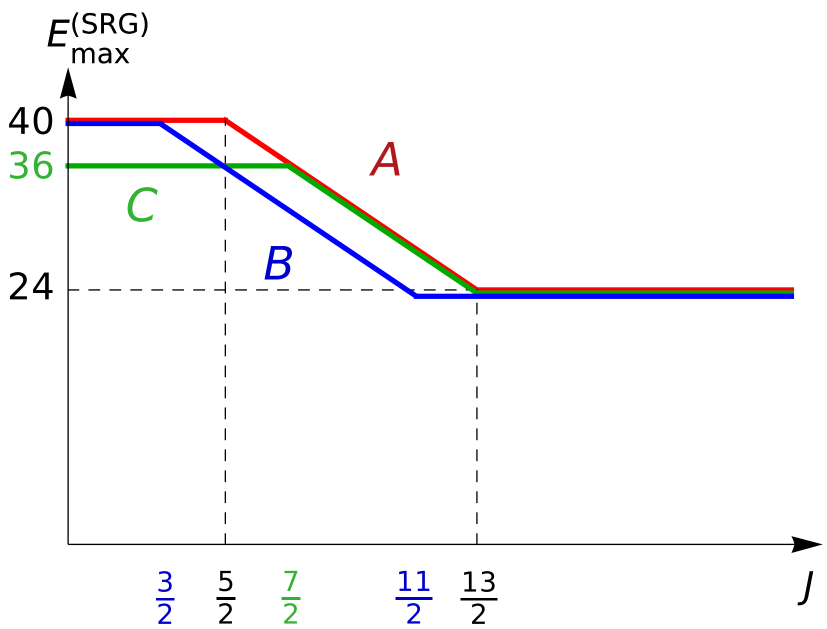


acceleration of convergence in many-body calculations

SRG Model Space

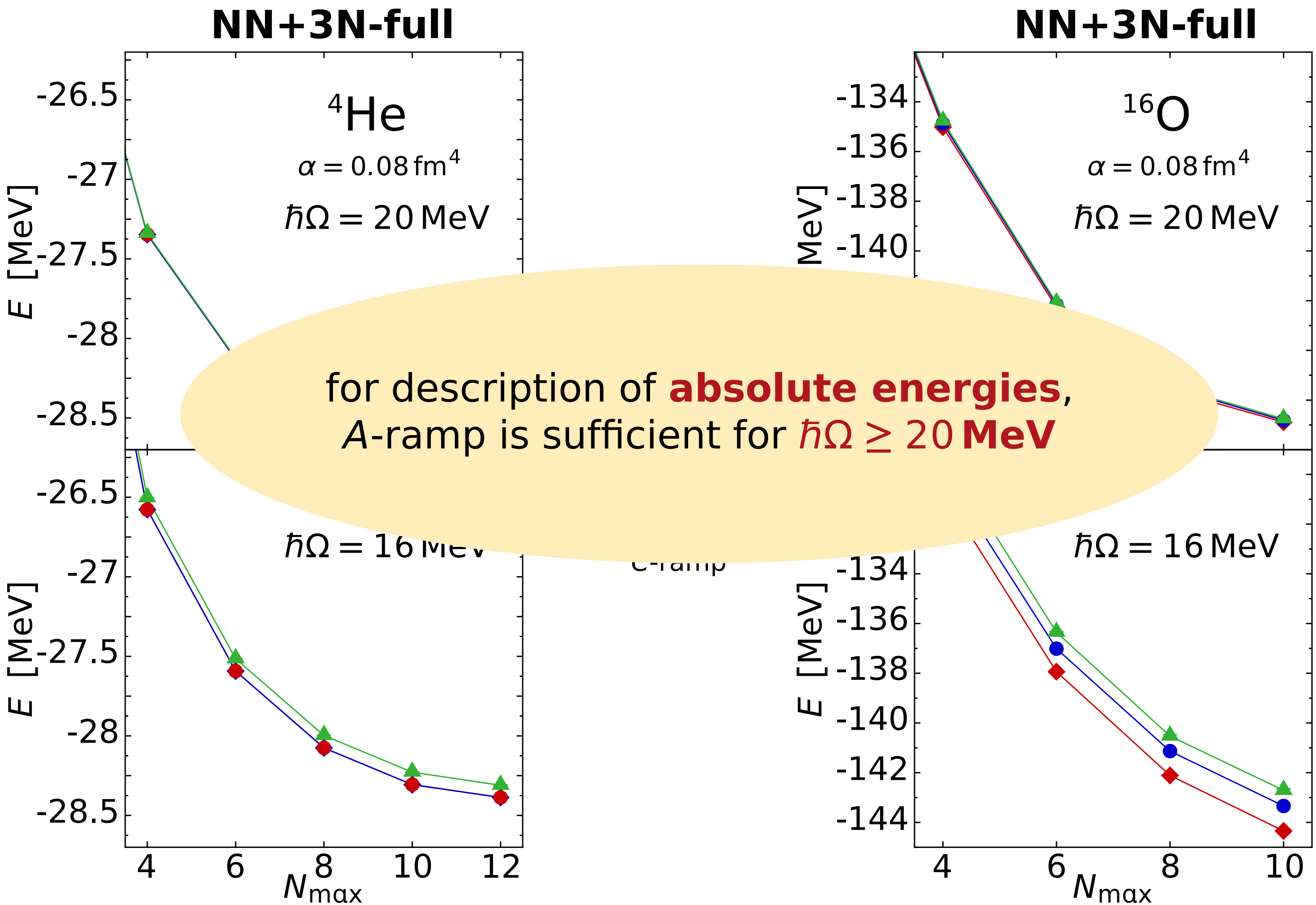
- model space in 3-body HO Jacobi basis defined by $E_{\text{max}}^{(\text{SRG})}$
- large angular momenta less important for low-energy properties
  - J-dependent model space truncation $E_{\text{max}}^{(\text{SRG})}(J)$

SRG model-space ramp



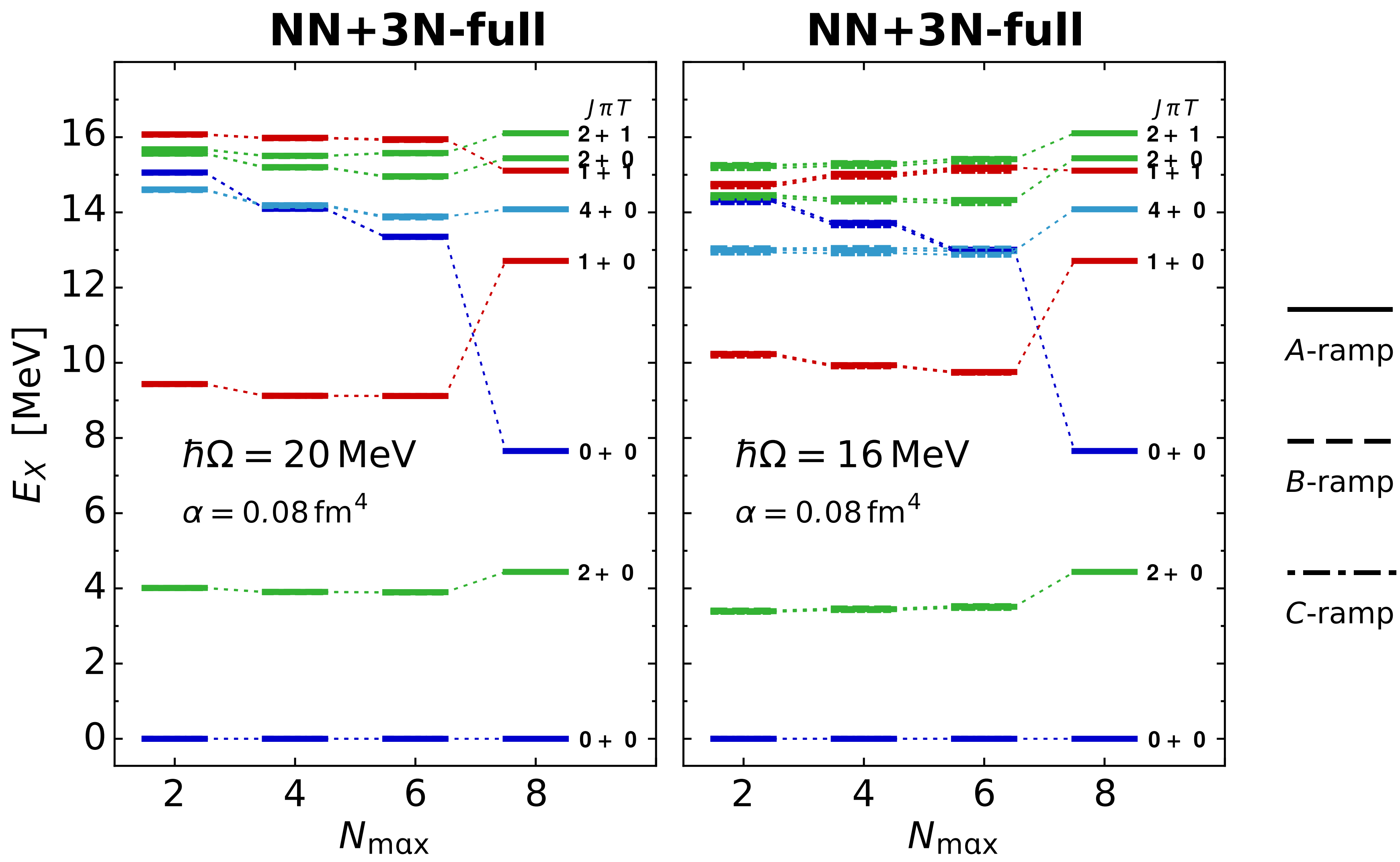
- use *A*-ramp as standard
- **investigate** sufficiency of **SRG model space**
  - use *B*- and *C*-ramp for comparison

SRG Model Space: ^{4}He & ^{16}O Ground-State



for description of **absolute energies**,
A-ramp is sufficient for $\hbar\Omega \geq 20\,$**MeV**

SRG Model Space: ^{12}C Spectrum



- excitation energies **independent** of SRG model space

SRG Evolution in *A*-Body Space

- SRG induces **irreducible** many-body **contributions**

$$U_\alpha^\dagger H U_\alpha = \widetilde{H}_\alpha^{[2]} + \widetilde{H}_\alpha^{[3]} + \cdots + \widetilde{H}_\alpha^{[A]}$$

- restricted to a SRG evolution in 2B or 3B space
- formal **violation of unitarity**

SRG-evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and evolve in two-body space
- **NN** … d evolve in three-b…
- **NN+3N-full**: start with NN+3N initial Hamiltonian and evolve in three-body space

application in talks by
R. Roth, J. Langhammer and S. Binder

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

SRG Evolution in Three-Body Space

cluster decomposition
decompose Hamiltonian in irreducible two- and three-body parts for use in *A*-body space

❶ **evolve** initial NN(+3N) Hamiltonian in **three-body** space

two- and three-body part in three-body space

❷ **evolve** initial NN Hamiltonian in **two-body** space

two-body part in two-body space

❸ **embed** evolved NN Hamiltonian in **three-body** space

two-body part in three-body space

❹ **subtract** ❸ from ❶ in **three-body** space

three-body part in three-body space

Transformation to $\mathcal{J}T$-Coupled Scheme

Roth, Langhammer, AC et al. — in preparation

From Jacobi to $\mathcal{J}$T-Coupled Scheme

effective interaction in 3B-Jacobi basis

first problem

many-body calculations ($A > 6$) in Jacobi coordinates not feasible

→ advantageous to use ***m*-scheme**

second problem

m-scheme matrix elements become intractable for $N_{\text{max}} > 8$ (p-shell)

transformation from Jacobi into $\mathcal{J}T$-coupled scheme

key to efficient NCSM calculations up to $N_{max} = 14$ for p-shell nuclei

decoupling on the fly

ab-initio many-body calculation

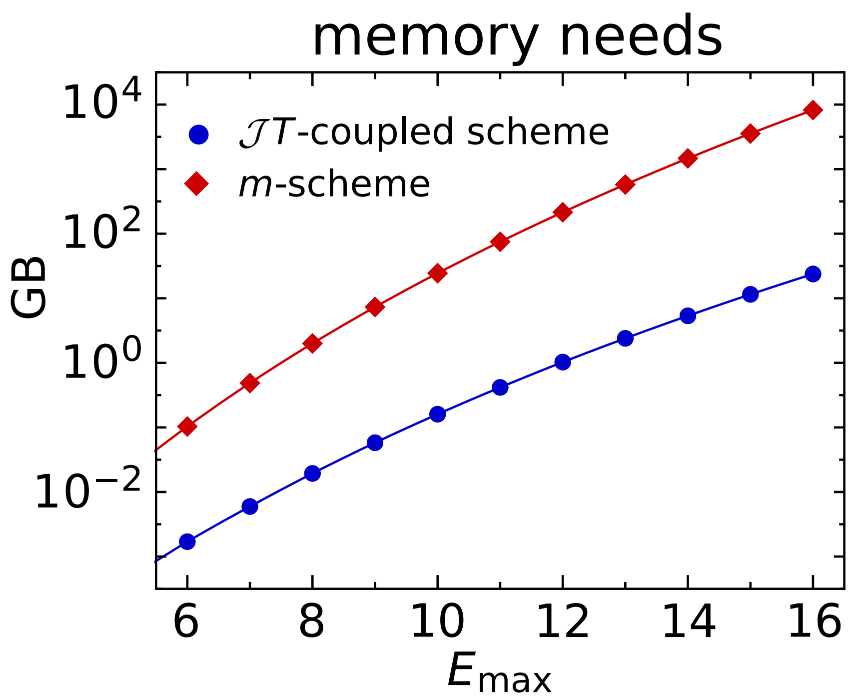
$\mathcal{J}T$-Coupled Scheme vs. m-Scheme

- m-scheme

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

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

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



- explicit consideration of interaction properties in $\mathcal{J}T$-coupled scheme
  - Hamiltonian connects only **equal $\mathcal{J}$ and T**
  - **memory needs decreases** by two orders of magnitude

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

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

$$
= 3! \sum_{l_{cm}} \sum_{\alpha} \tilde{T} \begin{pmatrix} a & b & c & J_{ab} & J & \mathcal{J} \\ n_{cm} & l_{cm} & n_{12} & l_{12} & n_3 & l_3 \\ s_{ab} & j_{12} & j_3 & & & \end{pmatrix}
$$

$$
\times \sum_{\alpha'} \tilde{T} \begin{pmatrix} a' & b' & c' & J'_{ab} & J & \mathcal{J} \\ n_{cm} & l_{cm} & n'_{12} & l'_{12} & n'_3 & l'_3 \\ s'_{ab} & j'_{12} & j'_3 & & & \end{pmatrix}
$$

$$
\times \sum_{i,i'} c_{\alpha,i}\, c_{\alpha',i'} \left\langle EiJT \right| \mathrm{H} \left| E'i'JT \right\rangle
$$

$\tilde{T}$ Coefficients...

$$\tilde{T}\begin{pmatrix} a & b & c & J_{ab} & J & \mathcal{J} \\ n_{cm} & l_{cm} & n_{12} & l_{12} & n_3 & l_3 \\ s_{ab} & j_{12} & j_3 & & & \end{pmatrix} = \{\langle n_{cm} l_{cm}| \otimes \langle \alpha|\}^{\mathcal{J}} |[(ab)J_{ab}t_{ab}, c]\mathcal{J}T\rangle$$

$$= \sum_{L_{ab}} \sum_{\mathcal{L}_{12}} \sum_{\mathcal{L}} \sum_{S_3} \sum_{\Lambda} \delta_{2n_a+l_a+2n_b+l_b+2n_c+l_c, 2n_{cm}+l_{cm}+2n_3+l_3+2n_{12}+l_{12}}$$

$$\times \langle\langle \mathcal{N}_{12}\mathcal{L}_{12}, n_{12}l_{12}; L_{ab}|n_b l_b, n_a l_a\rangle\rangle_1 \; \langle\langle n_{cm}l_{cm}, n_3 l_3; \Lambda|\mathcal{N}_{12}\mathcal{L}_{12}, n_c l_c\rangle\rangle_2$$

$$\times \begin{Bmatrix} l_a & l_b & L_{ab} \\ s_a & s_b & s_{ab} \\ j_a & j_b & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{ab} & l_c & \mathcal{L} \\ s_{ab} & s_c & S_3 \\ J_{ab} & j_c & \mathcal{J} \end{Bmatrix} \begin{Bmatrix} l_{12} & l_3 & L_3 \\ s_{ab} & s_c & S_3 \\ j_{12} & j_3 & J \end{Bmatrix}$$

$$\times \begin{Bmatrix} l_c & \mathcal{L}_{12} & \Lambda \\ l_{12} & \mathcal{L} & L_{ab} \end{Bmatrix} \begin{Bmatrix} l_{cm} & l_3 & \Lambda \\ l_{12} & \mathcal{L} & L_3 \end{Bmatrix} \begin{Bmatrix} l_{cm} & L_3 & \mathcal{L} \\ S_3 & \mathcal{J} & J \end{Bmatrix}$$

$$\times \hat{j}_a \hat{j}_b \hat{j}_c \hat{J}_{ab} \hat{j}_{12} \hat{j}_3 \hat{s}_{ab} \hat{J} \hat{S}_3^2 \hat{\mathcal{L}}^2 \hat{\Lambda}^2 \hat{L}_3^2 \hat{L}_{ab}^2 (-1)^{l_c+\Lambda+L_{ab}+\mathcal{L}+S_3+l_{12}+\mathcal{J}}$$

Storage Scheme

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

$$_a\langle\{[(n_a l_a, s_a)j_a, (n_b l_b, s_b)j_b]j_{ab}, (n_c l_c, s_c)j_c\}\mathcal{J}; [(t_a, t_b)t_{ab}, t_c]T|\,\mathrm{H}$$
$$|\{[(n'_a l'_a, s'_a)j'_a, (n'_b l'_b, s'_b)j'_b]j'_{ab}, (n'_c l'_c, s'_c)j'_c\}\mathcal{J}; [(t'_a, t'_b)t'_{ab}, t'_c]T\rangle_a$$

  - bra and ket have same **parity**
  - **antisymmetric** states: permutations are linear dependent
  - Hamiltonian is **hermitian**: save upper triangular matrix
  - use protons and neutrons: single-particle quantum numbers of (iso)-spin are ½

Storage Scheme

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

$$_a\langle\{[(n_a l_a)j_a,(n_b l_b)j_b]j_{ab},(n_c l_c)j_c\}\mathcal{J};[t_{ab}]T|\mathrm{H}|\{[(n'_a l'_a)j'_a,(n'_b l'_b)j'_b]j'_{ab},(n'_c l'_c)j'_c\}\mathcal{J};[t'_{ab}]T\rangle_a$$

- introduce **collective** single-particle **index** nlj
  - energetic ordering of n, l and j

nlj	1	2	3	4	...	nlj_{max}
n	0	0	1	0	...	0
l	1	1	0	2	...	l_{max}
j	1	3	1	3	...	j_{max}

Storage Scheme

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

$$_a\langle\{[nlj_a, nlj_b]j_{ab}, nlj_c\}\mathcal{J};[t_{ab}]T|\mathrm{H}|\{[nlj'_{a'}, nlj'_b]j'_{ab'}, nlj'_c\}\mathcal{J};[t'_{ab}]T\rangle_a$$

- loop over nlj indexes

$\mathtt{for}(\mathbf{nlj_a} = 0,\ \mathtt{nlj_a} \leq \mathtt{nlj_{max}},\ \mathtt{nlj_a}{+}{+})$

$\mathtt{for}(\mathbf{nlj_b} = 0,\ \mathtt{nlj_b} \leq \mathtt{nlj_a},\ \mathtt{nlj_b}{+}{+})$

$\mathtt{for}(\mathbf{nlj_c} = 0,\ \mathtt{nlj_c} \leq \mathtt{nlj_b},\ \mathtt{nlj_c}{+}{+})$

$\mathtt{for}(\mathbf{nlj'_a} = 0,\ \mathtt{nlj'_a} \leq \mathtt{nlj_a},\ \mathtt{nlj'_a}{+}{+})$

$\mathtt{for}(\mathbf{nlj'_b} = 0,\ \mathtt{nlj'_b} \leq \mathtt{nlj'_{b,max}},\ \mathtt{nlj'_b}{+}{+})$

$\mathtt{for}(\mathbf{nlj'_c} = 0,\ \mathtt{nlj'_c} \leq \mathtt{nlj'_{c,max}},\ \mathtt{nlj'_c}{+}{+})$

exploit symmetries of the Hamiltonian

inner loop contains all relevant quantum numbers for decoupling to *m*-scheme

Storage Scheme

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

$$ {}_a\langle \{[nlj_a, nlj_b]j_{ab}, nlj_c\}\mathcal{J}; [t_{ab}]T \,|\, \mathrm{H} \,|\, \{[nlj'_{a'}, nlj'_b]j'_{ab'}, nlj'_c\}\mathcal{J}; [t'_{ab}]T\rangle_a $$

- inner loop

for($\mathbf{j_{ab}} = |j_1 - j_2|,\ j_{ab} \le j_1 + j_2,\ j_{ab}++$)

for($\mathbf{j'_{ab}}$ …

for($\mathcal{J}$ … $_{ab} + j'_3],\ \mathcal{J}++$)

for($\mathbf{t_{ab}} = 0,\ t_{ab} \le 1,\ t_{ab}++$)

for($\mathbf{t'_{ab}} = 0,\ t'_{ab} \le 1,\ t'_{ab}++$)

for($\mathbf{T} = 1/2,\ T \le \mathrm{MIN}[t_{ab} + 1/2,\ t'_{ab} + 1/2],\ t'_{ab}++$)

storage scheme **already in use**
by other groups
(P. Navrátil and J. Vary)

details will be
published soon

write matrix element to file
quantum numbers specified by loop order

Conclusions

Conclusions

- **consistent SRG** evolution in 3B space
  - indispensable for converged NCSM calculations
- efficient transformation for Jacobi to $\mathcal{J}T$-coupled scheme
  - key for application to $\boldsymbol{N_{max} > 8}$ **calculations** (p-shell)
  - developed **optimized storage scheme**
- applications ahead (IT-NCSM, CC, ...)
- machinery ready to use **3N @ N3LO** in momentum Jacobi basis

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, B. Erler, E. Gebrerufael, A. Günther, H. Krutsch, **J. Langhammer**, S. Reinhardt, **R. Roth**, C. Stumpf, R. Trippel, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - J. Vary, P. Maris
    Iowa State University, USA
  - S. Quaglioni
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert
    Ohio State University, USA
  - P. Papakonstantinou
    IPN Orsay, F
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

JUROPA — JÜLICH FORSCHUNGSZENTRUM
LOEWE-CSC — CSC Center for Scientific Computing Frankfurt
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COMPUTING TIME

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