No-Core Shell Model

and Related Areas (NCSM*)

Lecture 2: Light Nuclei

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Overview

- **Lecture 1: Hamiltonian**

  Prelude ● Nuclear Hamiltonian ● Matrix Elements ● Two-Body Problem ● Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**

  Similarity Renormalization Group ● Many-Body Problem ● Configuration Interaction ● No-Core Shell Model ● Hypernuclei

- **Lecture 3: Beyond Light Nuclei**

  Normal Ordering ● Coupled-Cluster Theory ● In-Medium Similarity Renormalization Group

- **Hands-On: Do-It-Yourself NCSM**

  Three-Body Problem ● Numerical SRG Evolution ● NCSM Eigenvalue Problem ● Lanczos Algorithm

Similarity Renormalization Group

Similarity Renormalization Group

continuous unitary transformation to
pre-diagonalize the Hamiltonian with respect
to a given basis

- start with an **explicit unitary transformation** of the Hamiltonian with a unitary operator U_α with continuous **flow parameter α**

$$H_\alpha = {U_\alpha}^\dagger H\, U_\alpha$$

- **differentiate both sides** with respect to flow parameter

$$\begin{aligned}
\frac{d}{d\alpha} H_\alpha &= \left(\frac{d}{d\alpha}{U_\alpha}^\dagger\right) H\, U_\alpha + {U_\alpha}^\dagger H \left(\frac{d}{d\alpha} U_\alpha\right) \\
&= \left(\frac{d}{d\alpha}{U_\alpha}^\dagger\right) U_\alpha {U_\alpha}^\dagger H\, U_\alpha + {U_\alpha}^\dagger H\, U_\alpha {U_\alpha}^\dagger \left(\frac{d}{d\alpha} U_\alpha\right) \\
&= \left(\frac{d}{d\alpha}{U_\alpha}^\dagger\right) U_\alpha H_\alpha + H_\alpha {U_\alpha}^\dagger \left(\frac{d}{d\alpha} U_\alpha\right)
\end{aligned}$$

Similarity Renormalization Group

- define the **antihermitian generator** of the unitary transformation via

$$\eta_\alpha = -U_\alpha{}^\dagger\left(\frac{d}{d\alpha}U_\alpha\right) = \left(\frac{d}{d\alpha}U_\alpha{}^\dagger\right)U_\alpha = -\eta_\alpha{}^\dagger$$

where the antihermiticity follows explicitly from differentiating the unitarity condition $1 = U_\alpha{}^\dagger U_\alpha$

- we thus obtain for the derivative of the transformed Hamiltonian

$$\begin{aligned}\frac{d}{d\alpha}H_\alpha &= \eta_\alpha H_\alpha - H_\alpha \eta_\alpha \\ &= [\eta_\alpha, H_\alpha]\end{aligned}$$

thus, that change of the Hamiltonian as function of the flow parameter is governed by the **commutator of the generator with the Hamiltonian**

- this is the **SRG flow equation**, which has a close resemblance to the Heisenberg equation of motion

Similarity Renormalization Group

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

continuous unitary transformation to pre-diagonalize the Hamiltonian with respect to a given basis

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

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

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

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

- the physics of the transformation is governed by the **dynamic generator η_α** and we choose an ansatz depending on the type of "pre-diaognalization" we want to achieve

SRG Generator & Fixed Points

- **standard choice** for antihermitian generator: commutator of intrinsic kinetic energy and the Hamiltonian

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

- this **generator vanishes** if
  - kinetic energy and Hamiltonian commute
  - kinetic energy and Hamiltonian have a simultaneous eigenbasis
  - the Hamiltonian is diagonal in the eigenbasis of the kinetic energy, i.e., in a momentum eigenbasis

- a vanishing generator implies a **trivial fix point** of the SRG flow equation — the r.h.s. of the flow equation vanishes and the Hamiltonian is stationary

- SRG flow **drives the Hamiltonian towards the fixed point**, i.e., towards the diagonal in momentum representation

Solving the SRG Flow Equation

- convert operator equations into a basis representation to obtain **coupled evolution equations for *n*-body matrix elements** of the Hamiltonian

  n=2: two-body relative momentum $\quad |q\,(LS)\,JT\rangle$

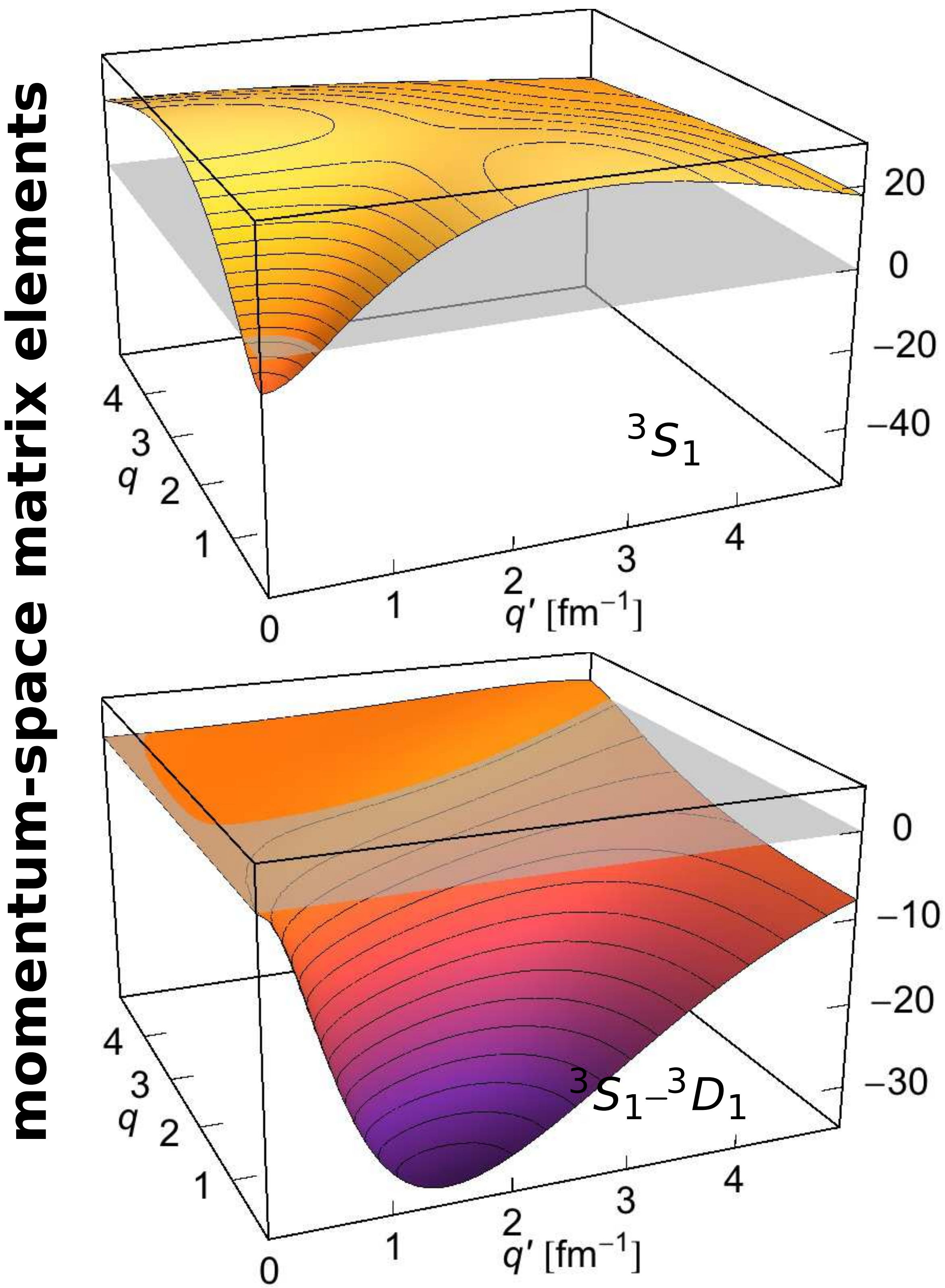
  n=3: antisym. three-body Jacobi HO $\quad |E i J^{\pi} T\rangle$

- matrix-evolution equations for n=3 with antisym. three-body Jacobi HO states:

$$
\begin{aligned}
\frac{d}{d\alpha}\langle E i J^{\pi} T|\,\mathrm{H}_{\alpha}\,|E' i' J^{\pi} T\rangle = (2\mu)^2 \sum_{E'',i''}^{E_{\mathrm{SRG}}} \sum_{E''',i'''}^{E_{\mathrm{SRG}}} \Big[\\
\langle E i \ldots|\,\mathrm{T}_{\mathrm{int}}\,|E'' i'' \ldots\rangle\,\langle E'' i'' \ldots|\,\mathrm{H}_{\alpha}\,|E''' i''' \ldots\rangle\,\langle E''' i''' \ldots|\,\mathrm{H}_{\alpha}\,|E' i' \ldots\rangle \\
-2\langle E i \ldots|\,\mathrm{H}_{\alpha}\,|E'' i'' \ldots\rangle\,\langle E'' i'' \ldots|\,\mathrm{T}_{\mathrm{int}}\,|E''' i''' \ldots\rangle\,\langle E''' i''' \ldots|\,\mathrm{H}_{\alpha}\,|E' i' \ldots\rangle \\
+\langle E i \ldots|\,\mathrm{H}_{\alpha}\,|E'' i'' \ldots\rangle\,\langle E'' i'' \ldots|\,\mathrm{H}_{\alpha}\,|E''' i''' \ldots\rangle\,\langle E''' i''' \ldots|\,\mathrm{T}_{\mathrm{int}}\,|E' i' \ldots\rangle \Big]
\end{aligned}
$$

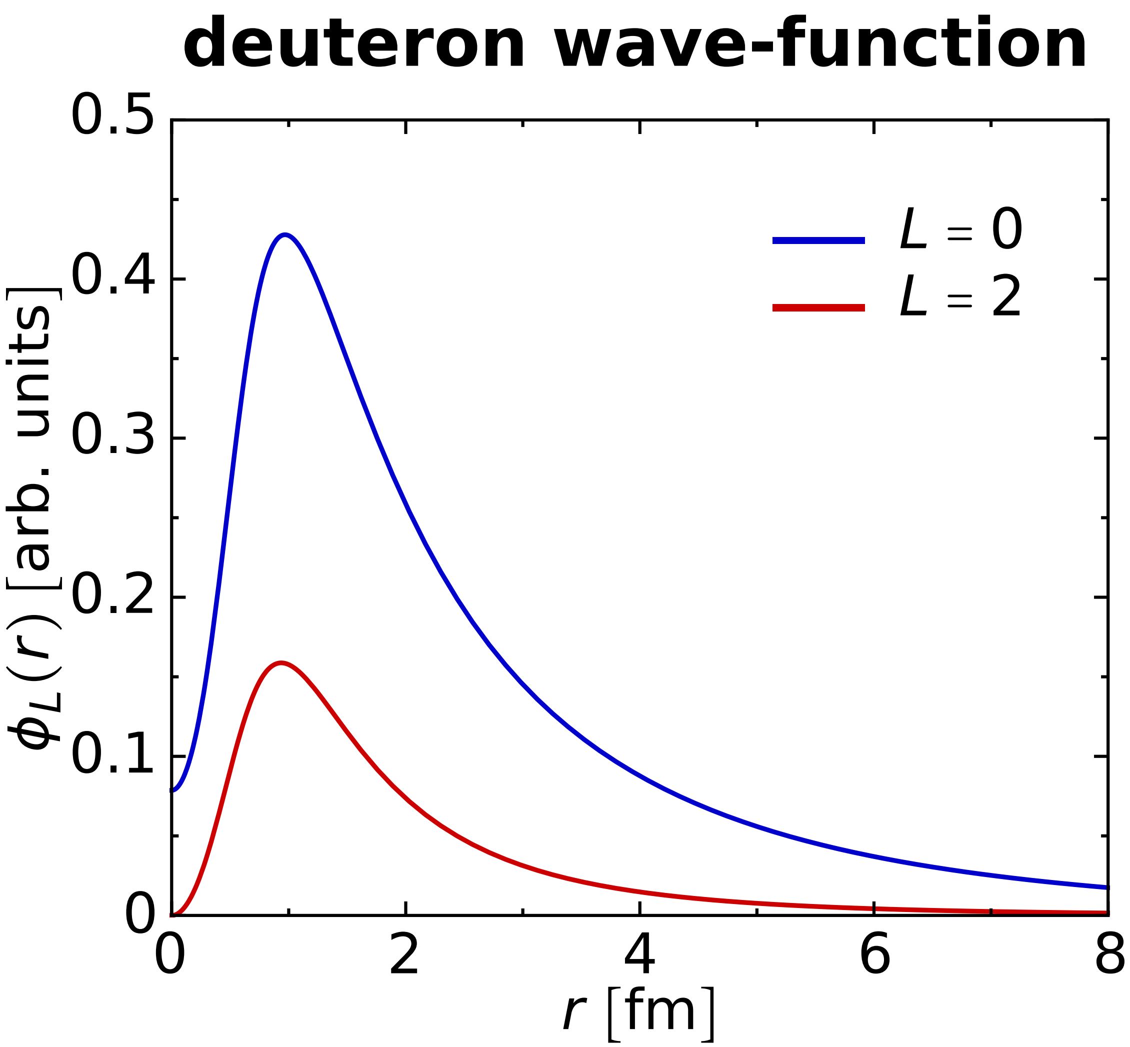
- **note**: when using *n*-body matrix elements, components of the evolved Hamiltonian with particle-rank > *n* are discarded

SRG Evolution in Two-Body Space



Argonne V18

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



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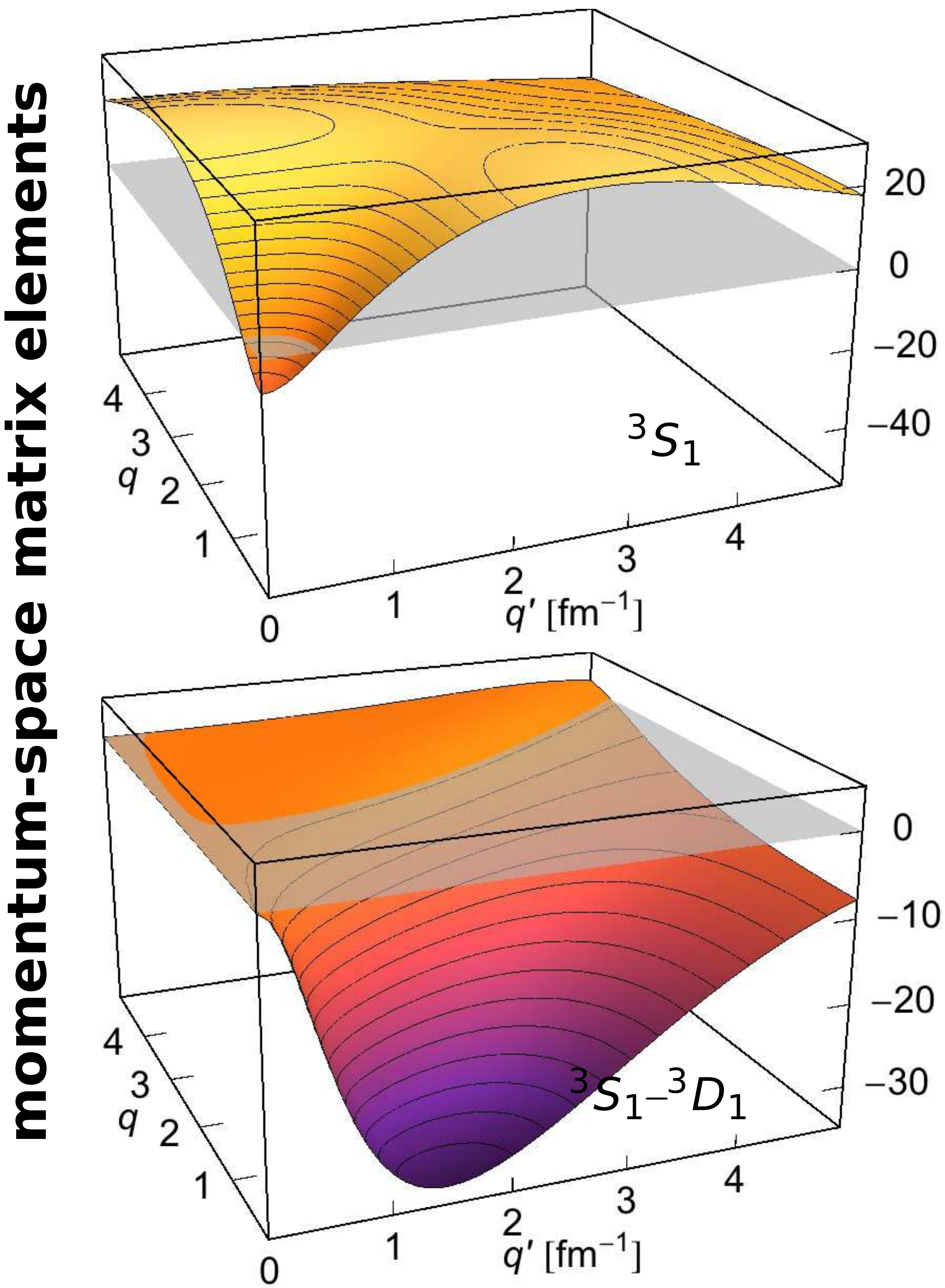

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$\Lambda = \infty\,\text{fm}^{-1}$

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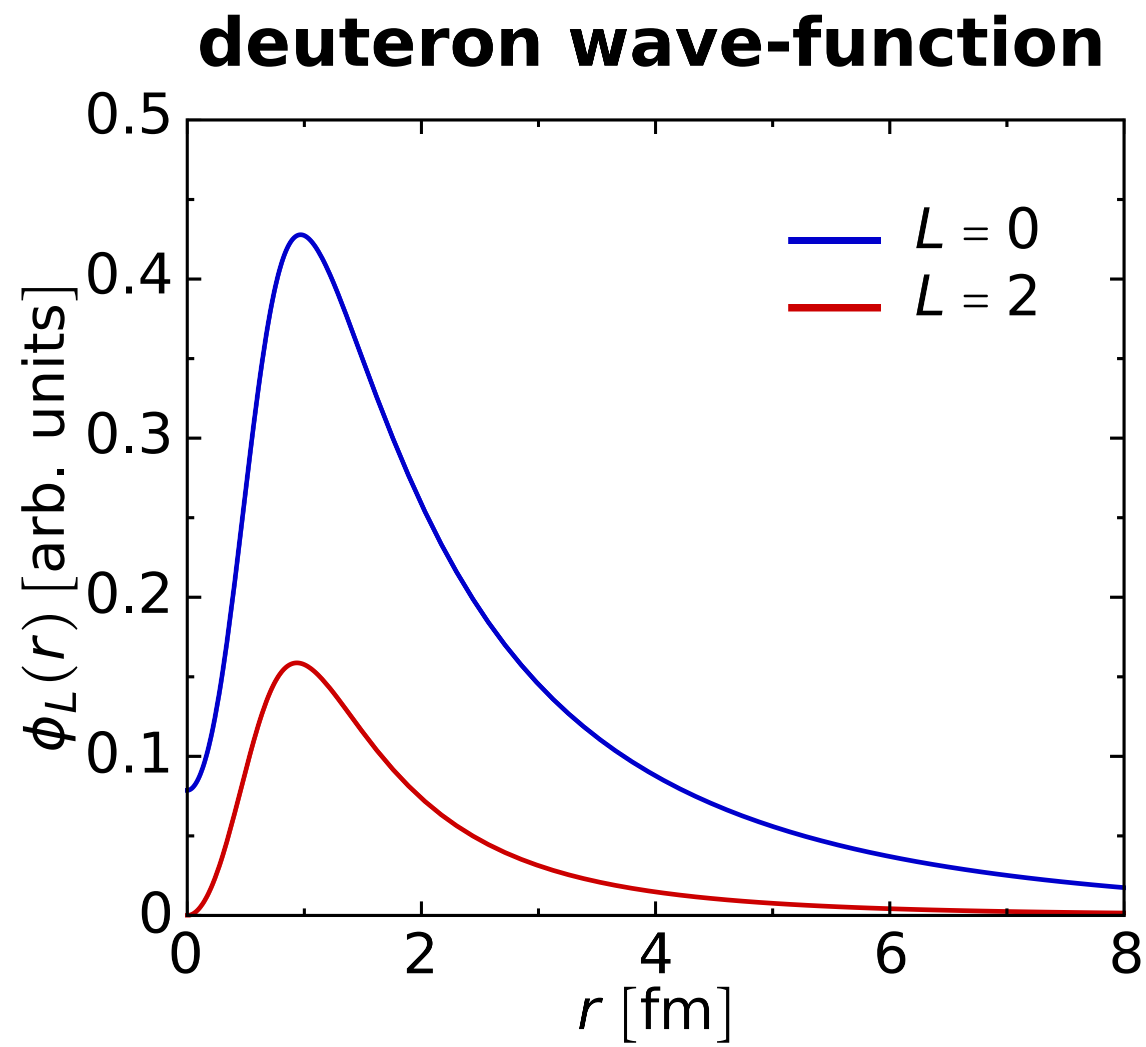

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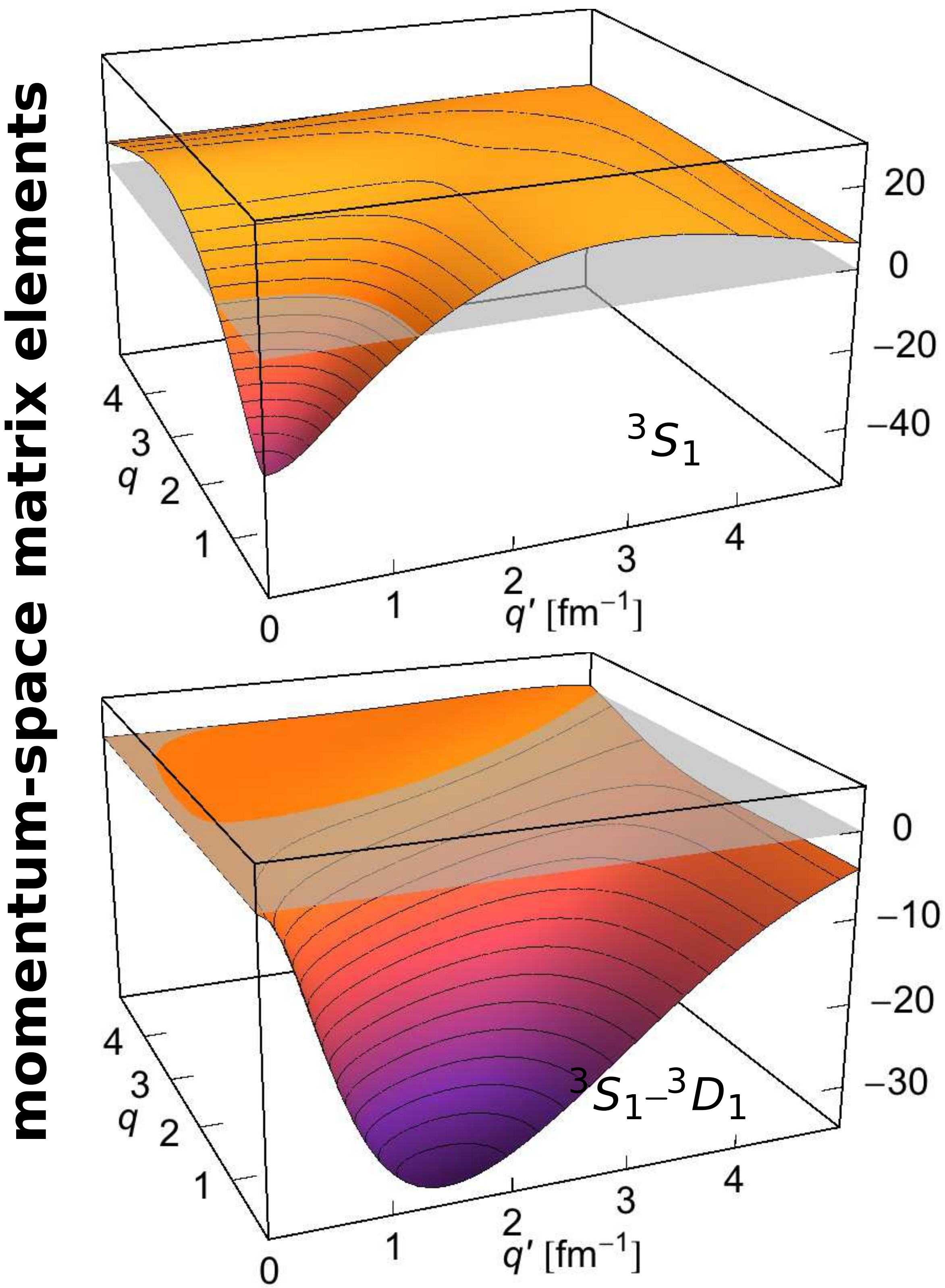

$\alpha = 0.001\,\mathrm{fm}^4$

$\Lambda = 5.62\,\mathrm{fm}^{-1}$

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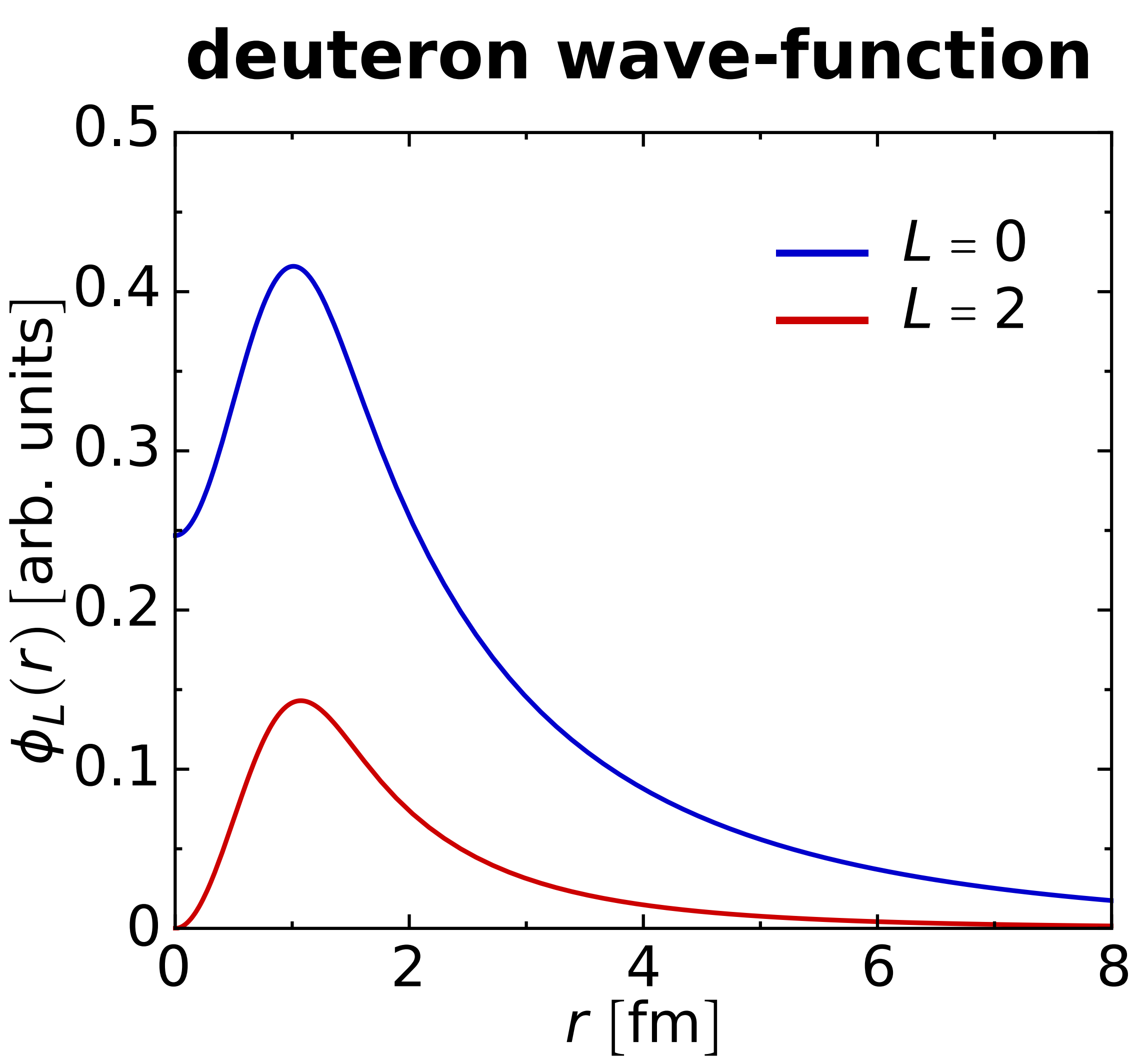

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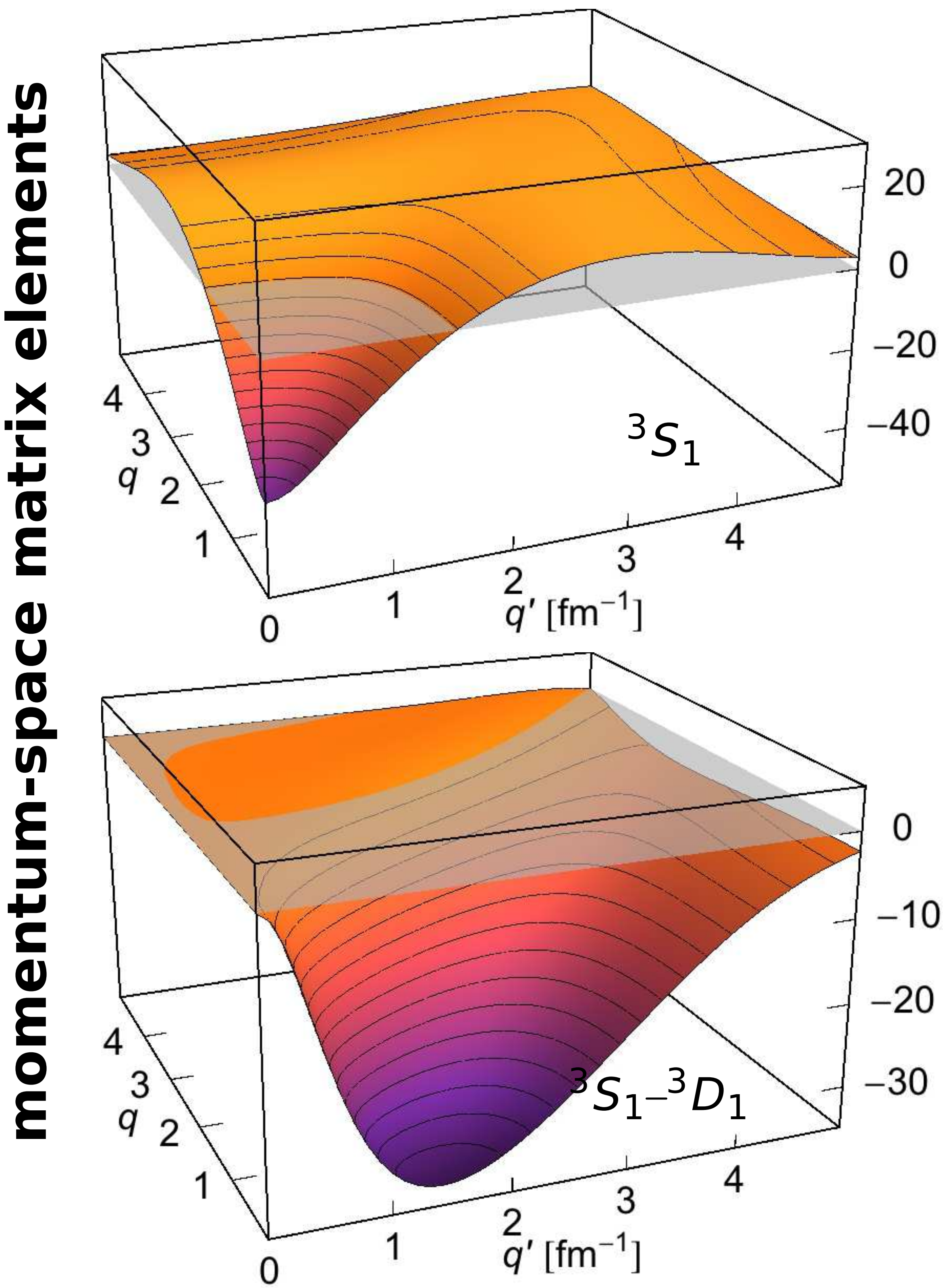

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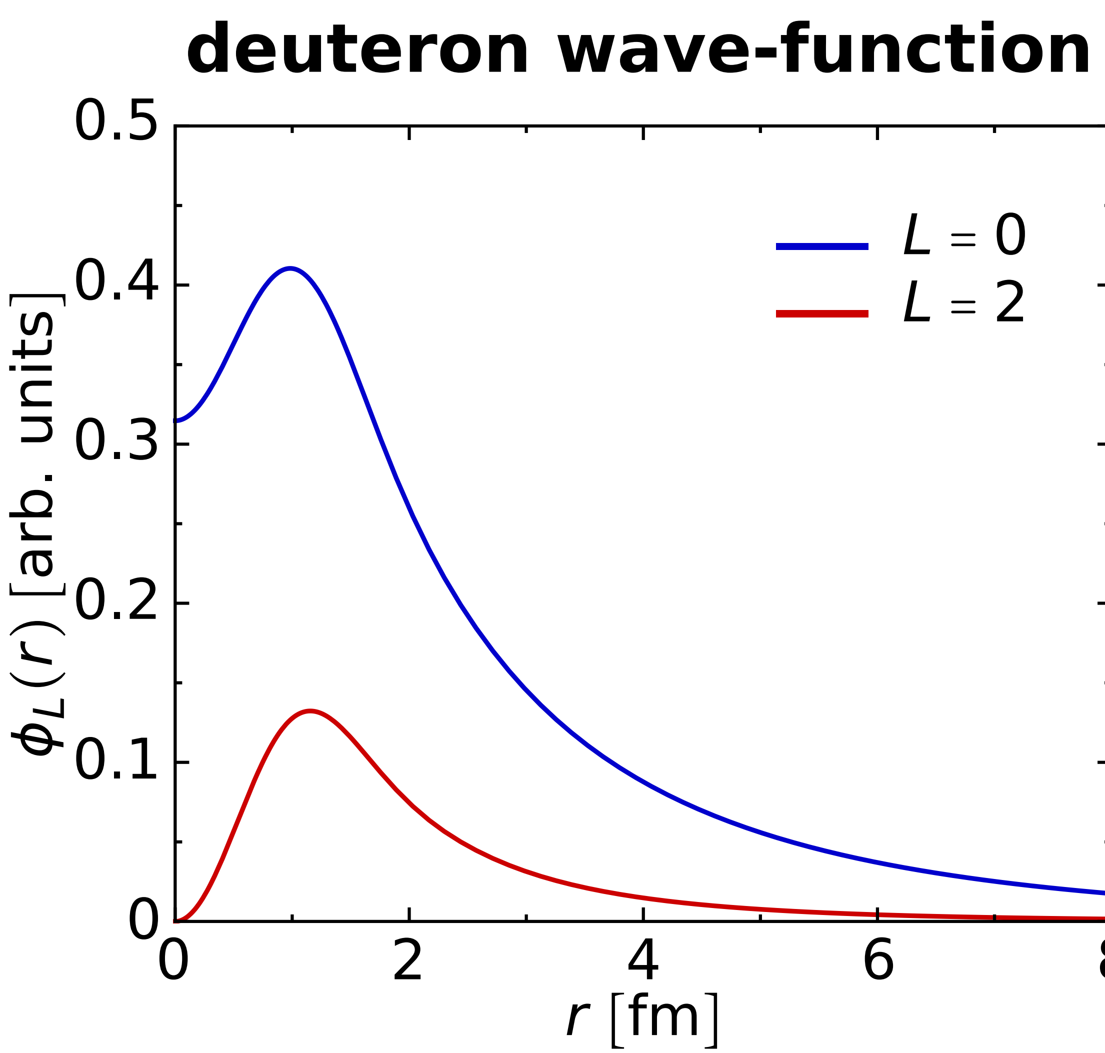
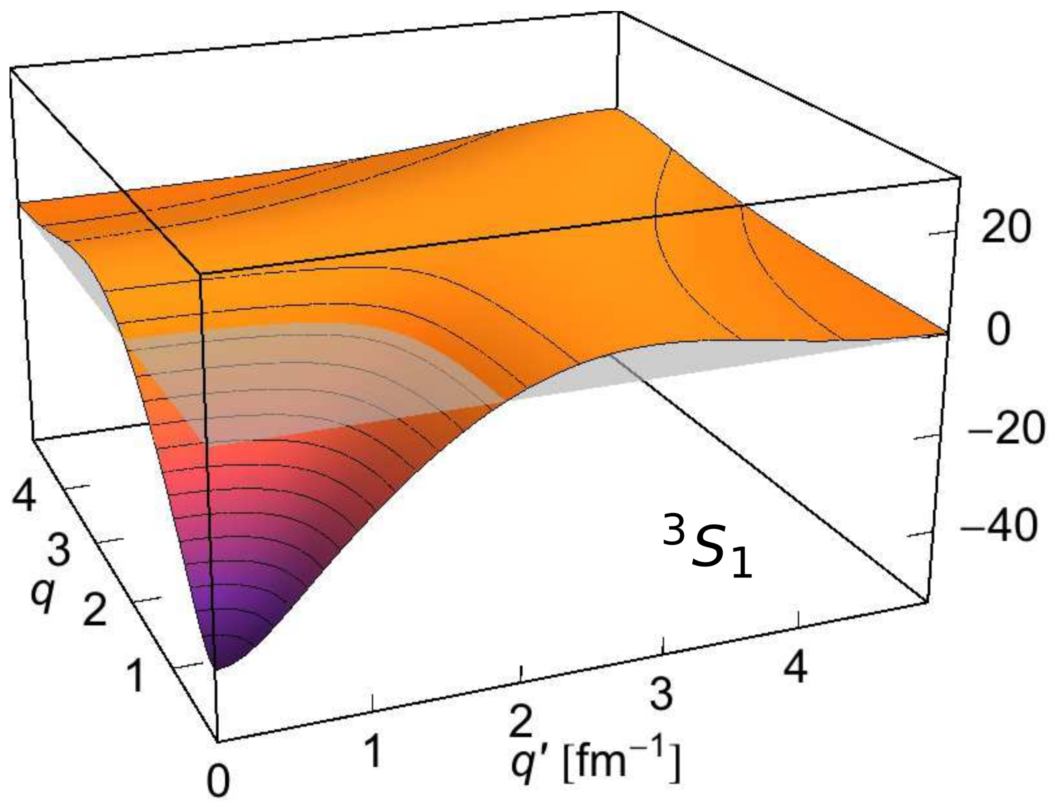
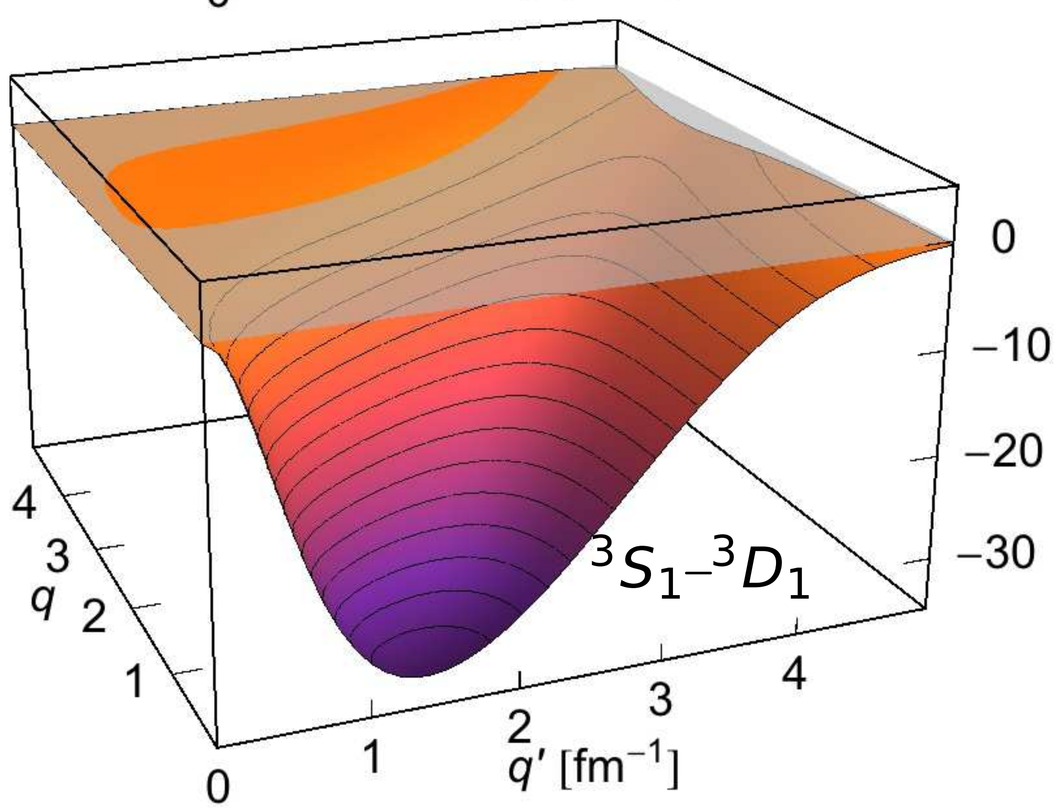


SRG Evolution in Two-Body Space

momentum-space matrix elements





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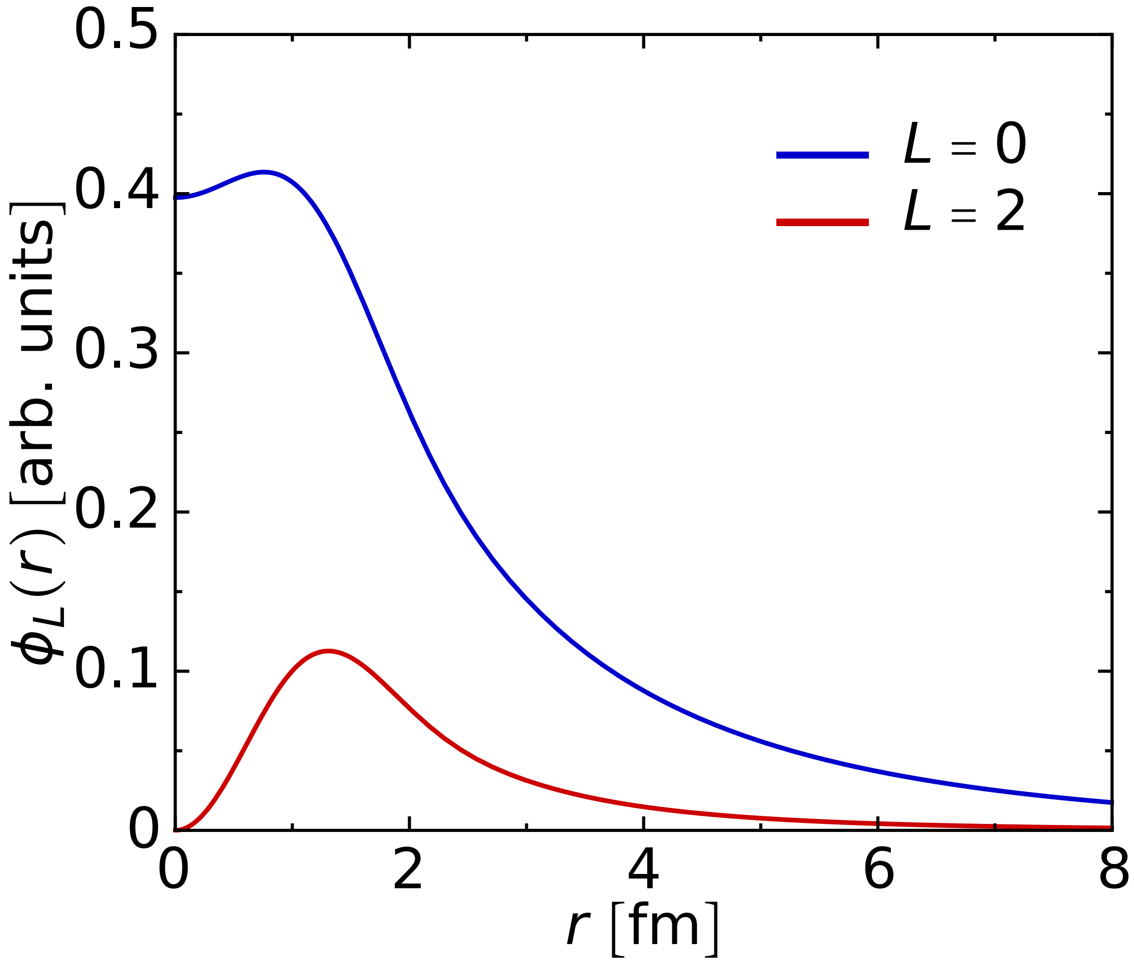
deuteron wave-function



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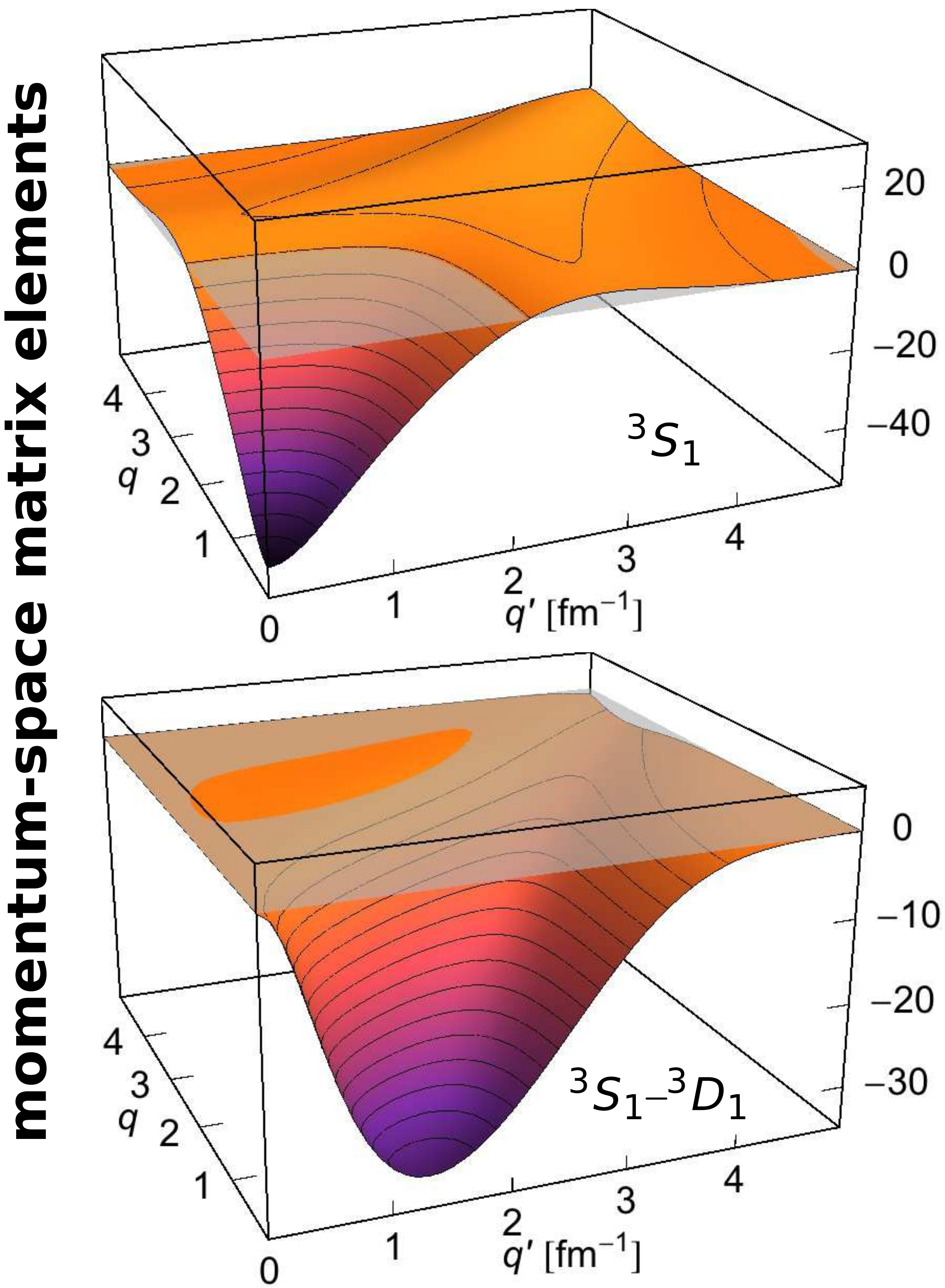

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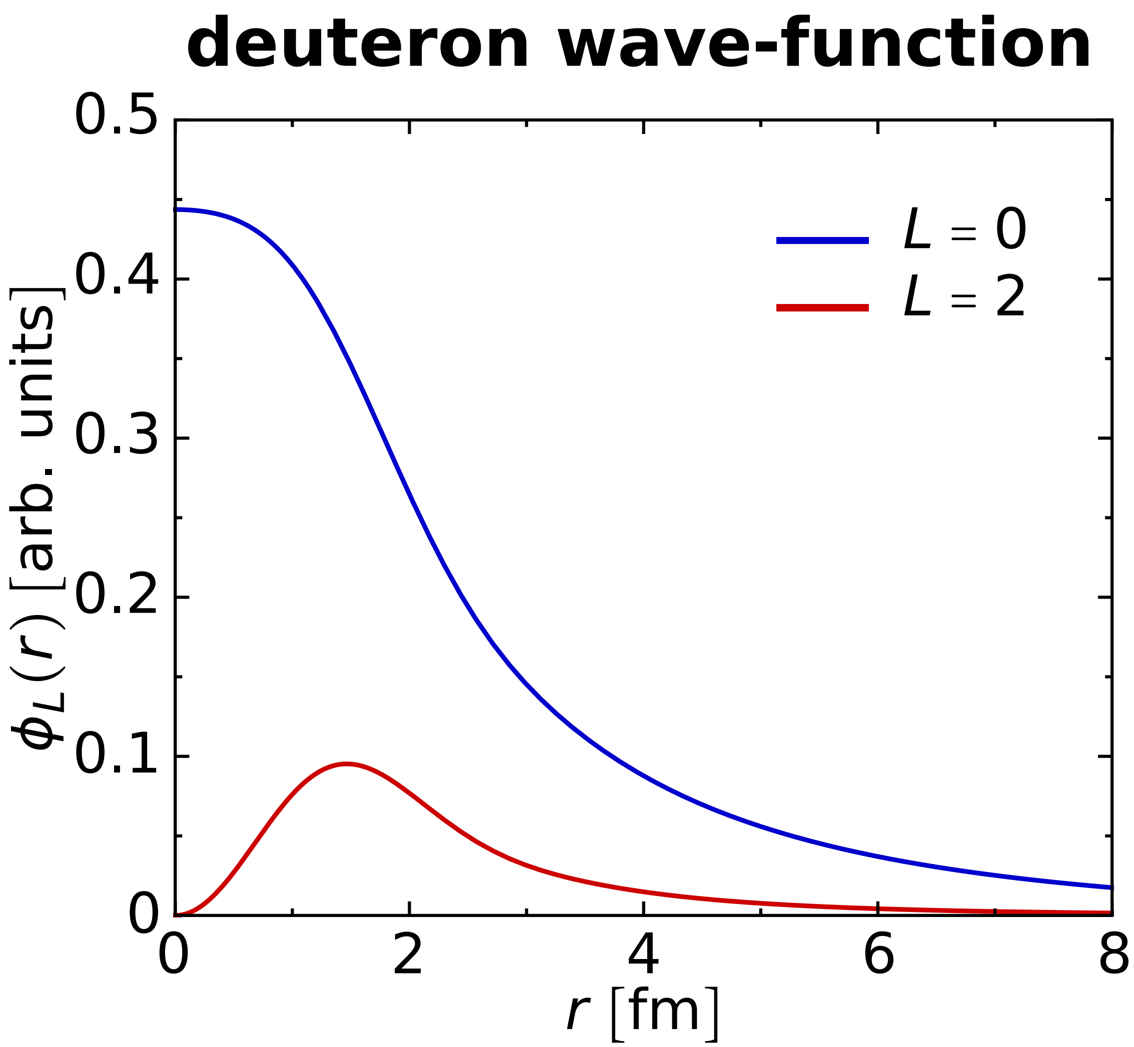

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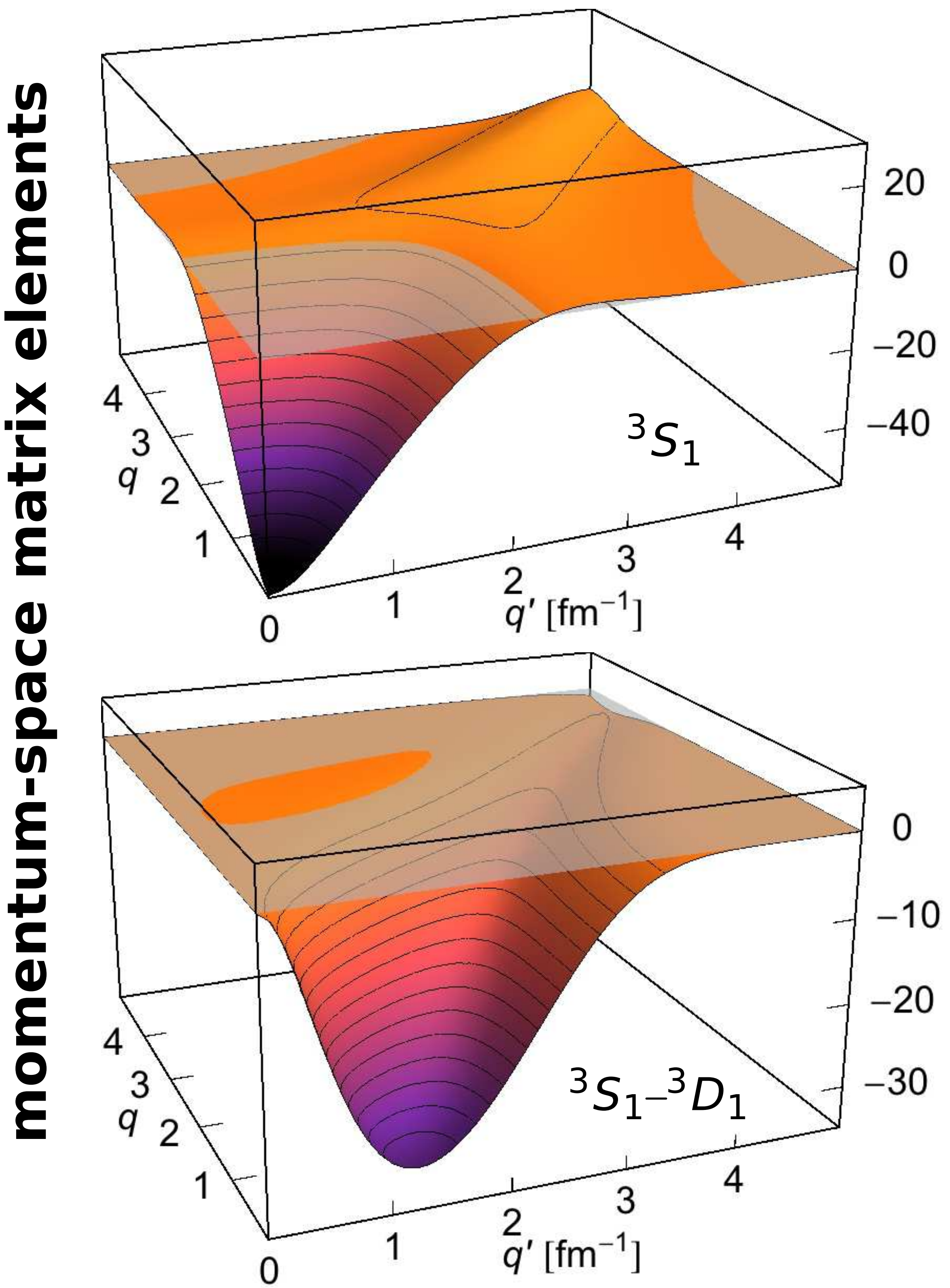

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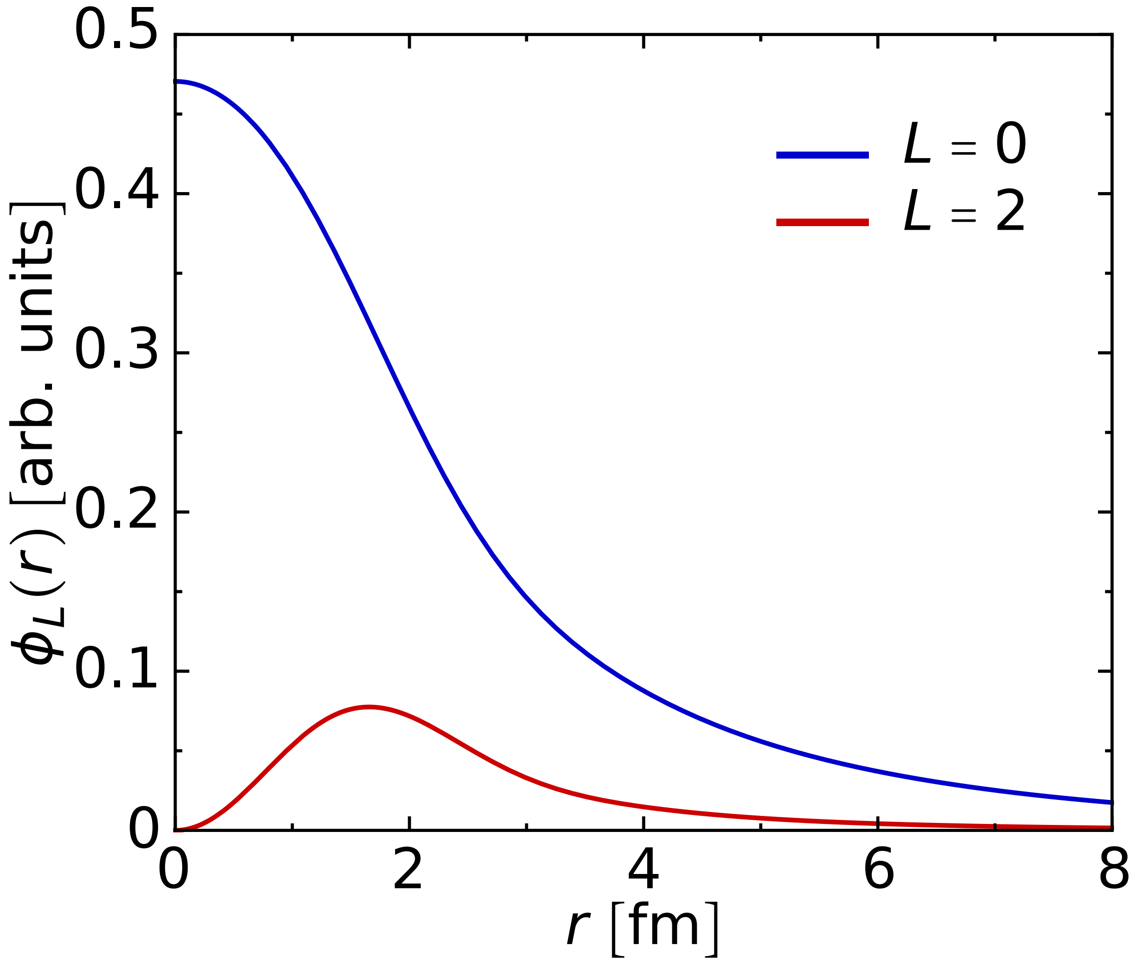

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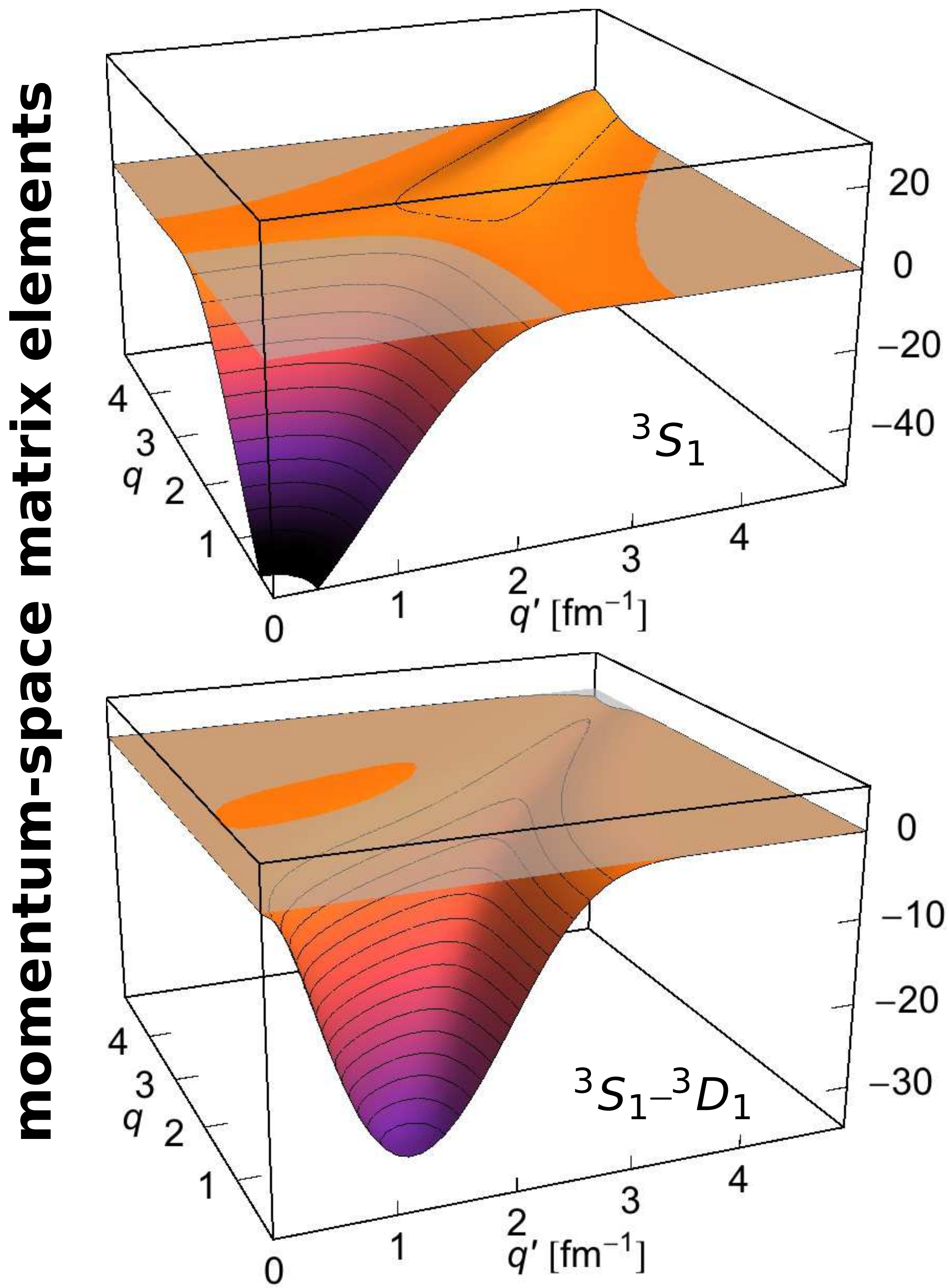

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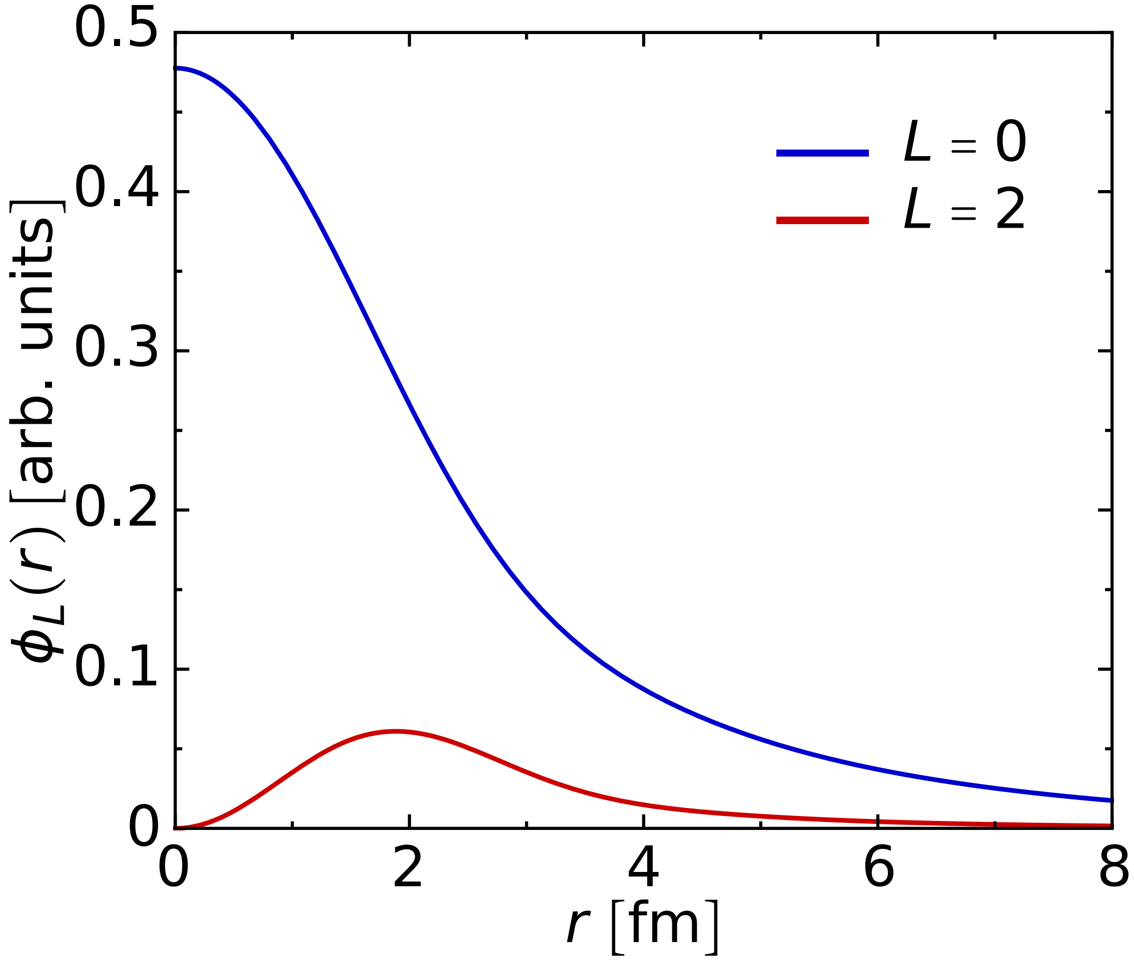

SRG Evolution in Two-Body Space

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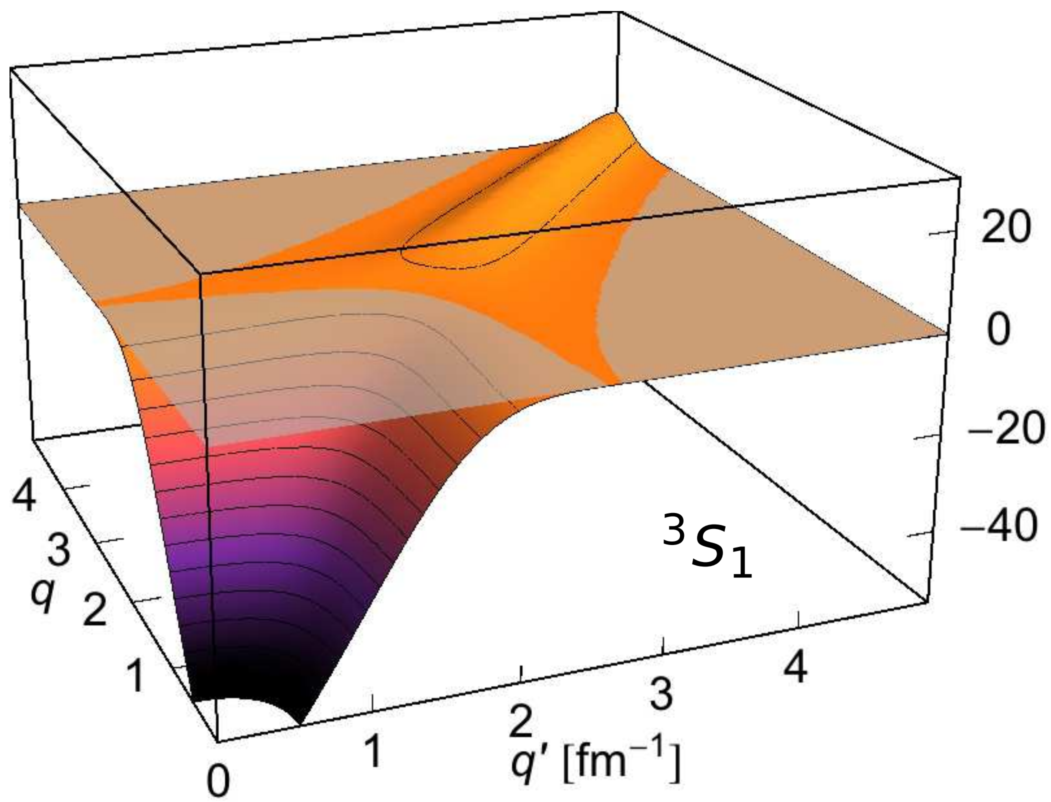

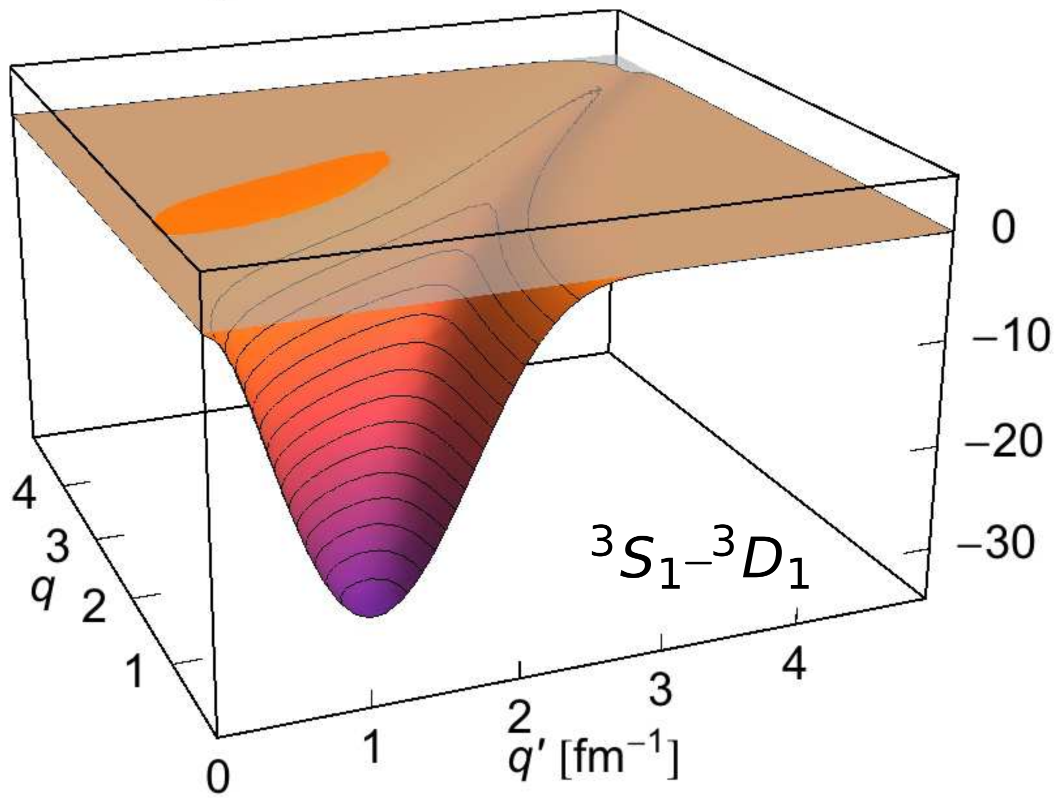

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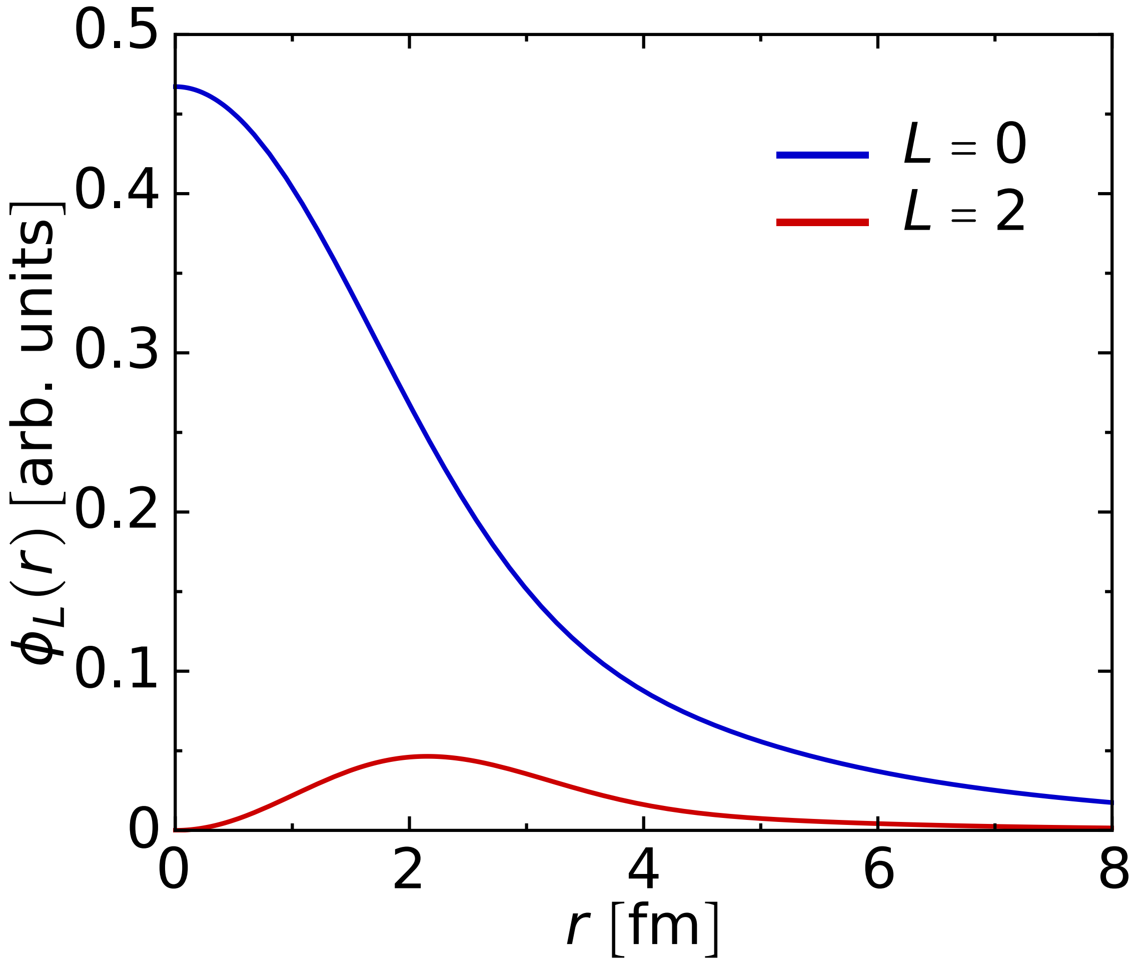

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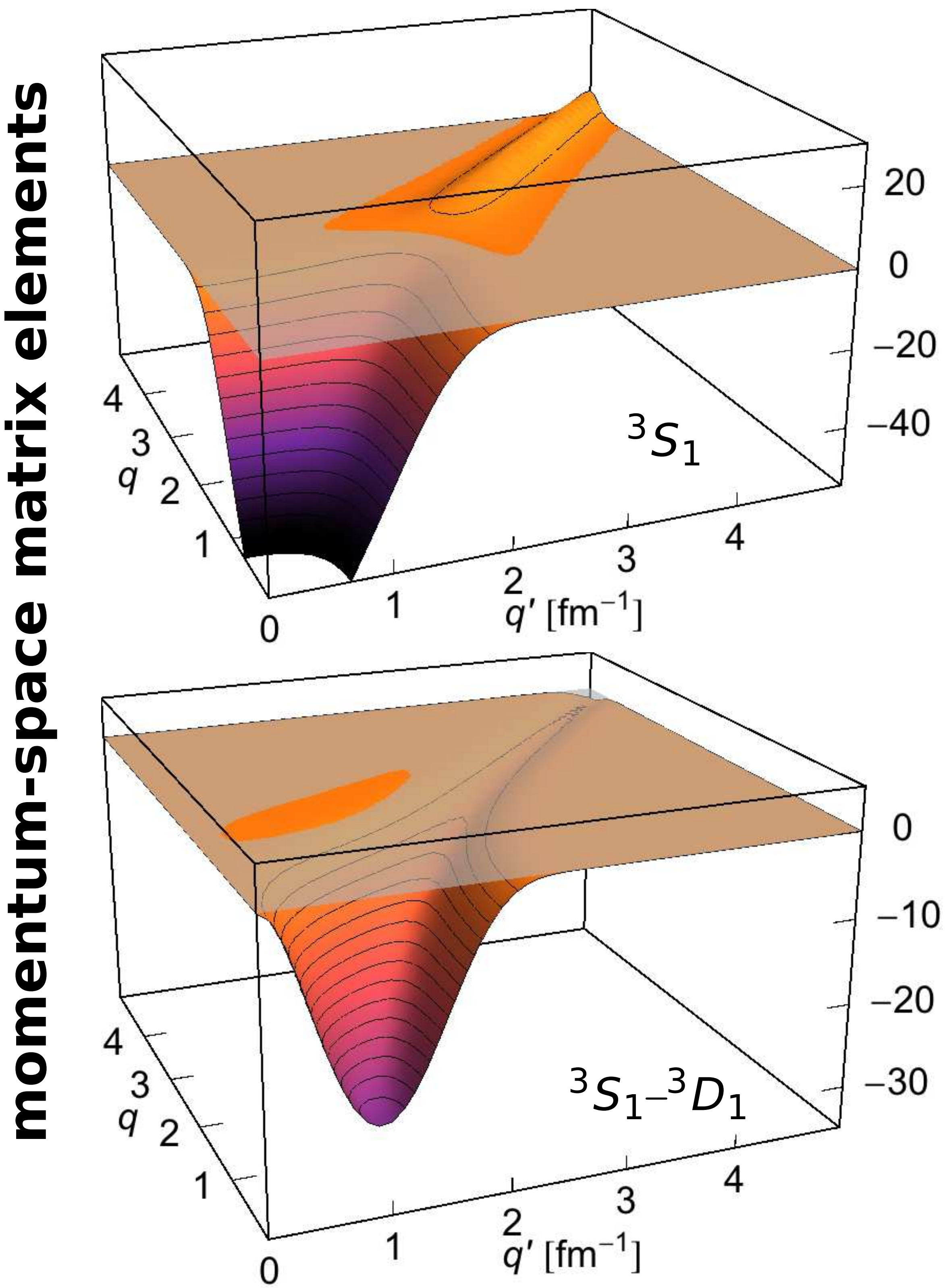

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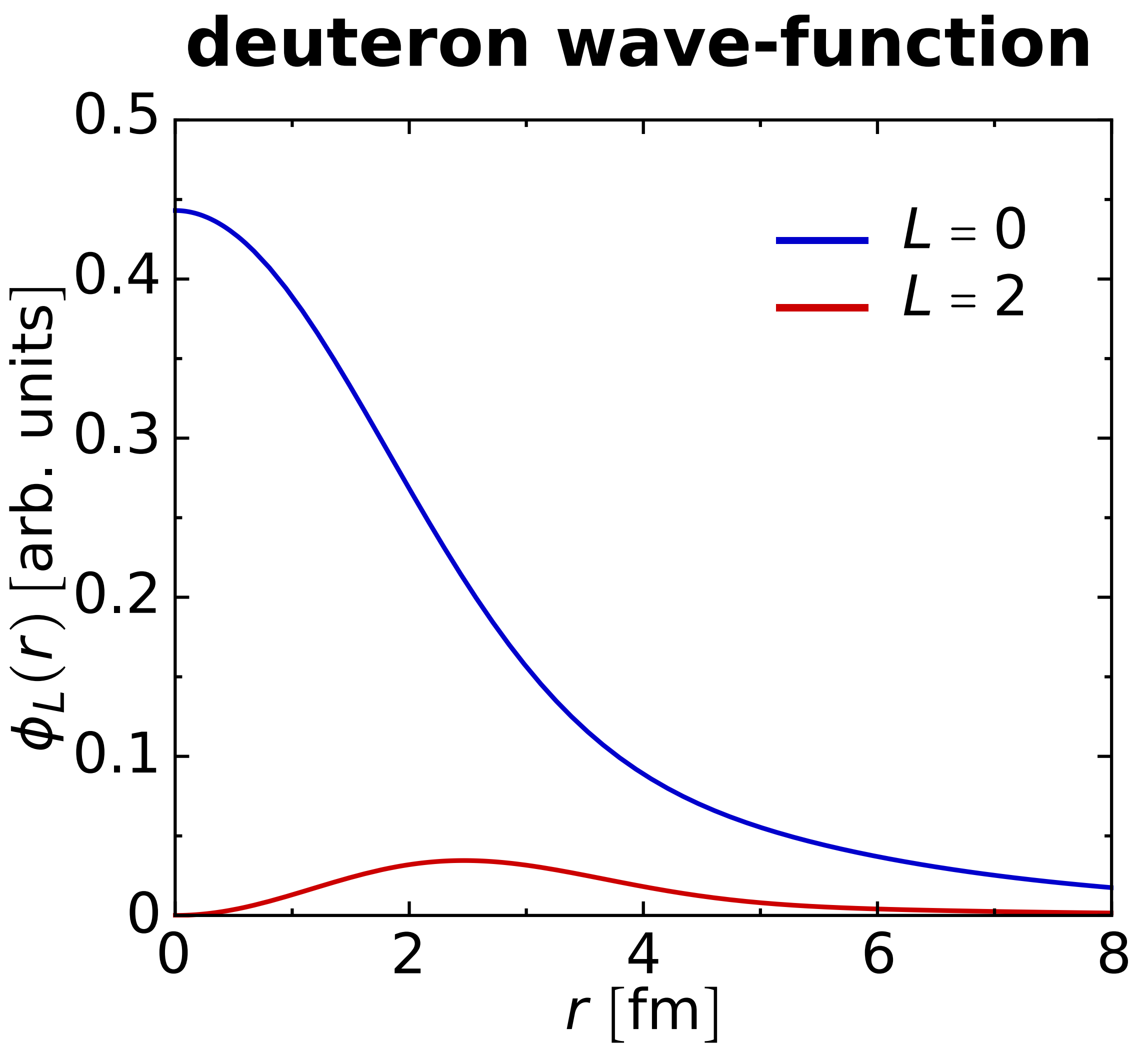

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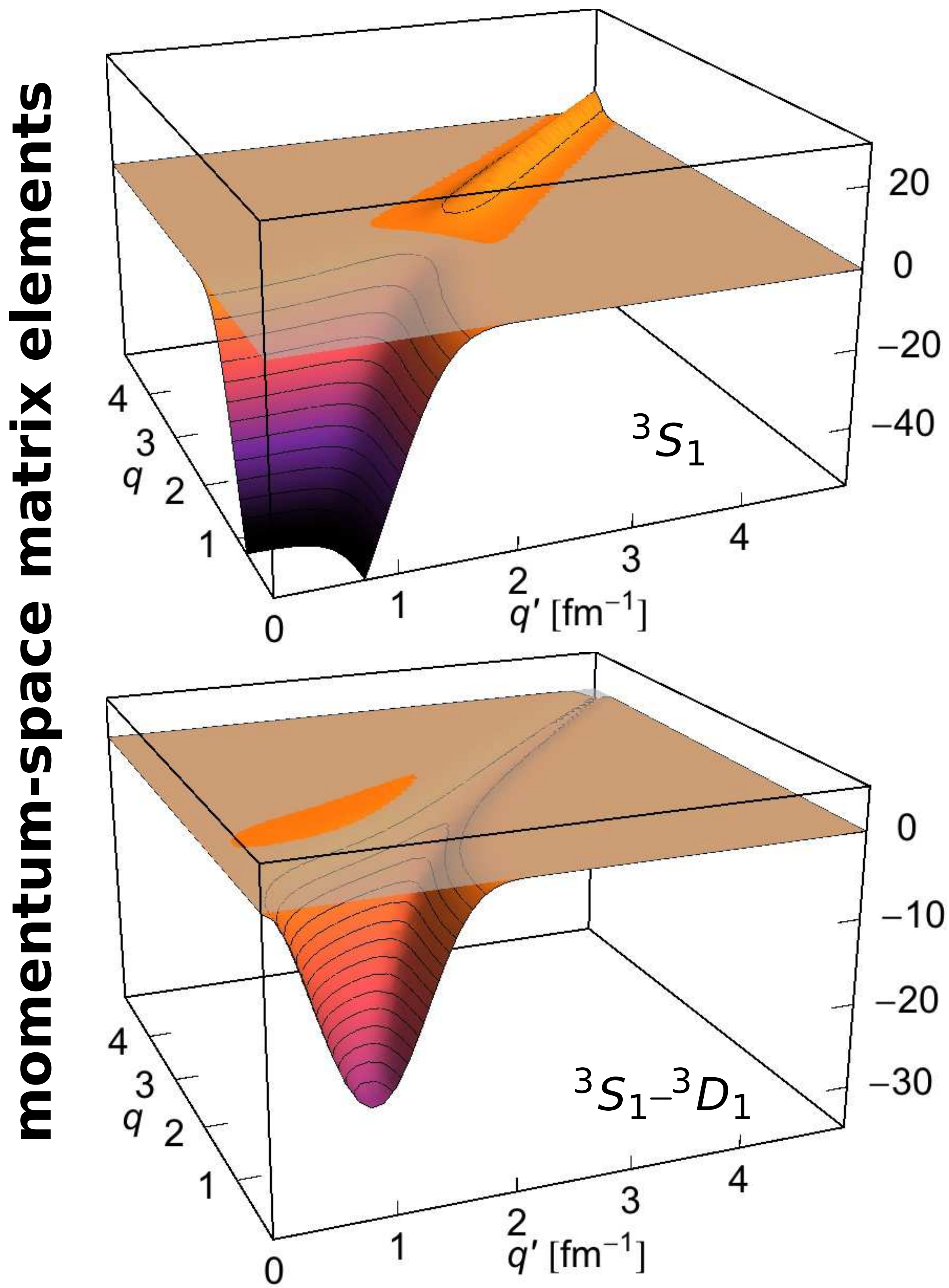

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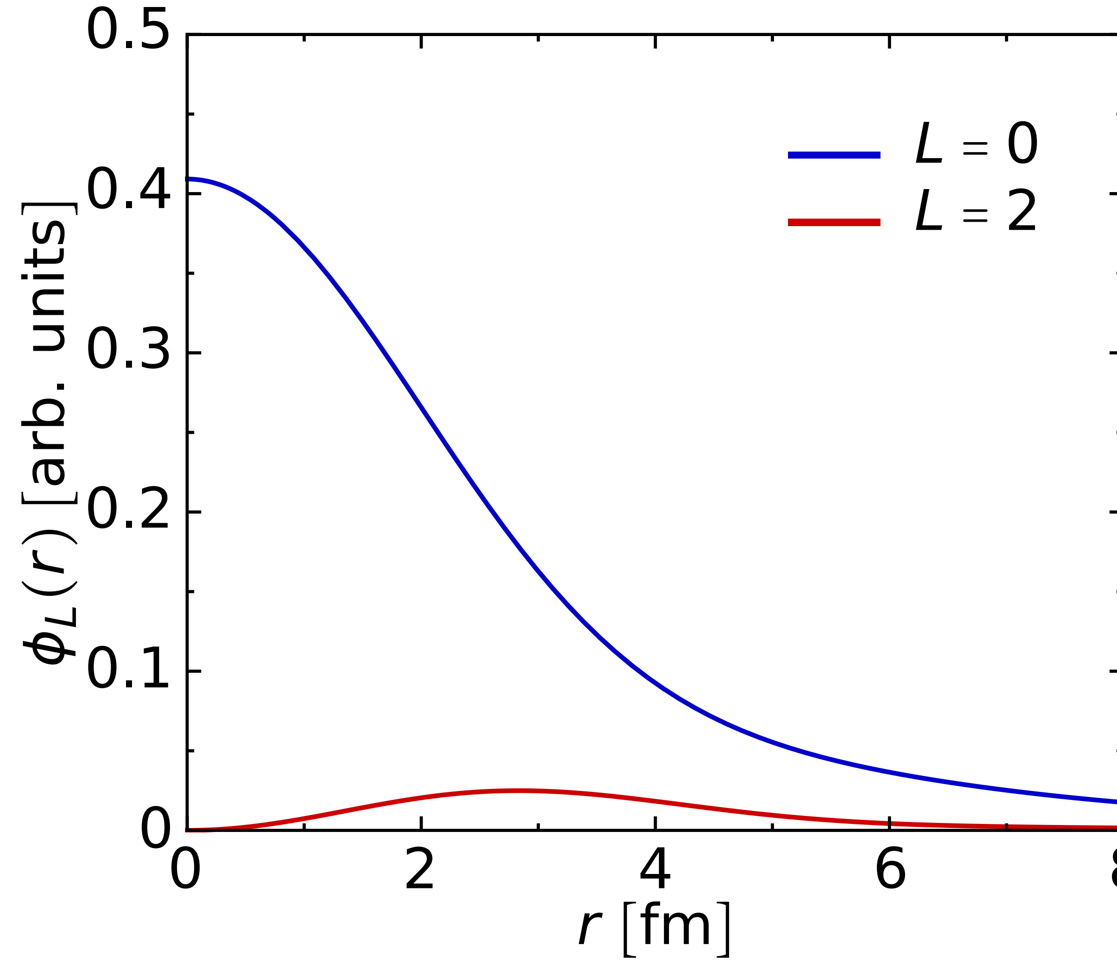
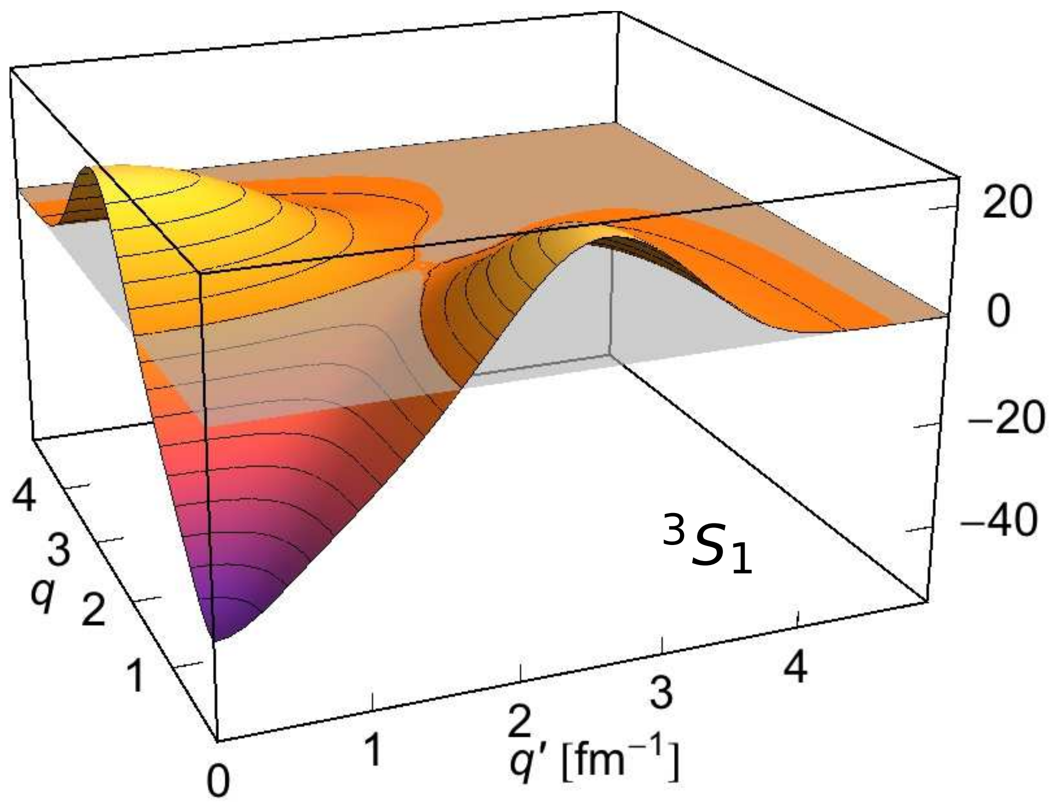
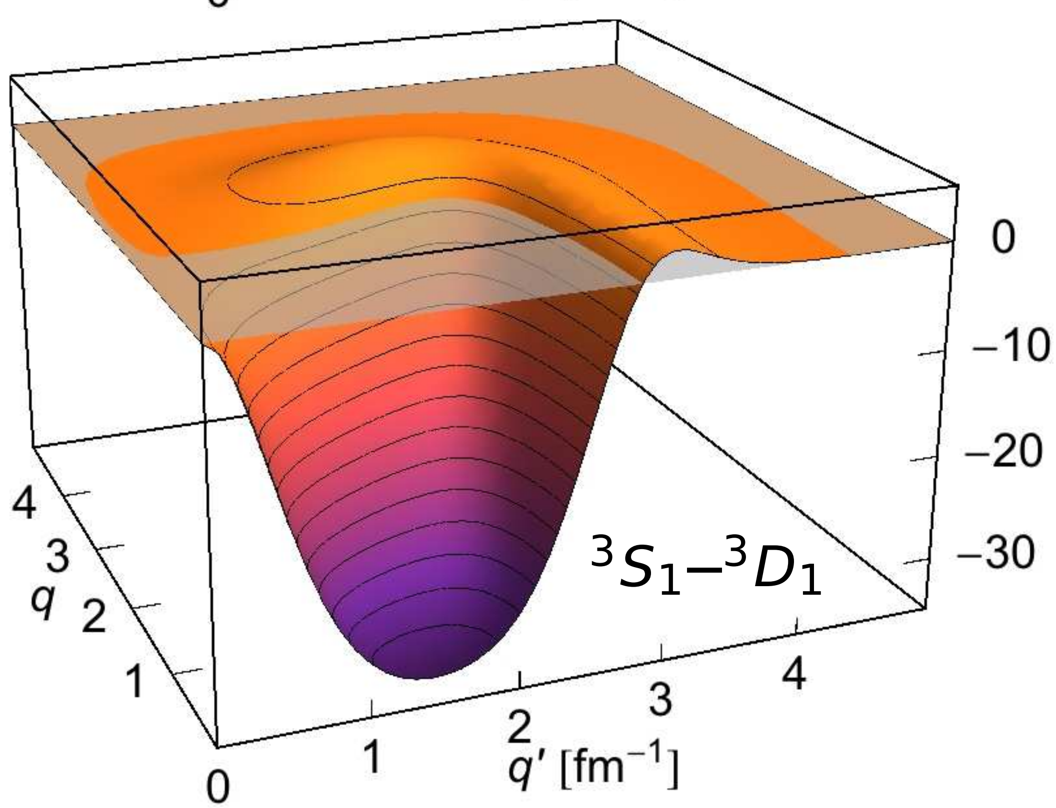


SRG Evolution in Two-Body Space

momentum-space matrix elements



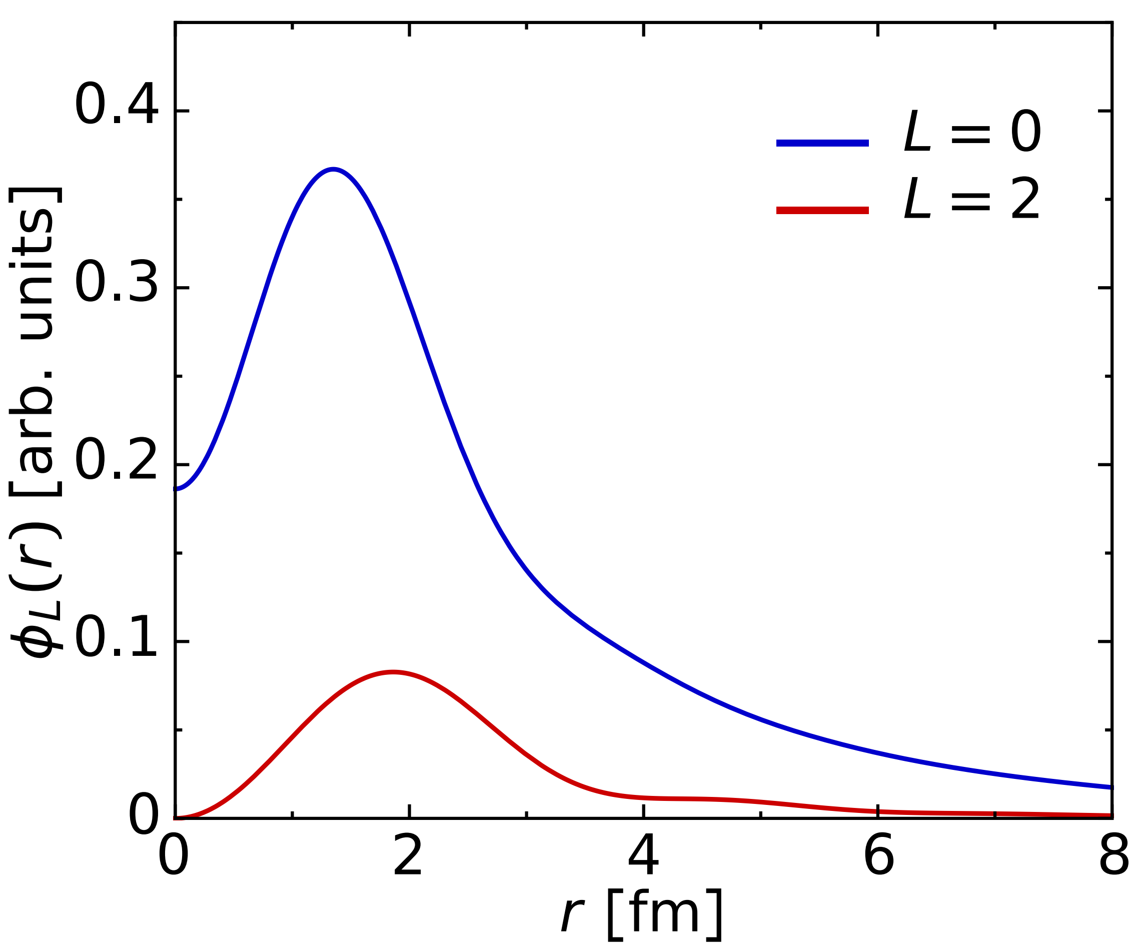


chiral NN

Entem & Machleidt. N^{3}LO, 500 MeV

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

deuteron wave-function



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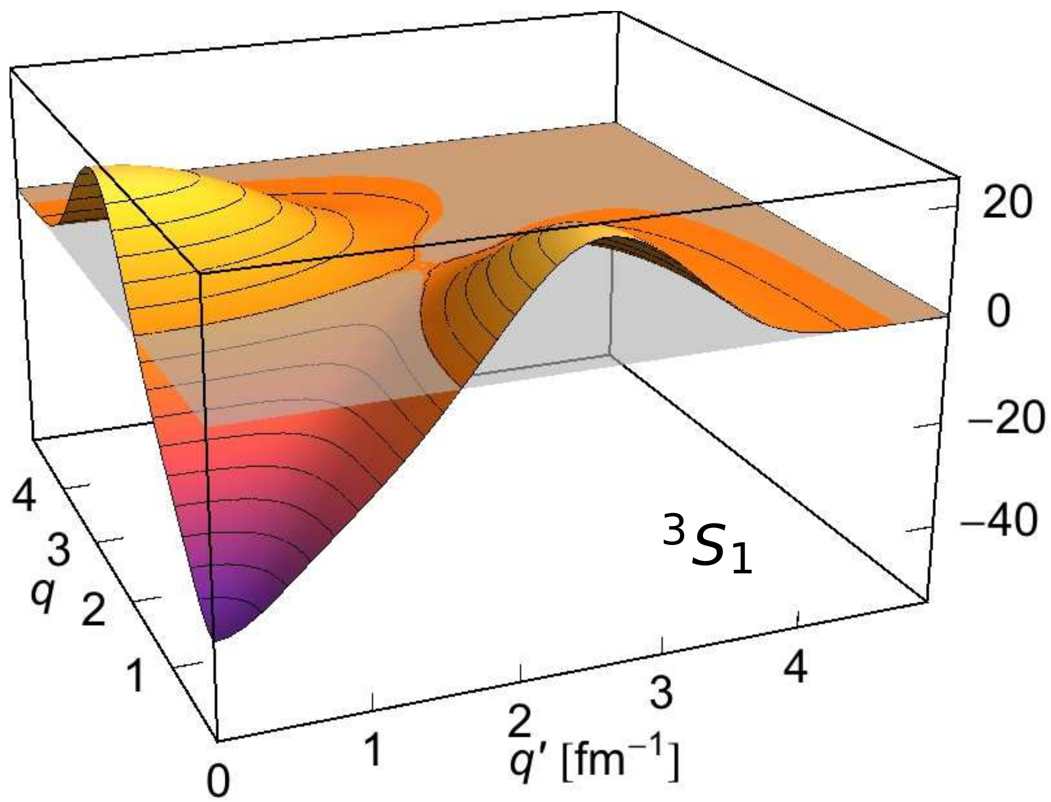

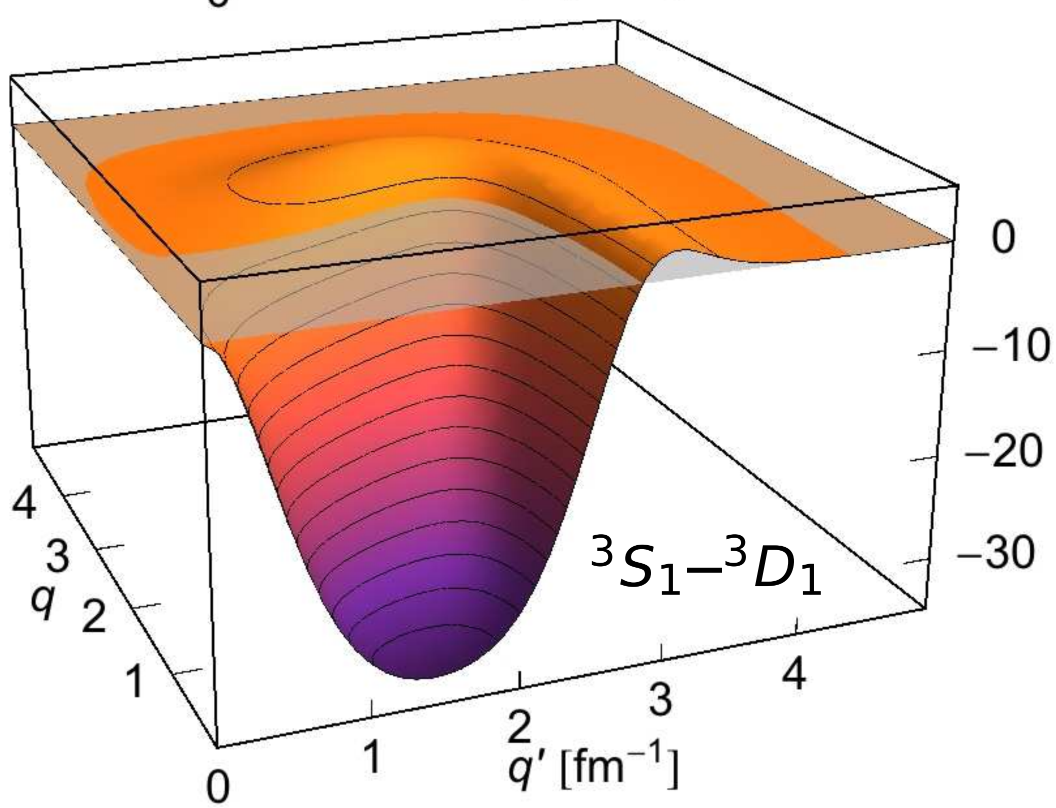

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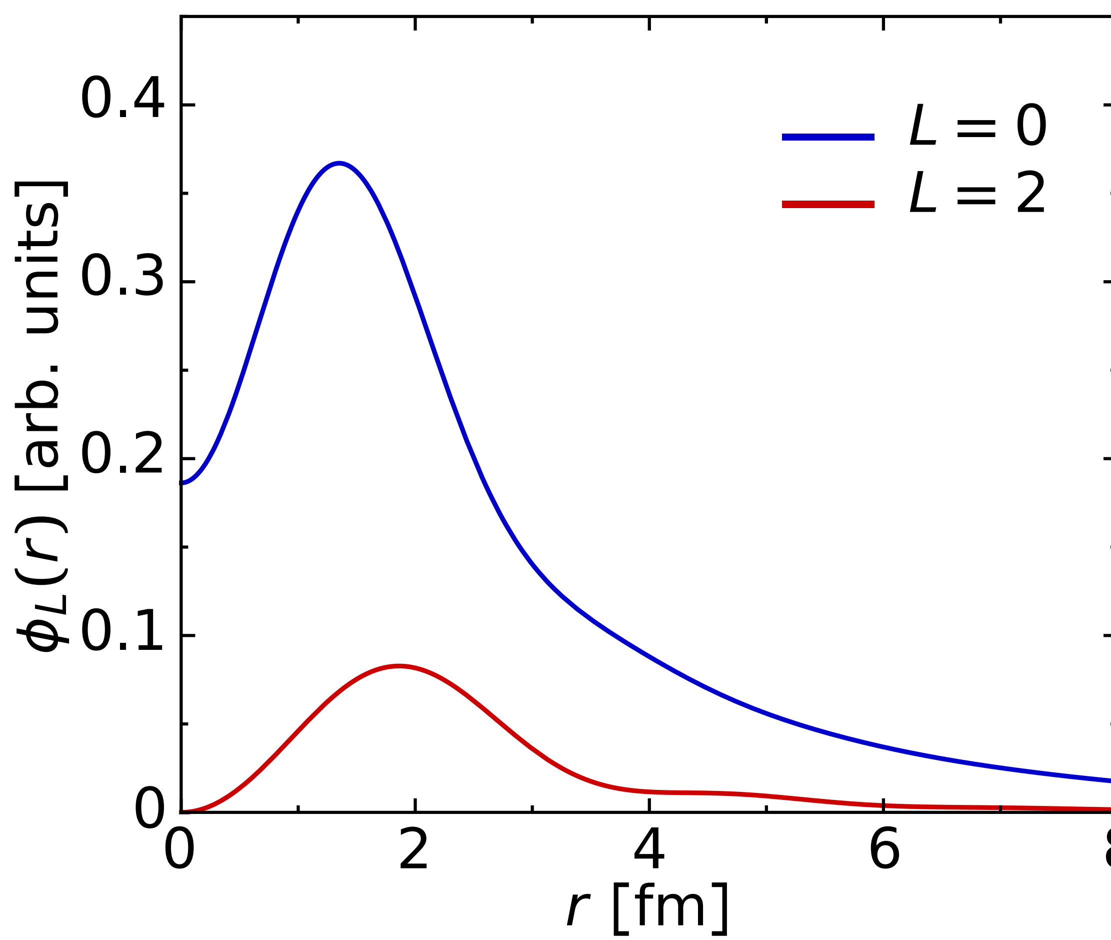

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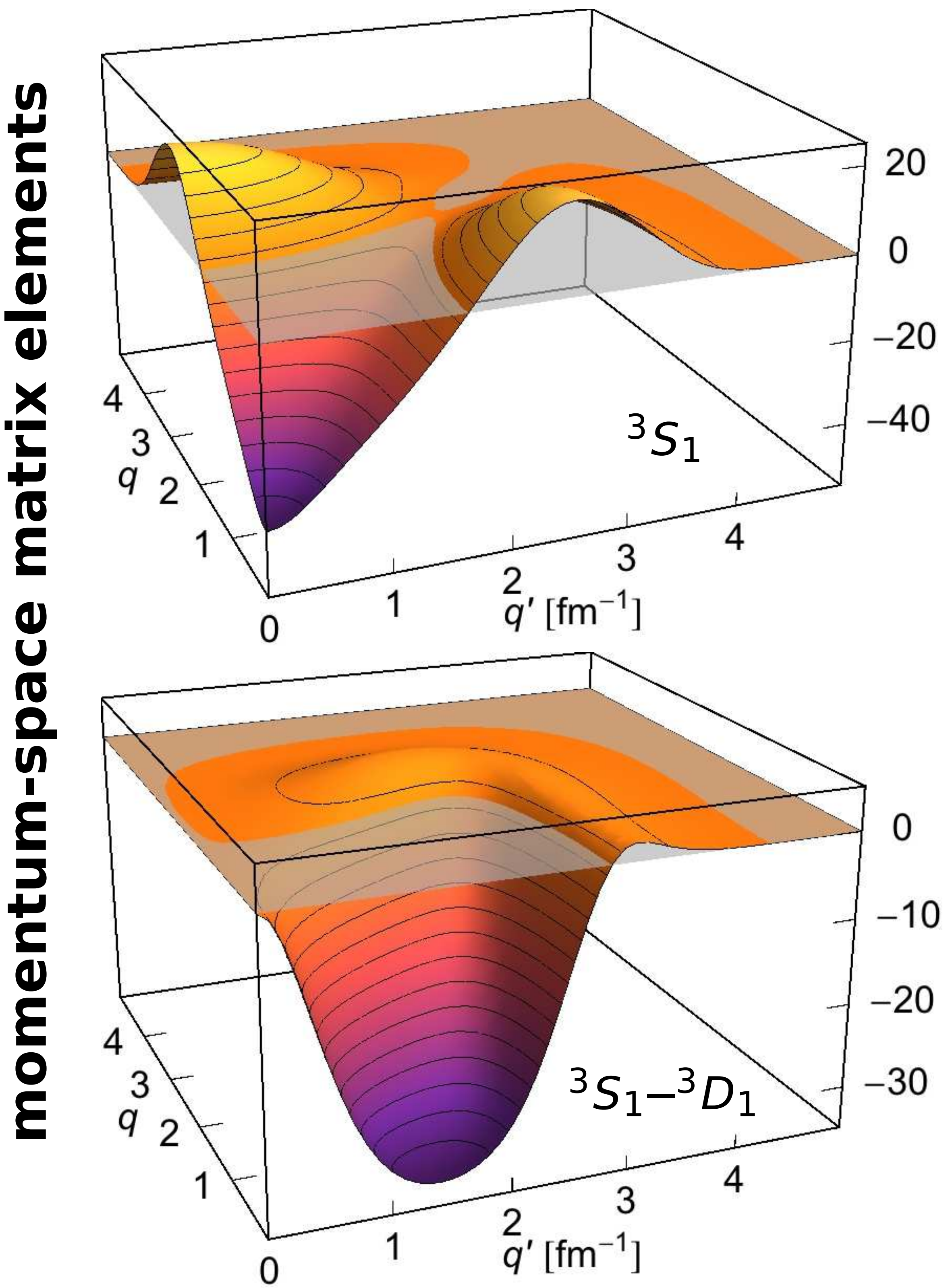

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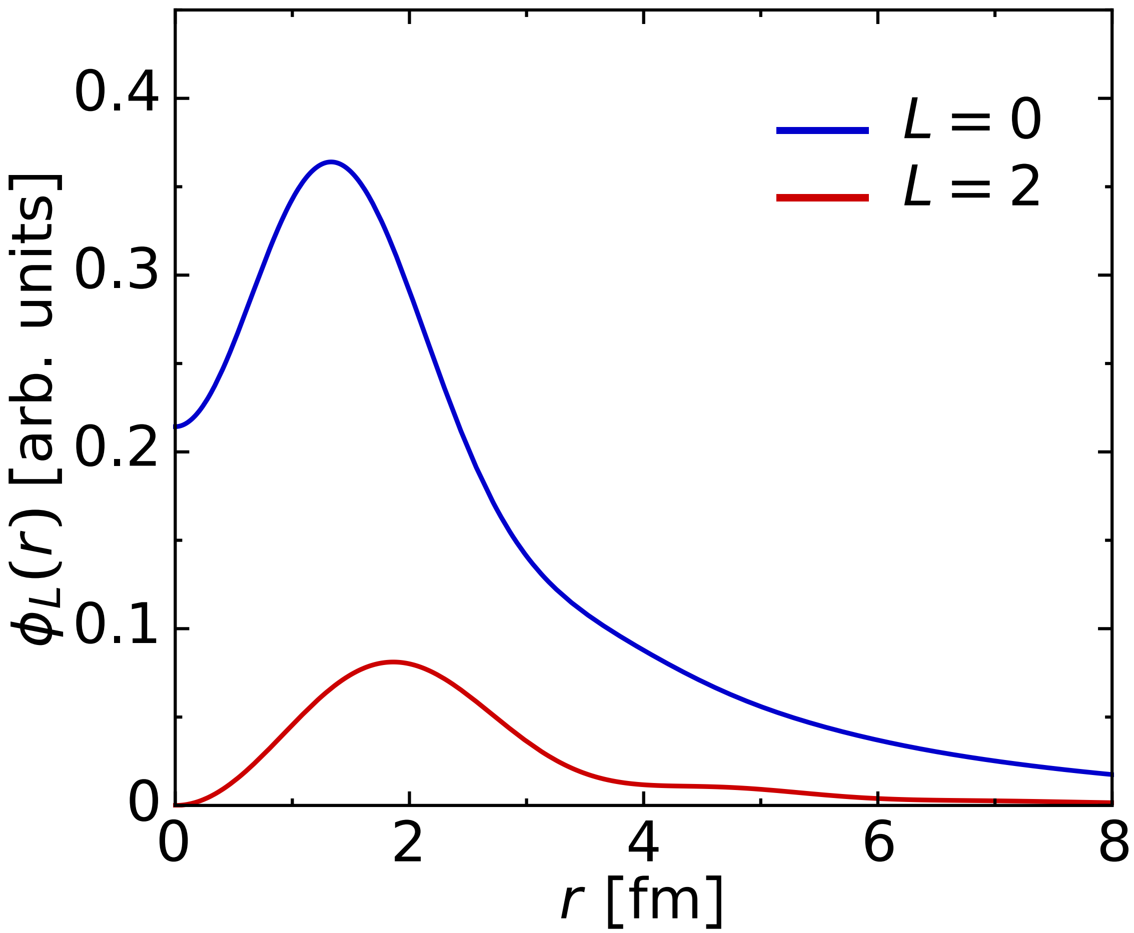

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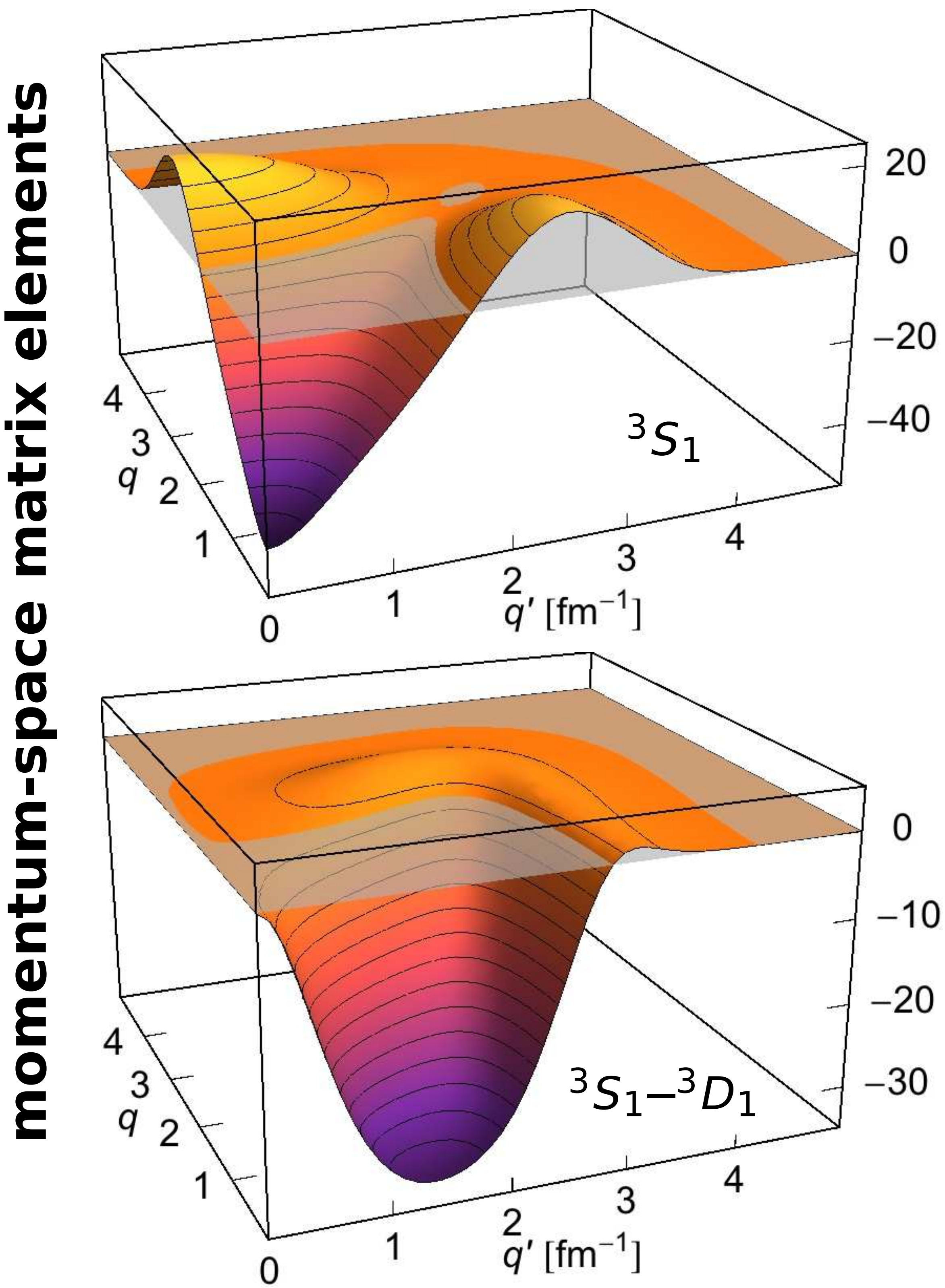

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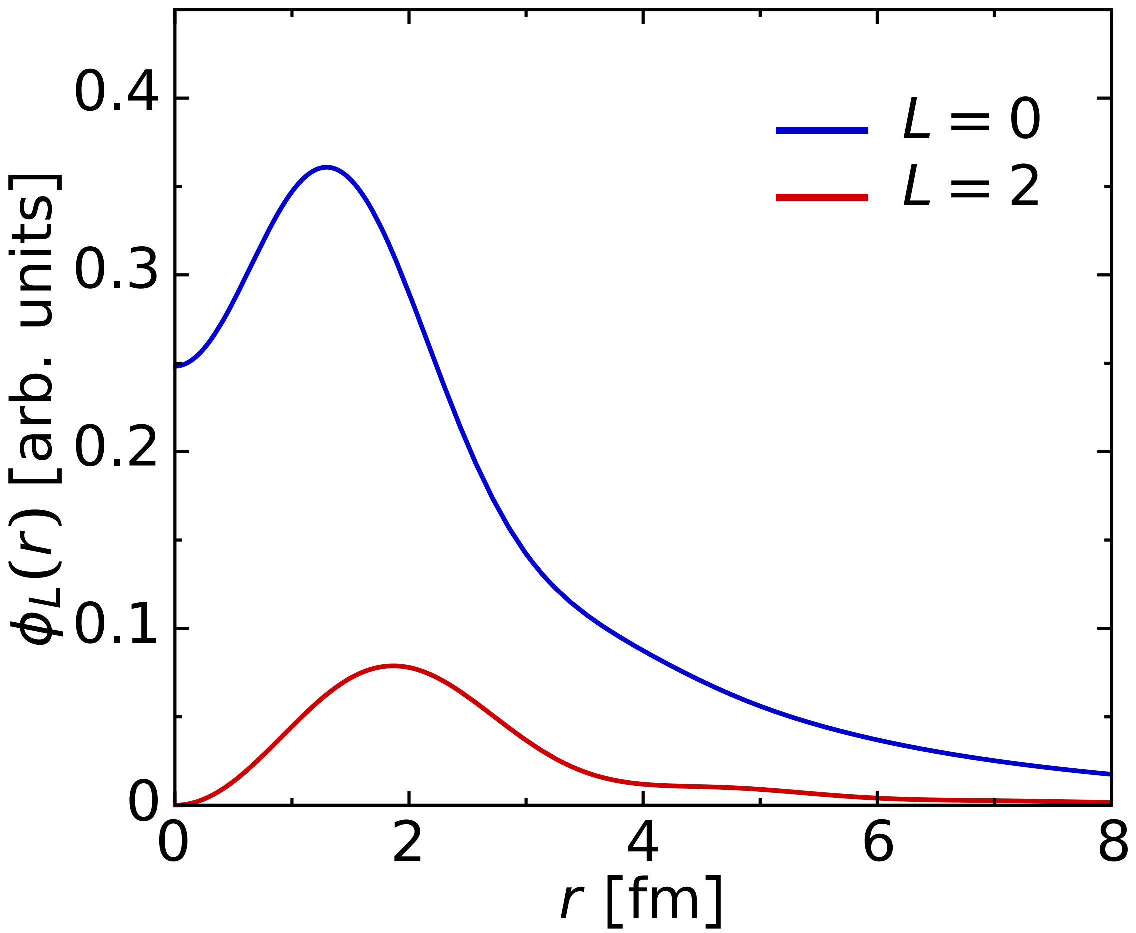
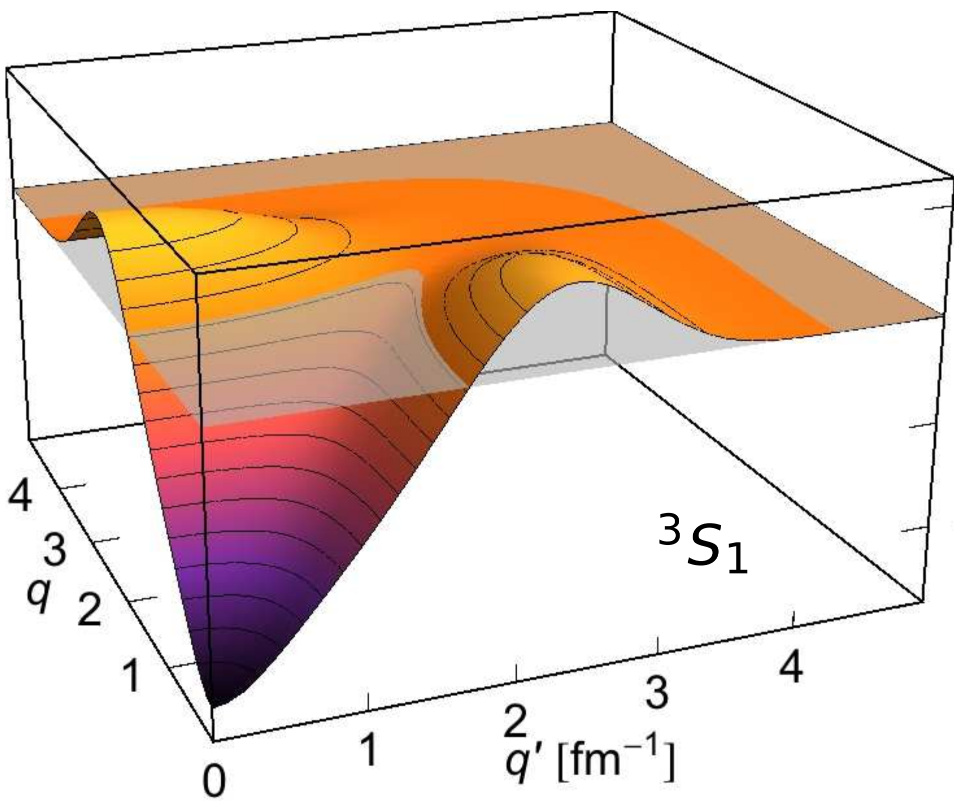
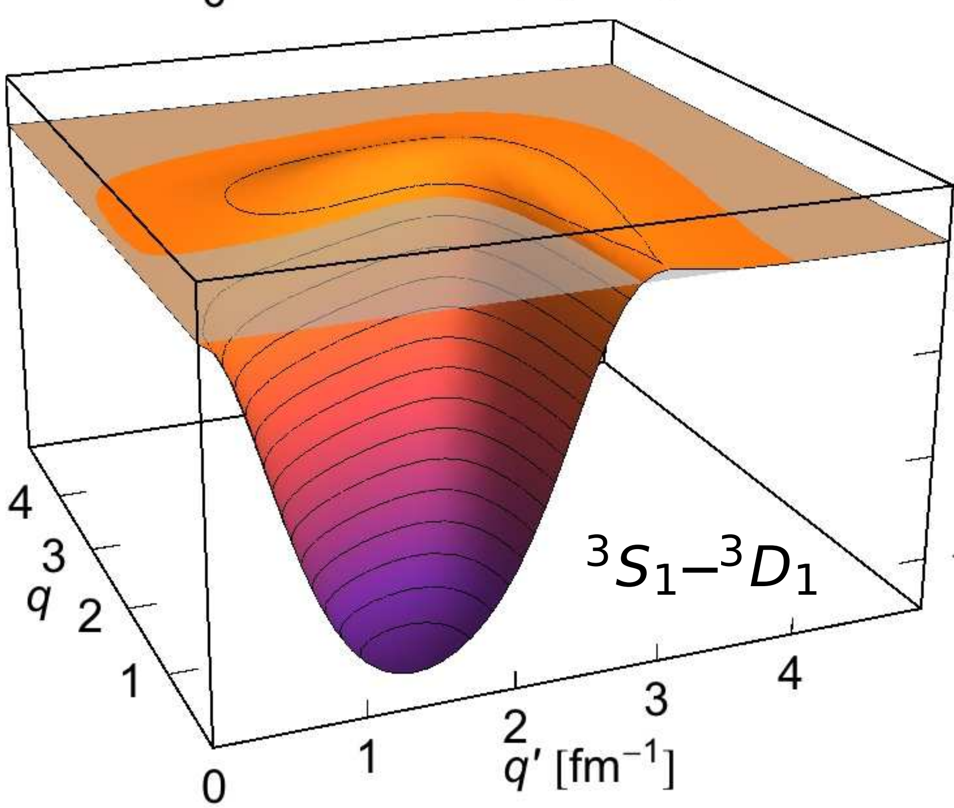


SRG Evolution in Two-Body Space

momentum-space matrix elements





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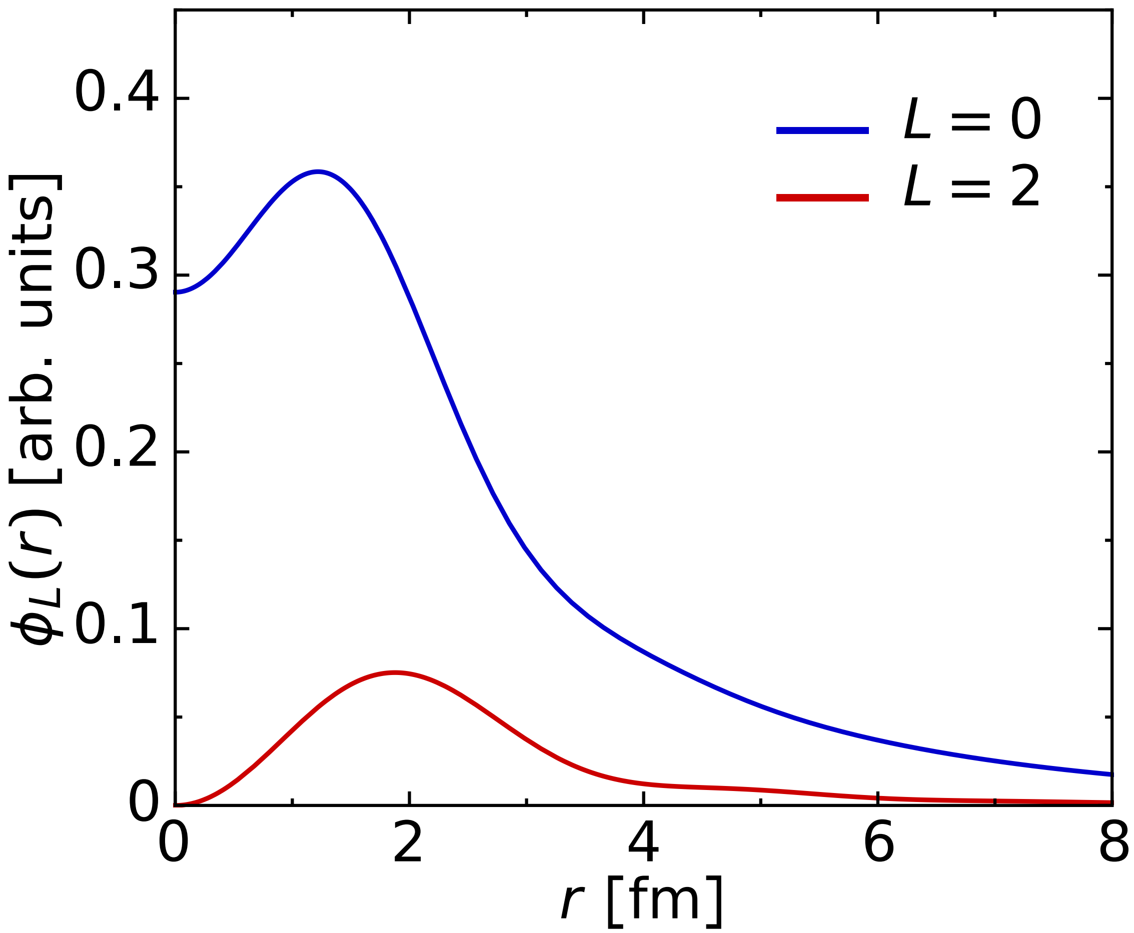

SRG Evolution in Two-Body Space

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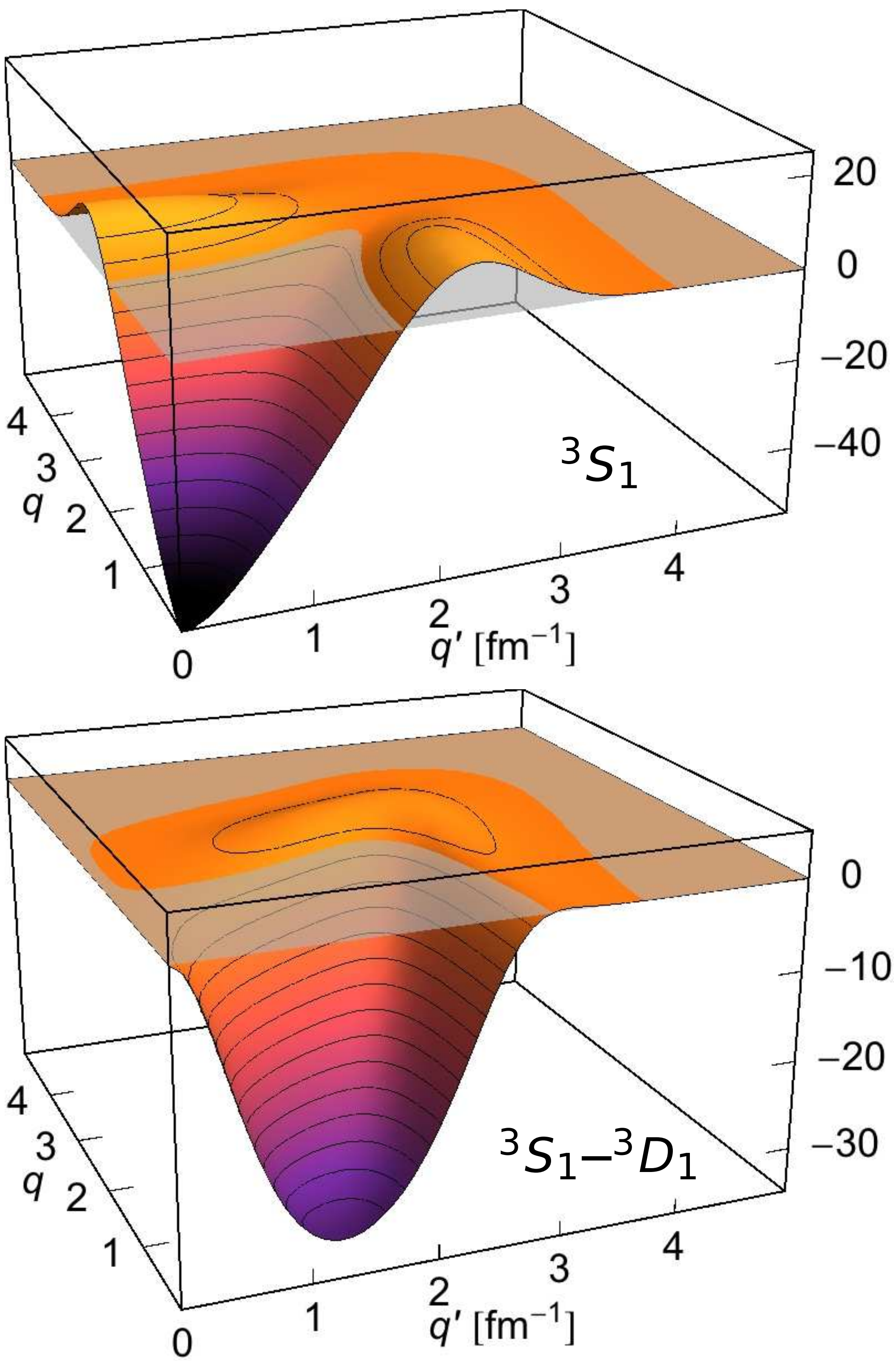

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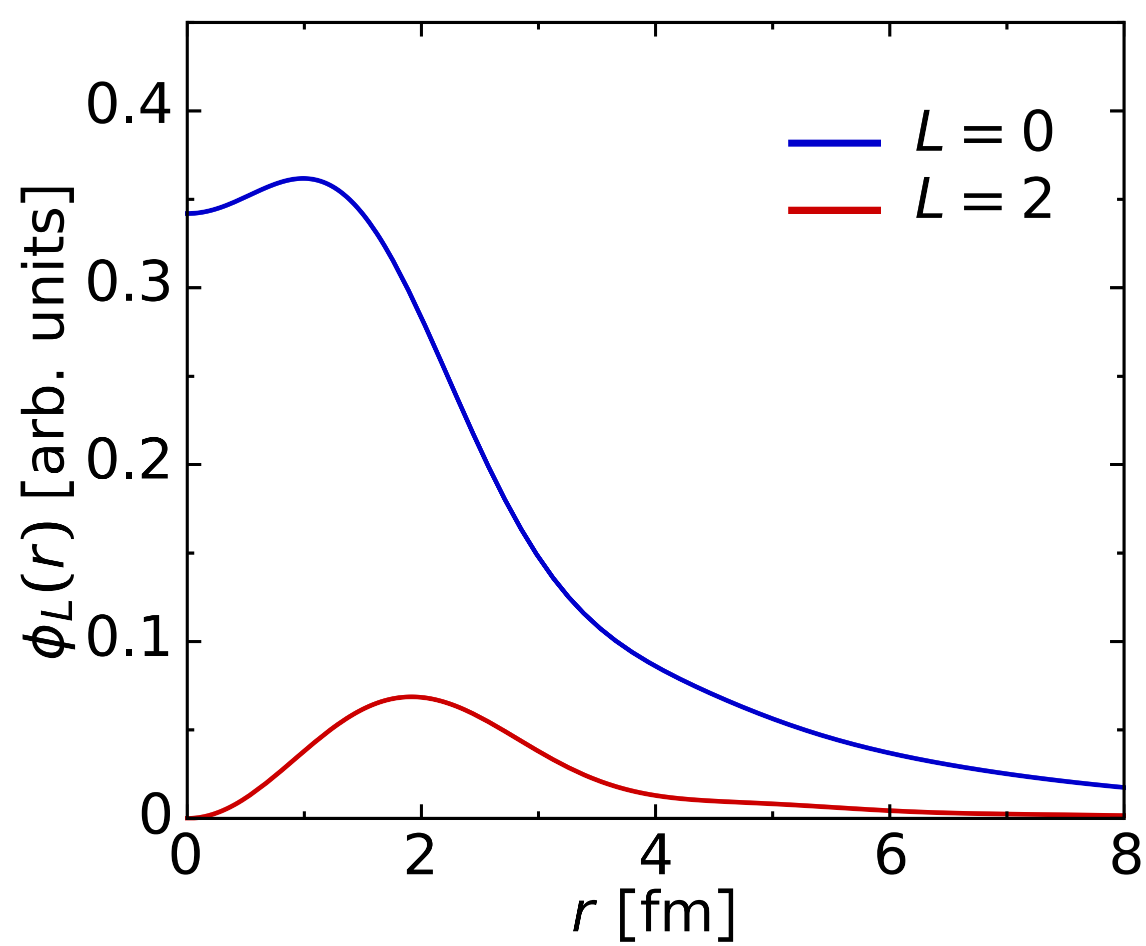

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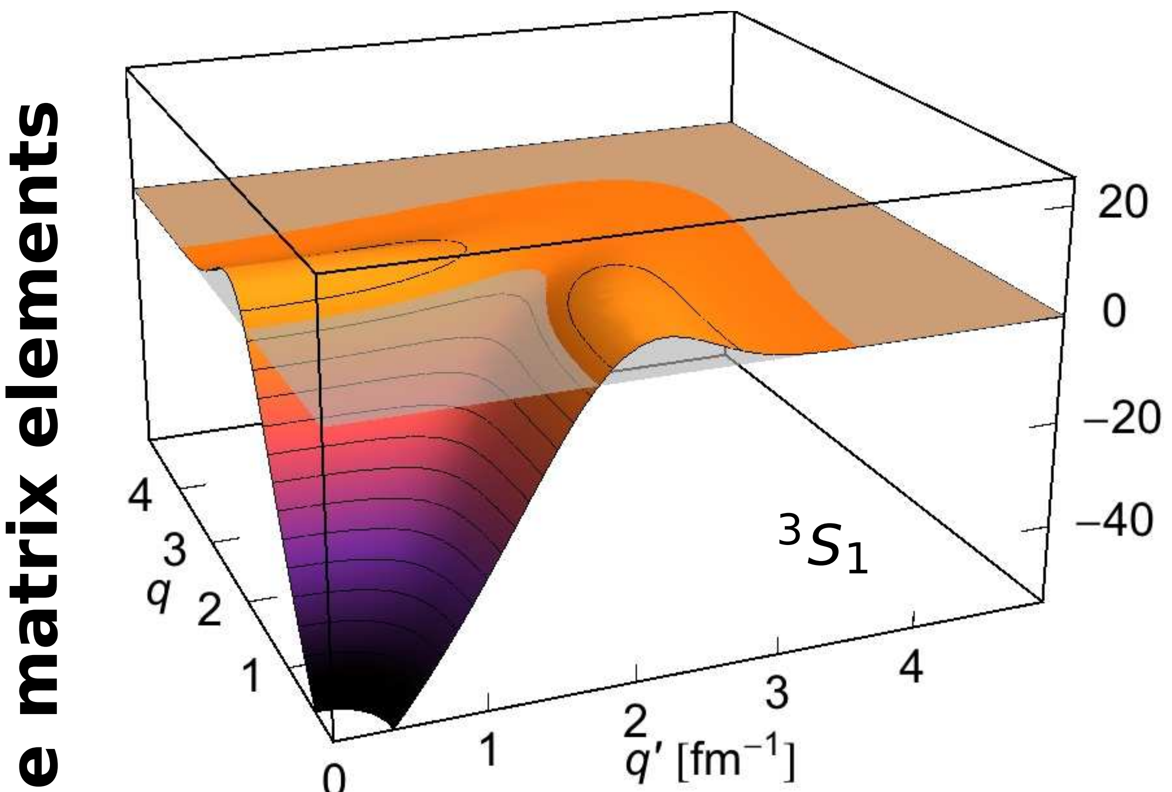

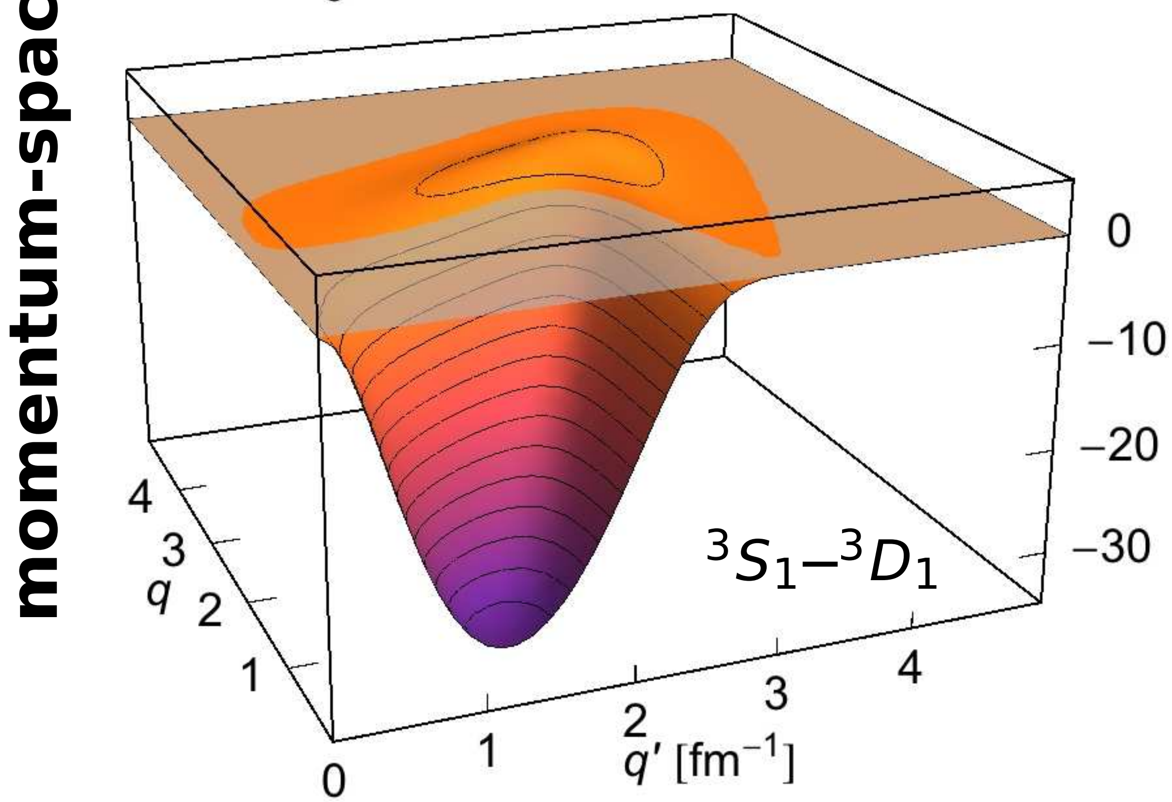

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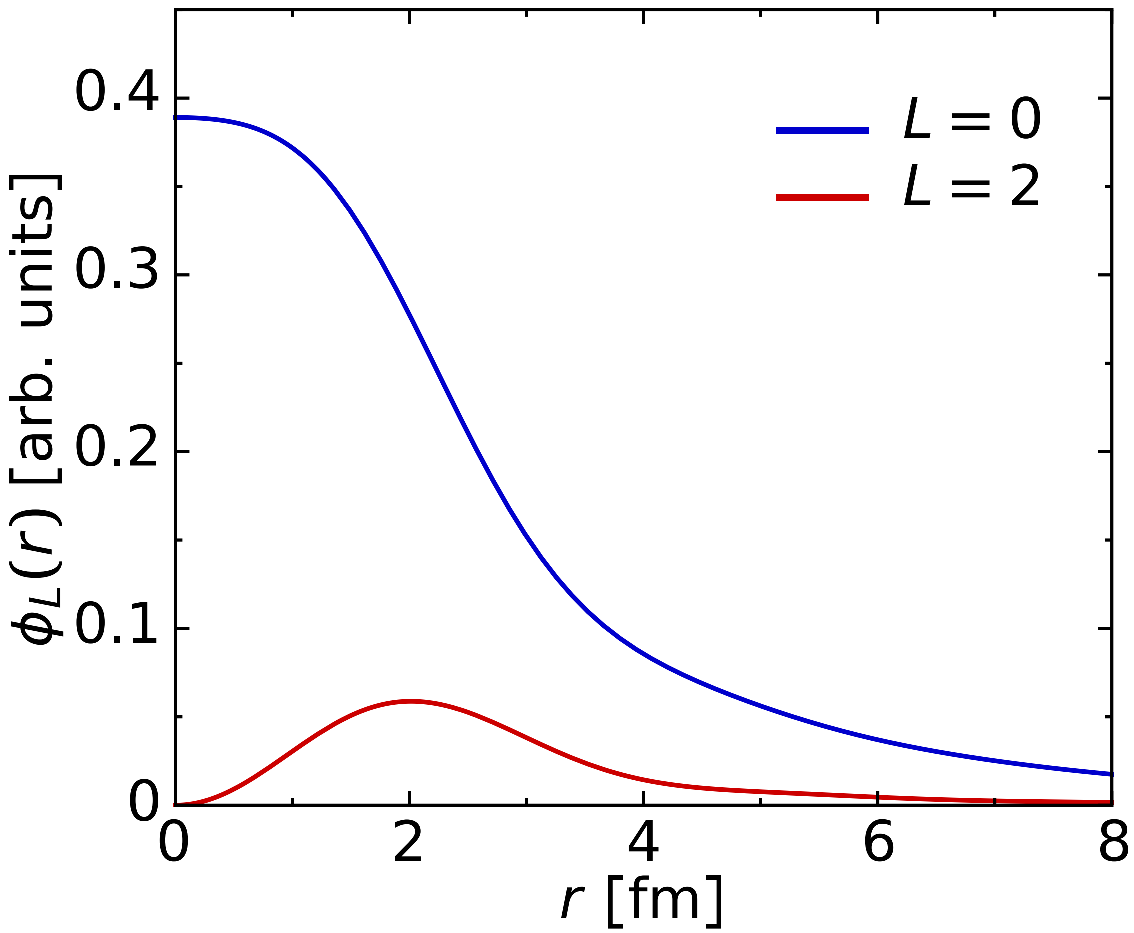

SRG Evolution in Two-Body Space

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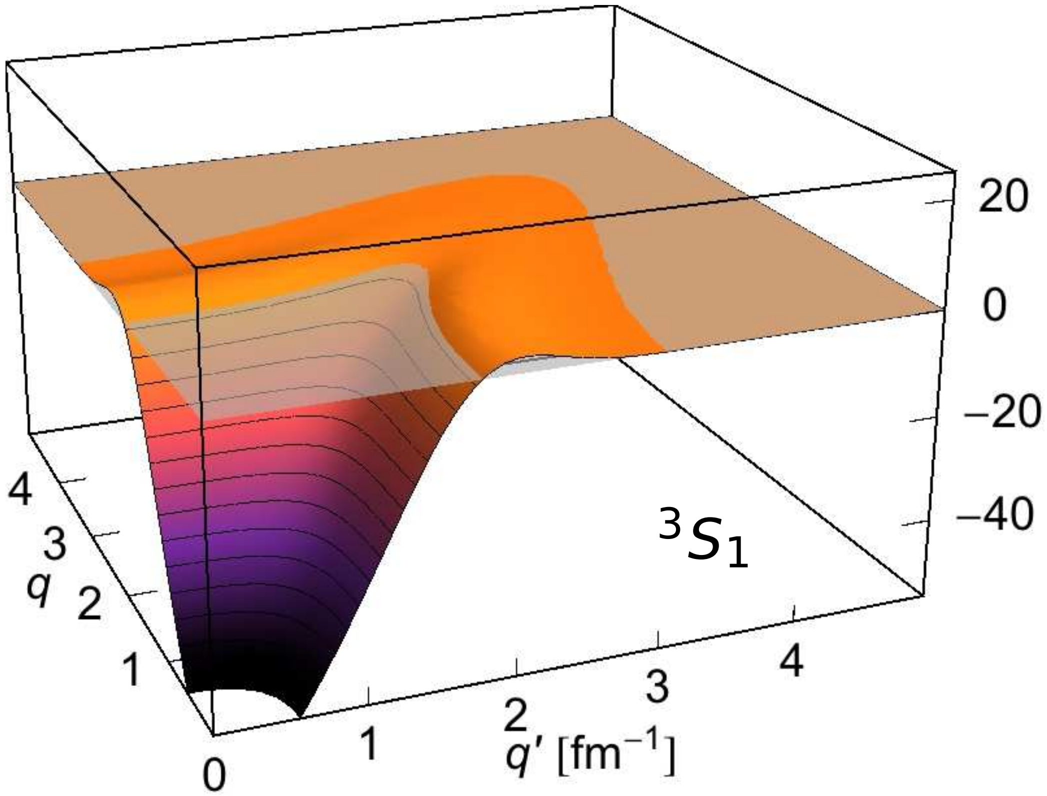

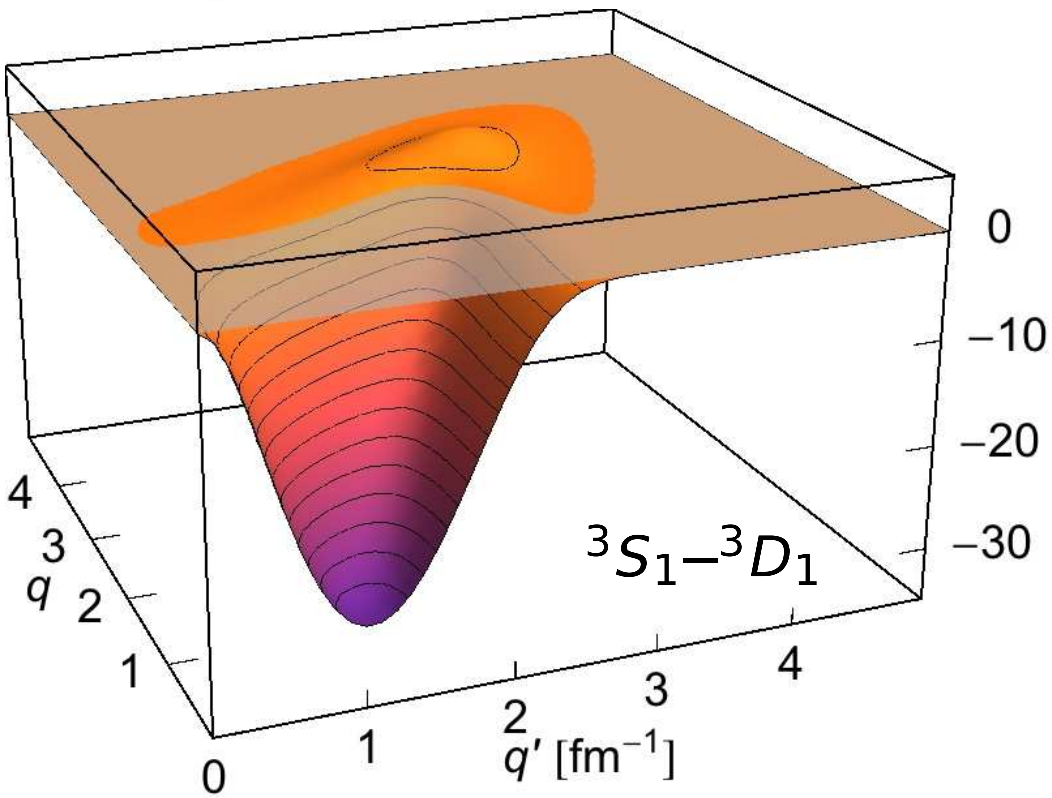

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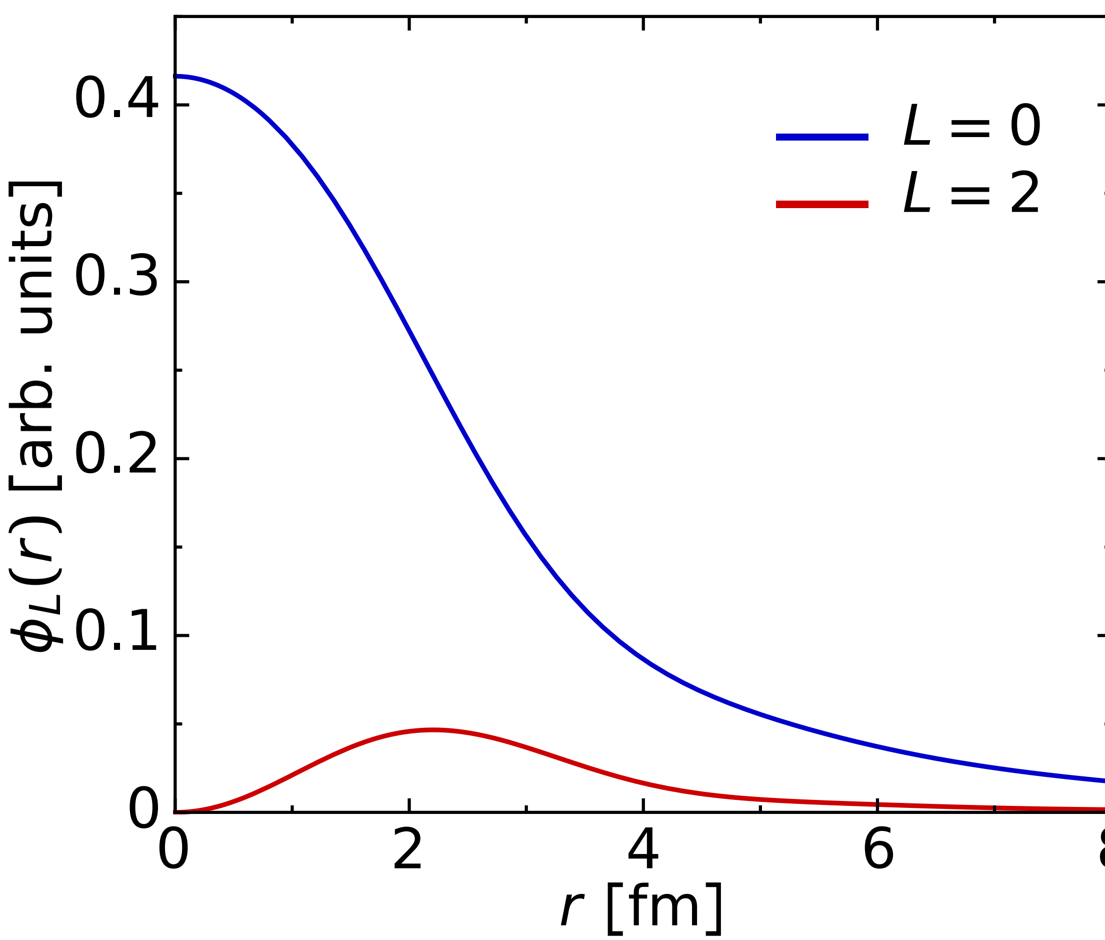
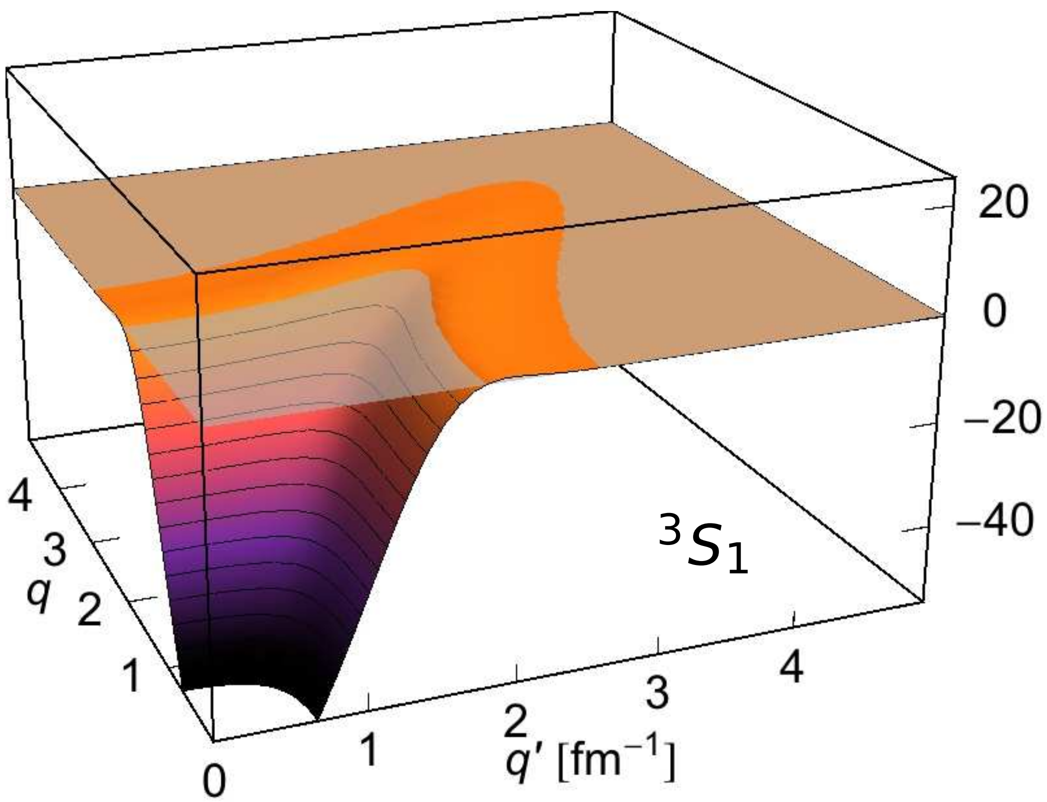
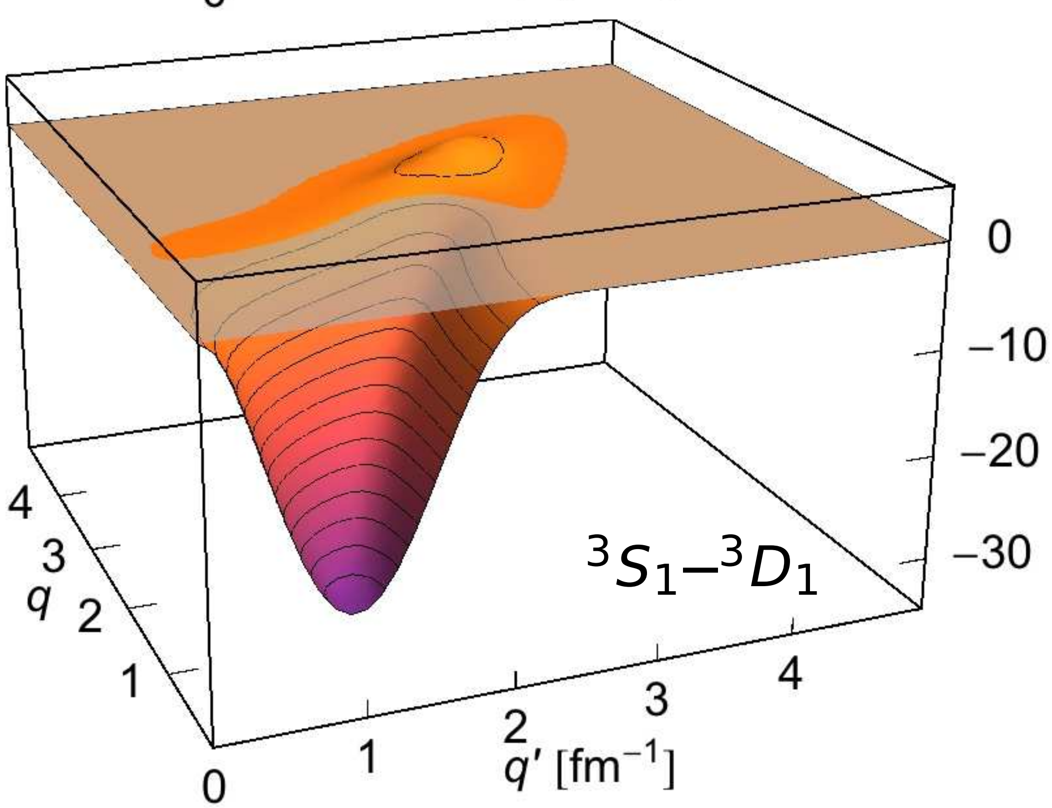


SRG Evolution in Two-Body Space

momentum-space matrix elements





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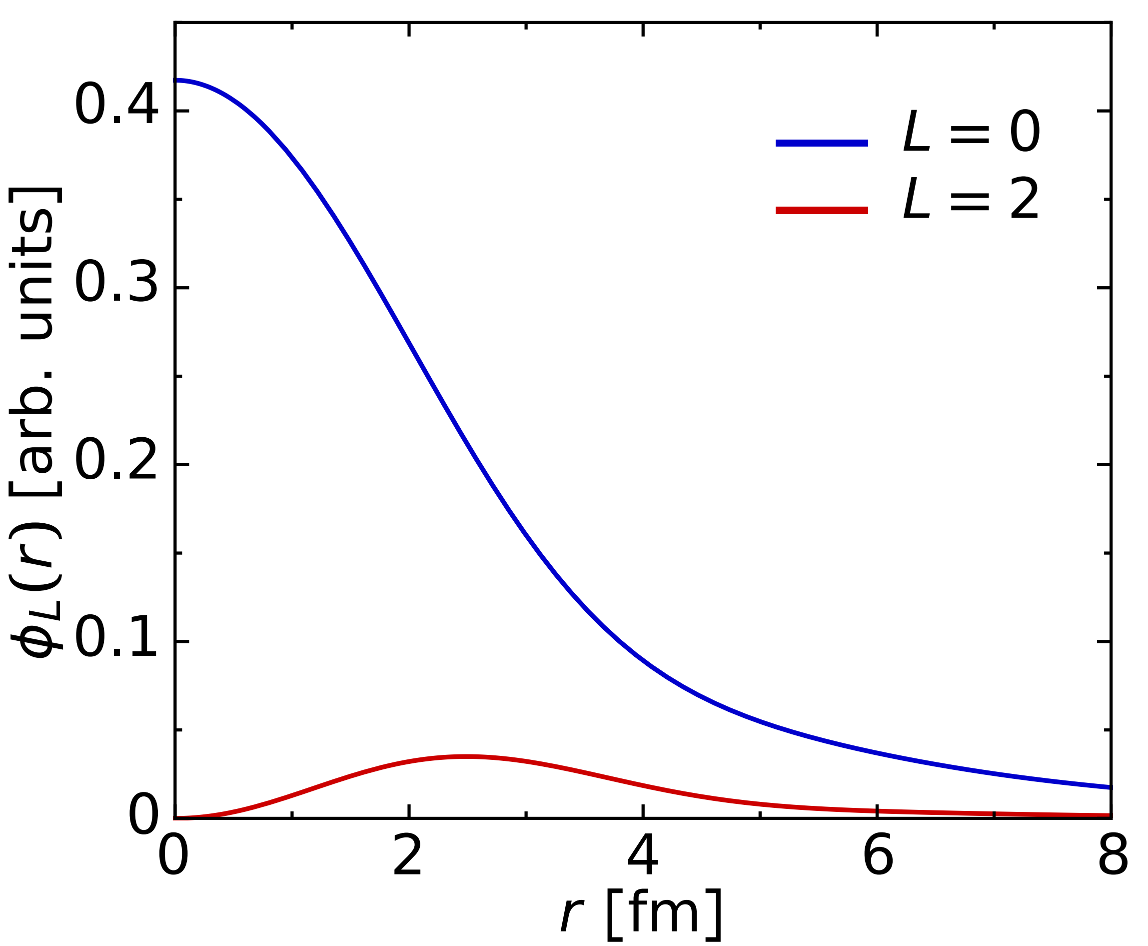

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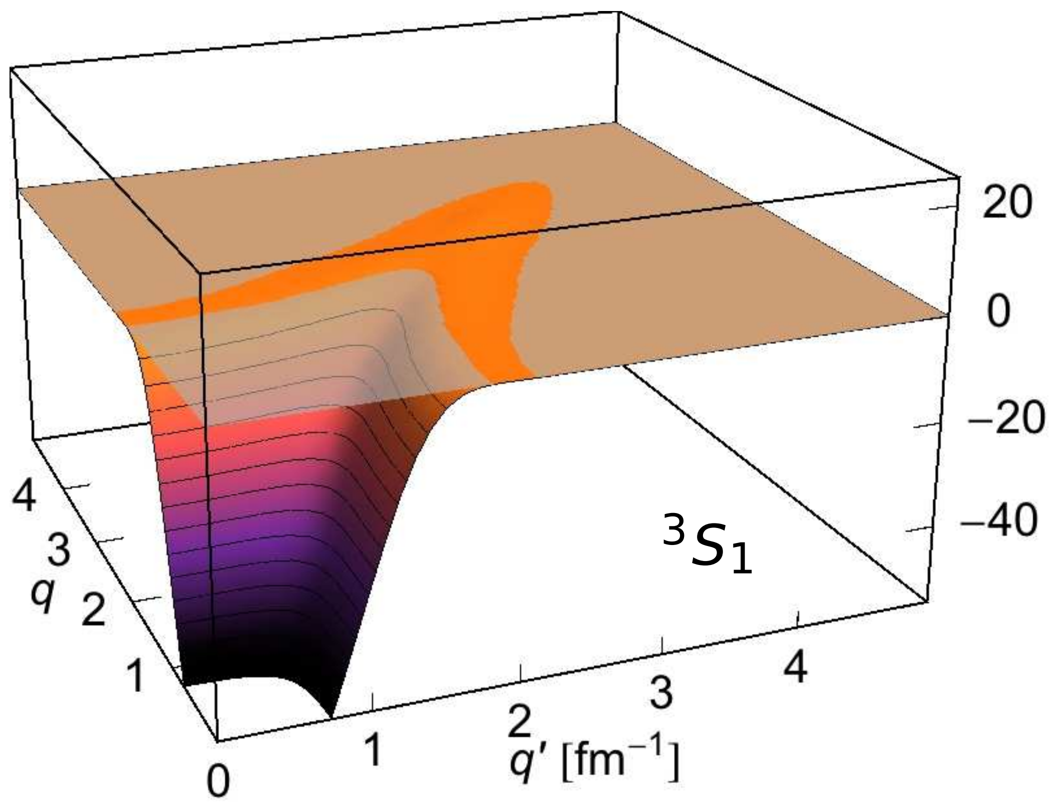

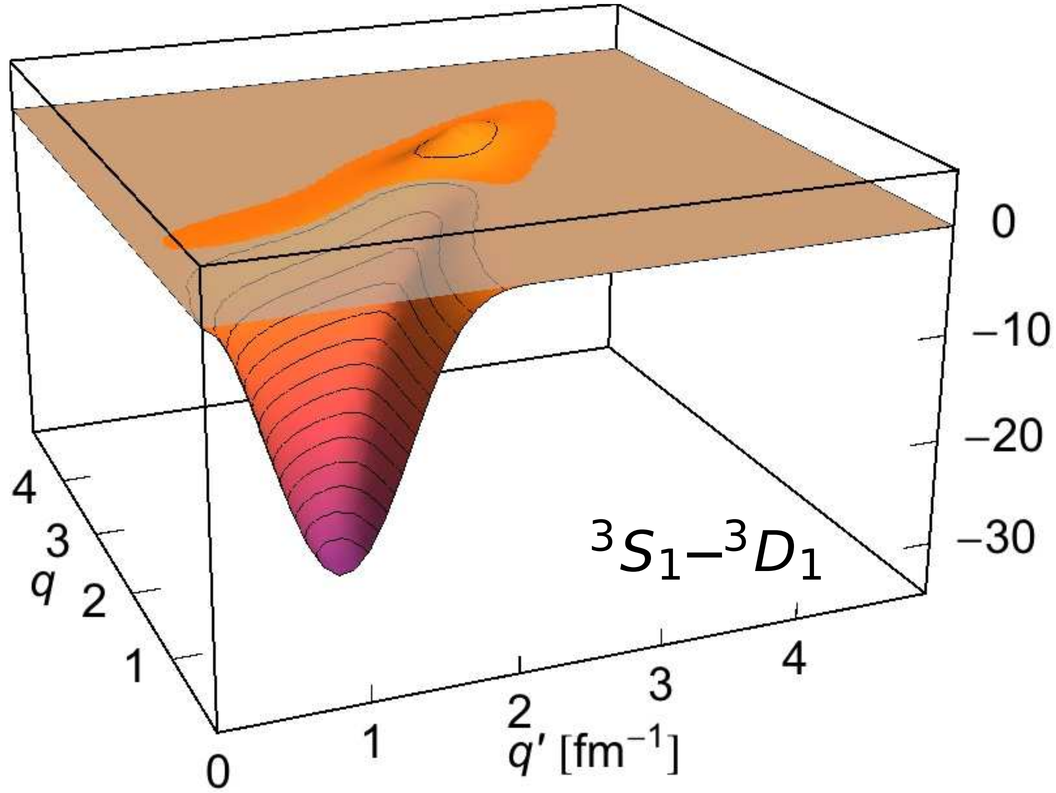

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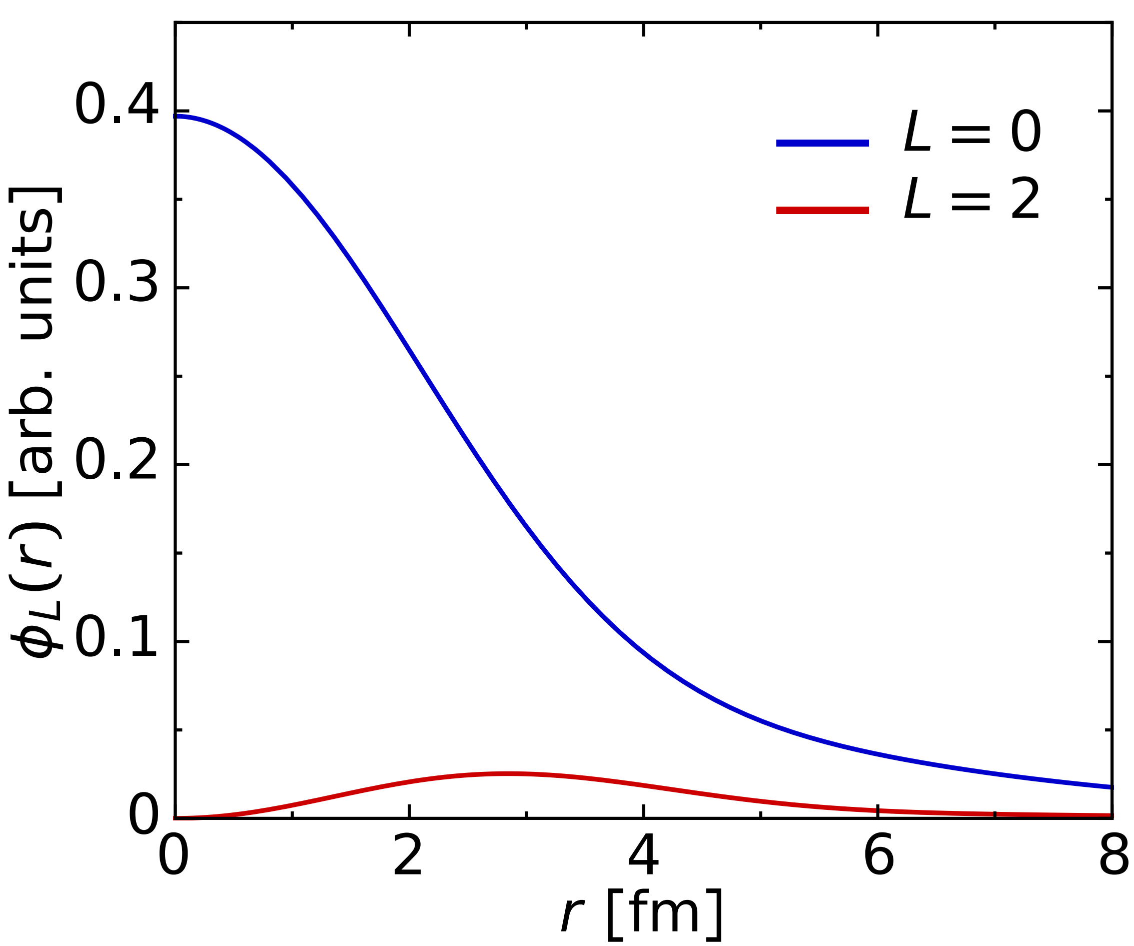
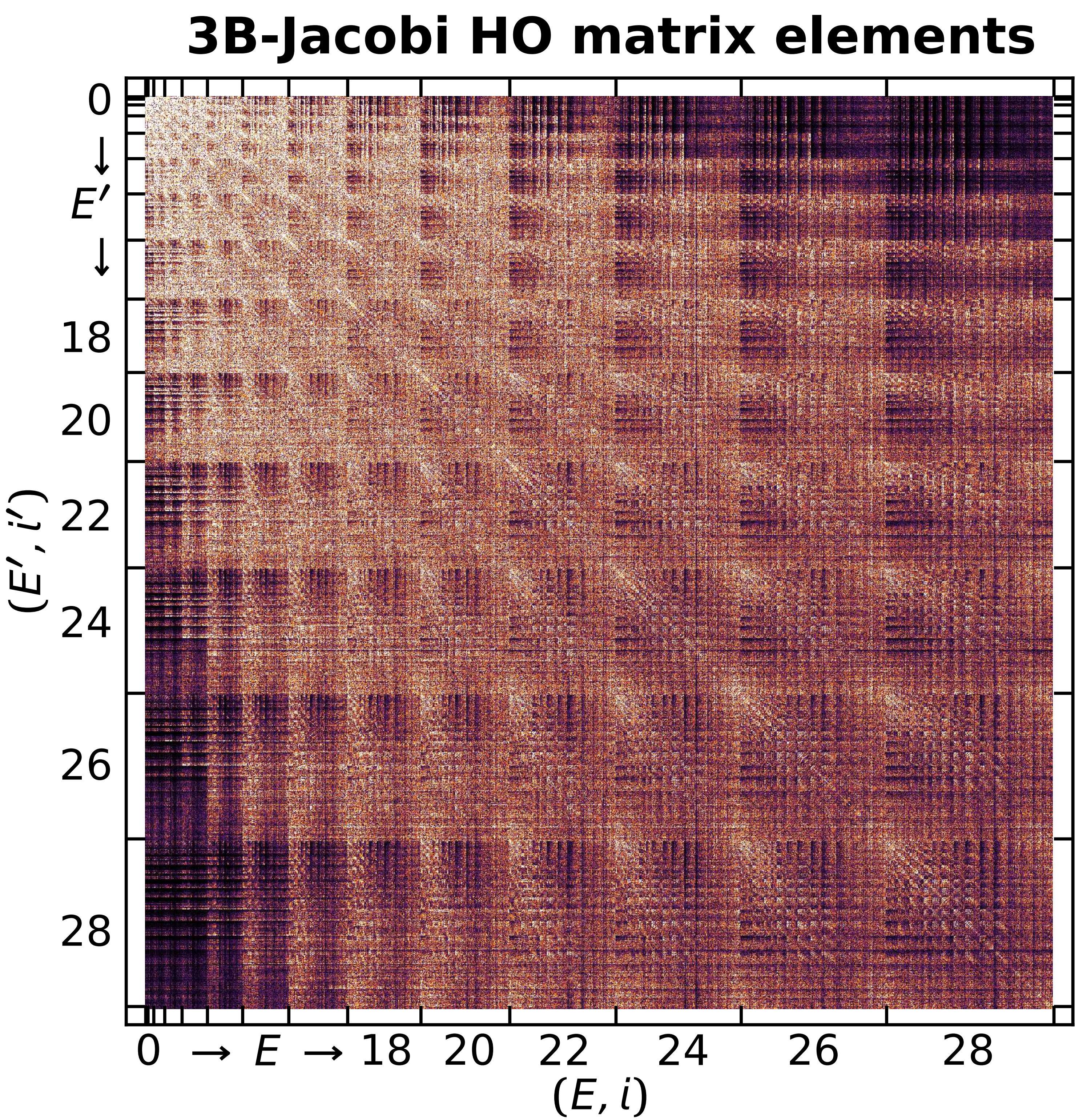
$J^\pi = 1^+, T = 0$

deuteron wave-function



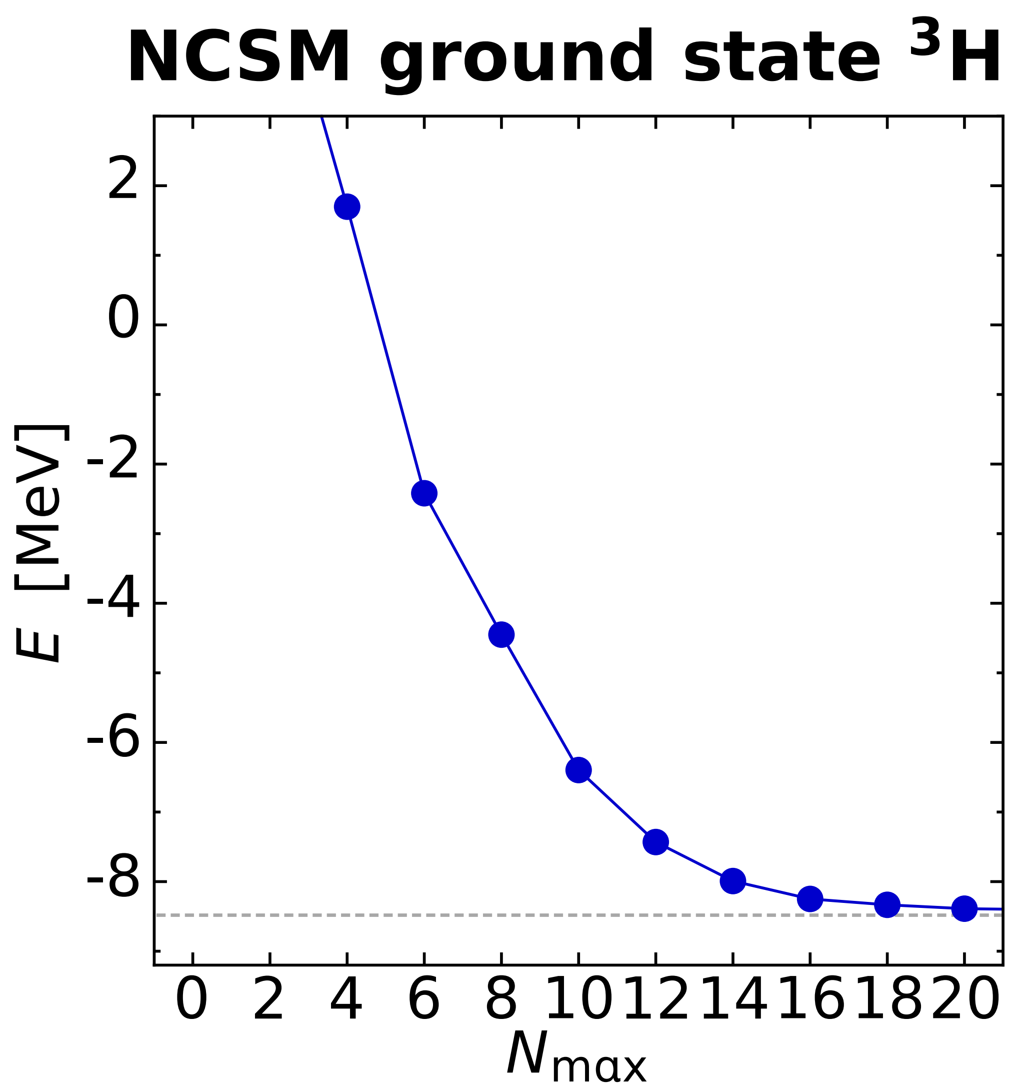
SRG Evolution in Three-Body Space



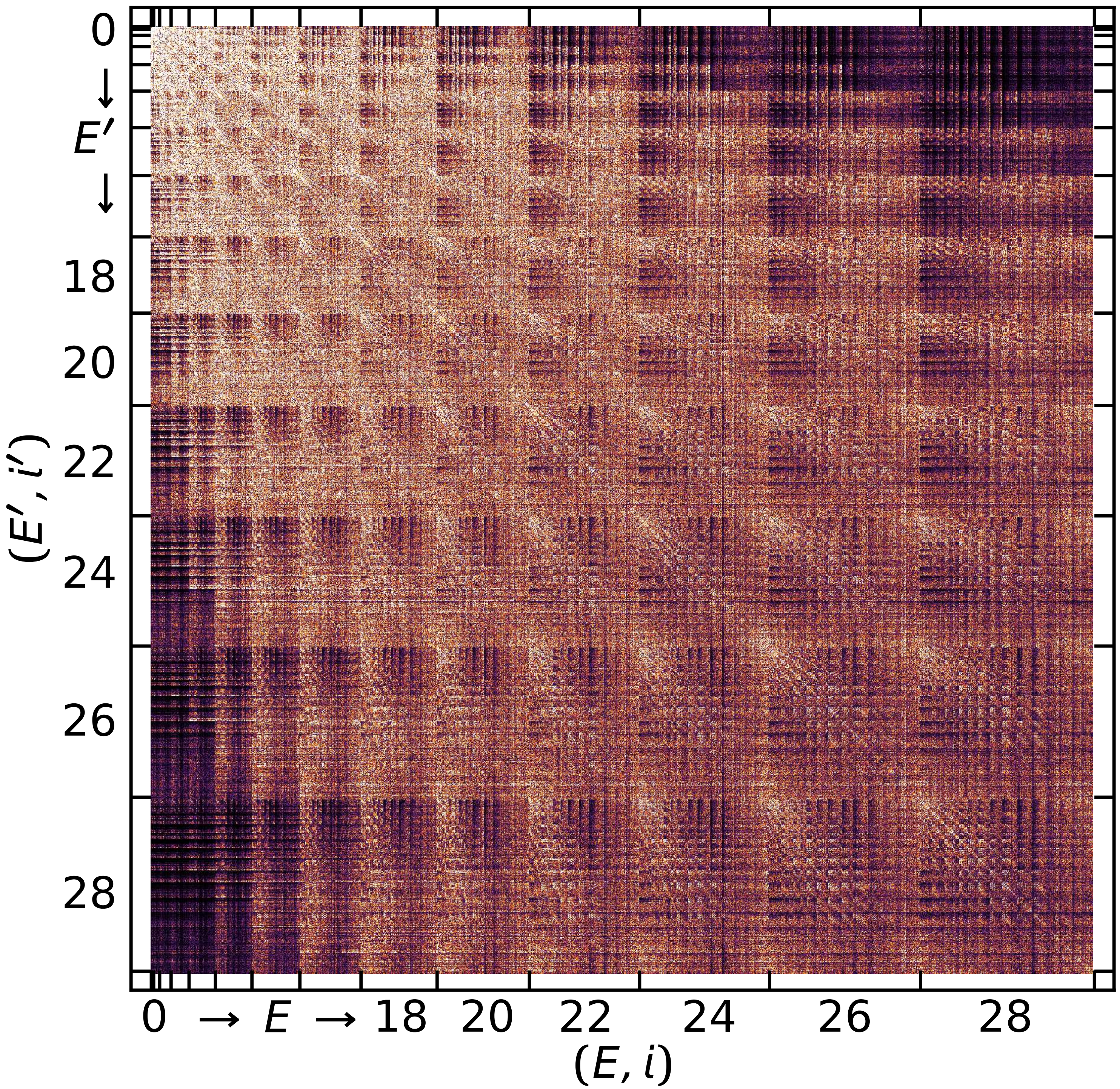
chiral NN+3N

$N^3LO + N^2LO$, triton-fit, 500 MeV

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



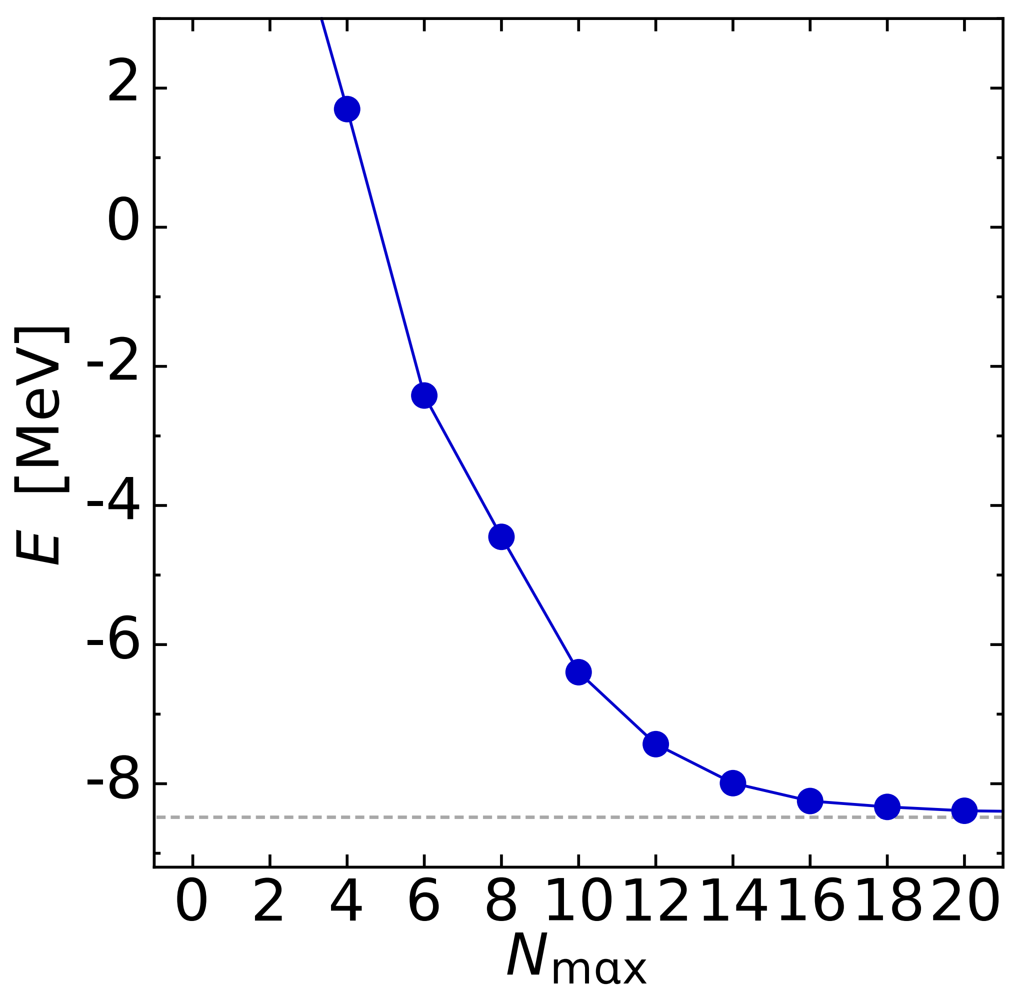
SRG Evolution in Three-Body Space



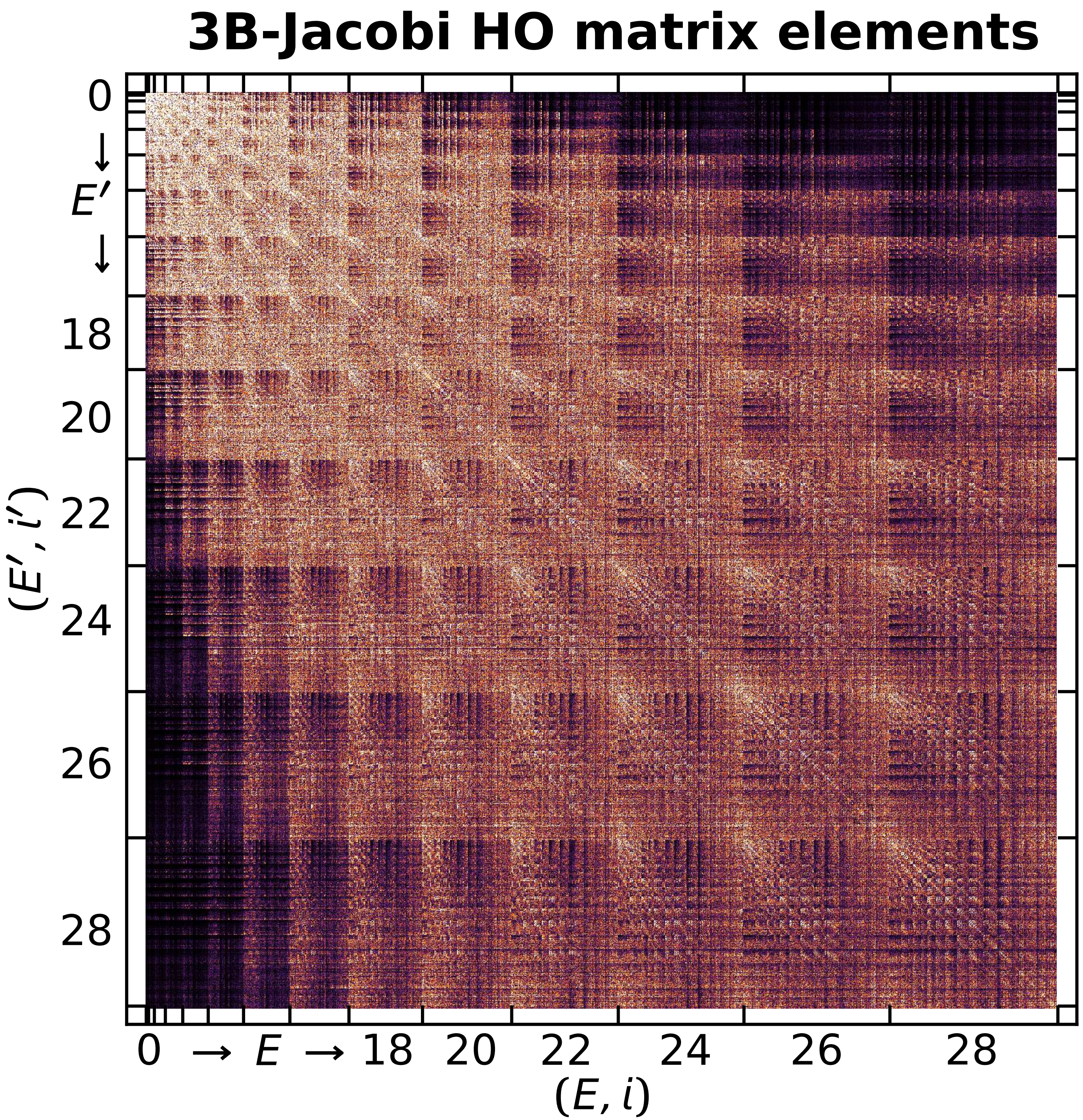
$\alpha = 0.000\,\mathrm{fm}^4$

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

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



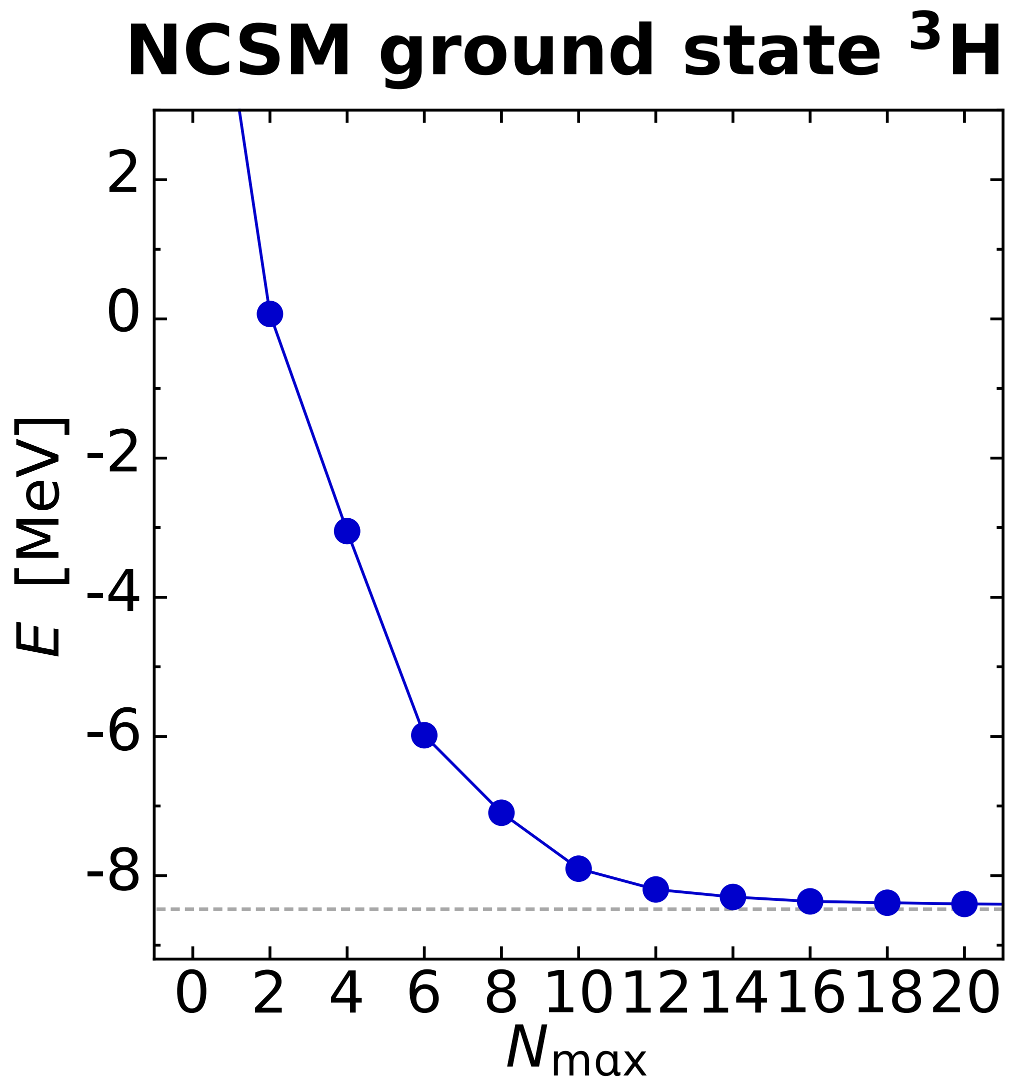
SRG Evolution in Three-Body Space



$$\alpha = 0.010\,\mathrm{fm}^4$$

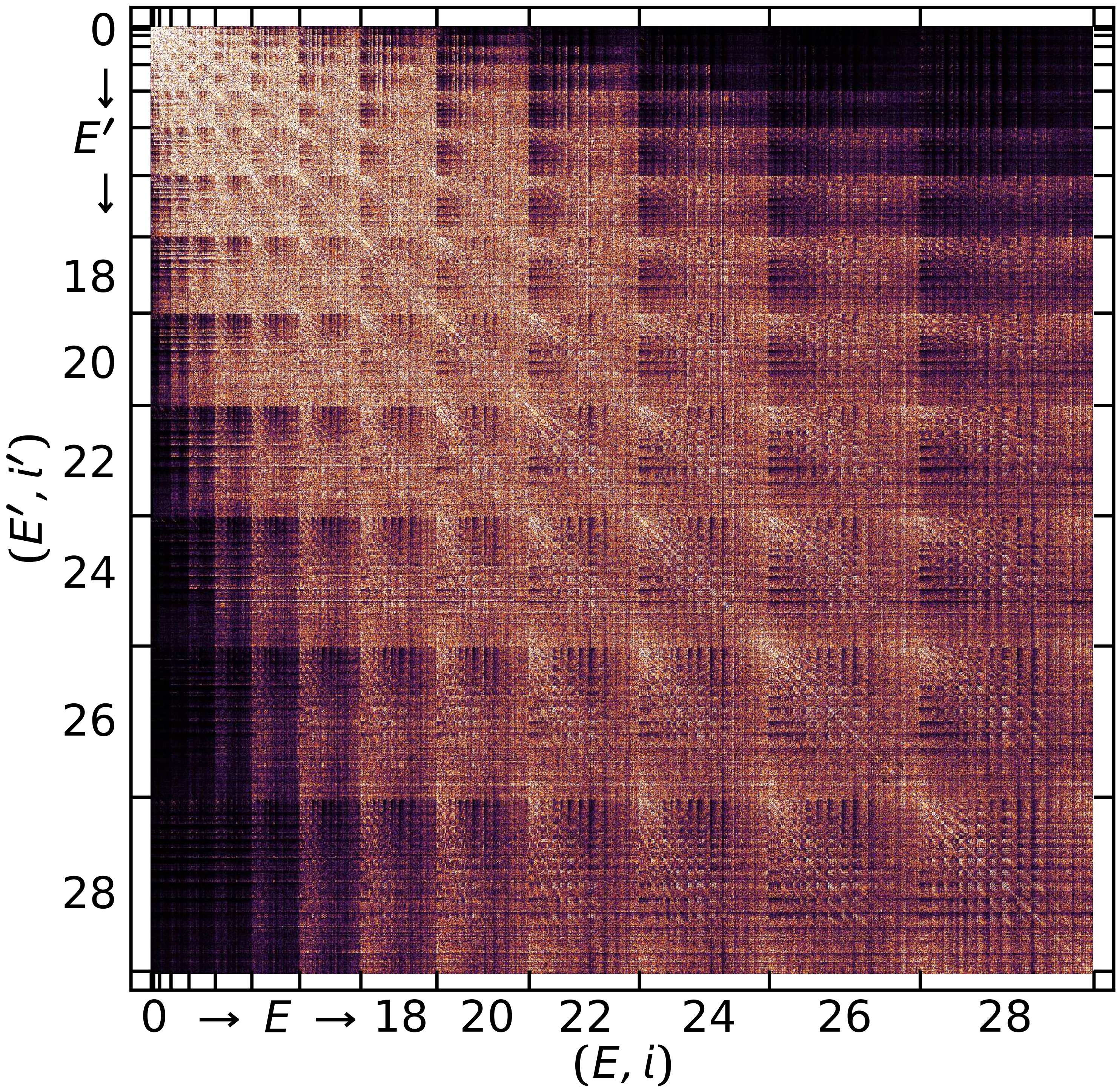
$\Lambda = 3.16\,\mathrm{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

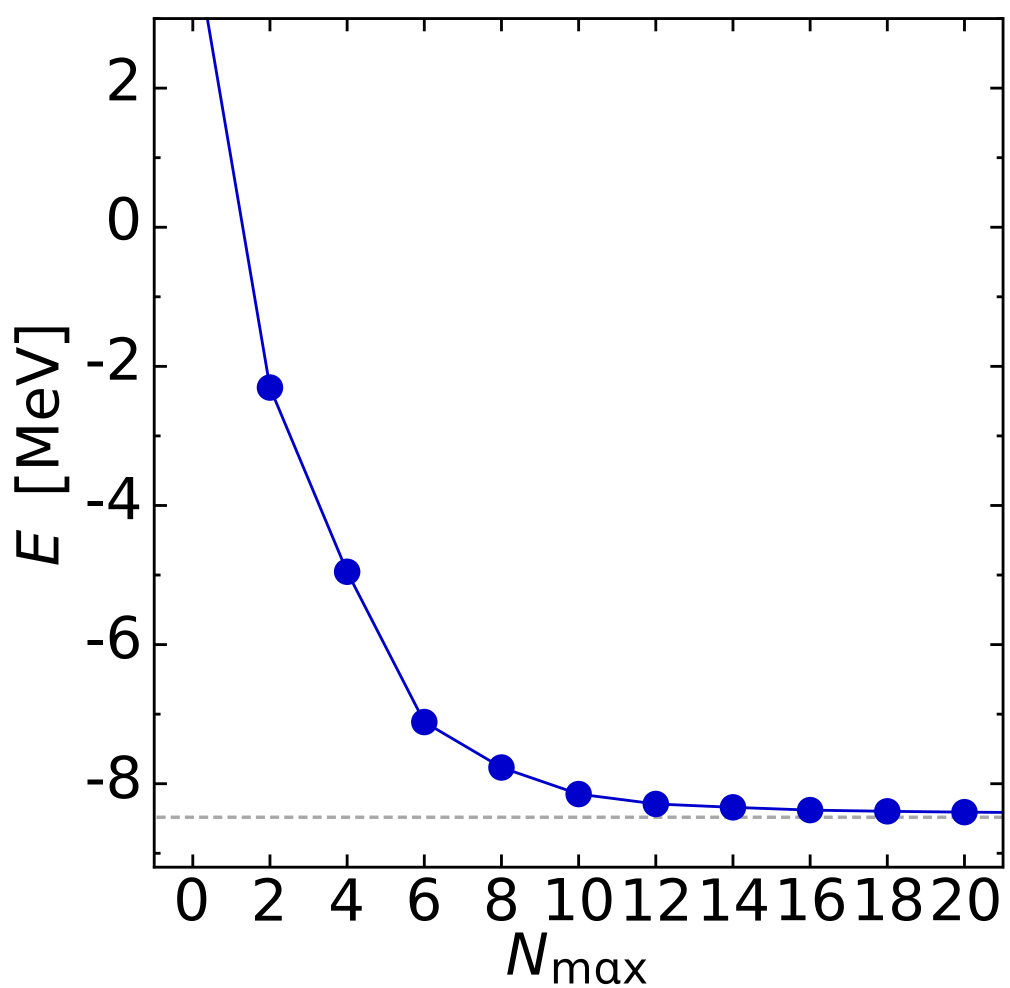


$\alpha = 0.020\,\text{fm}^4$

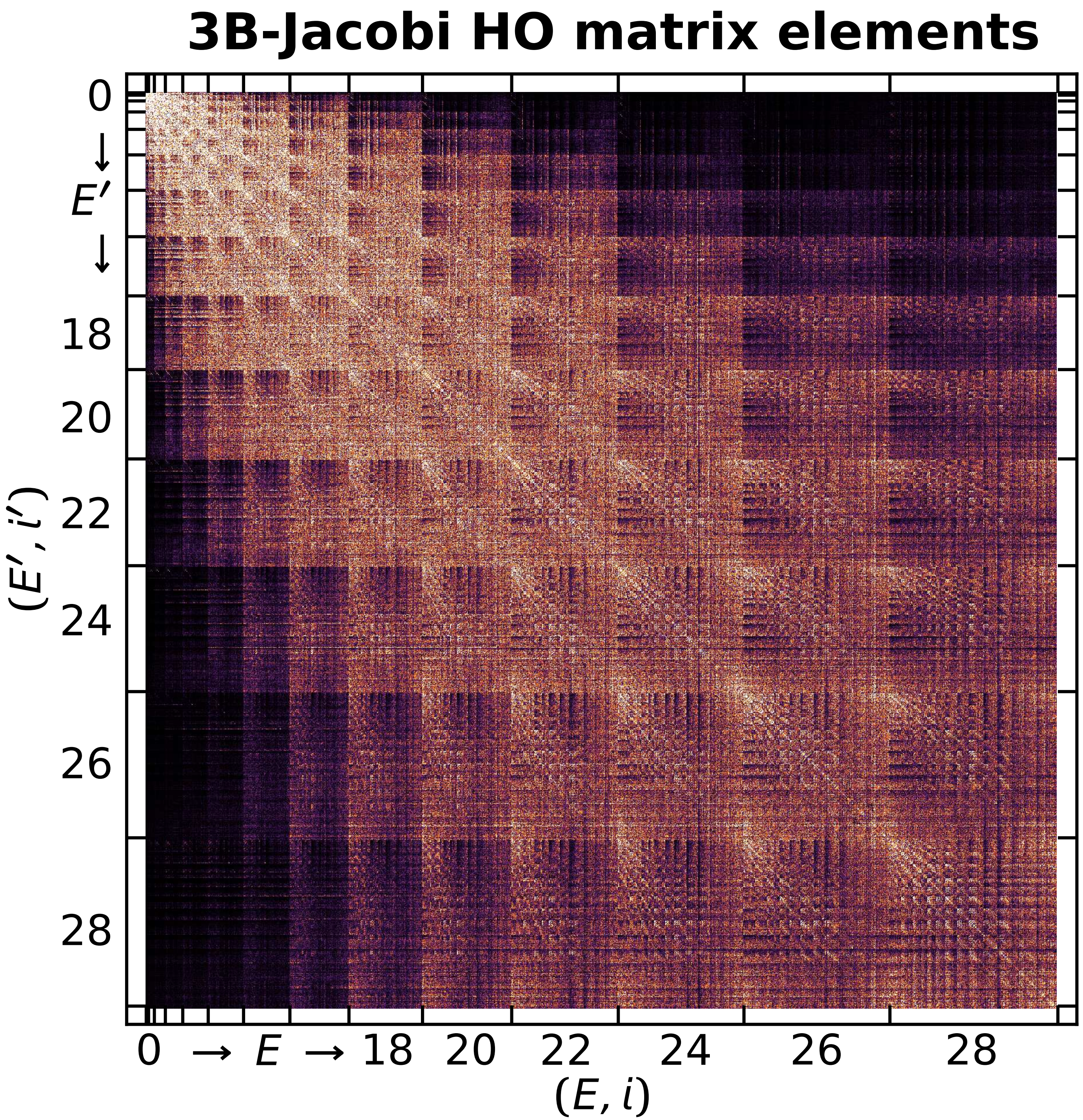
$\Lambda = 2.66\,\text{fm}^{-1}$

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

NCSM ground state ^{3}H



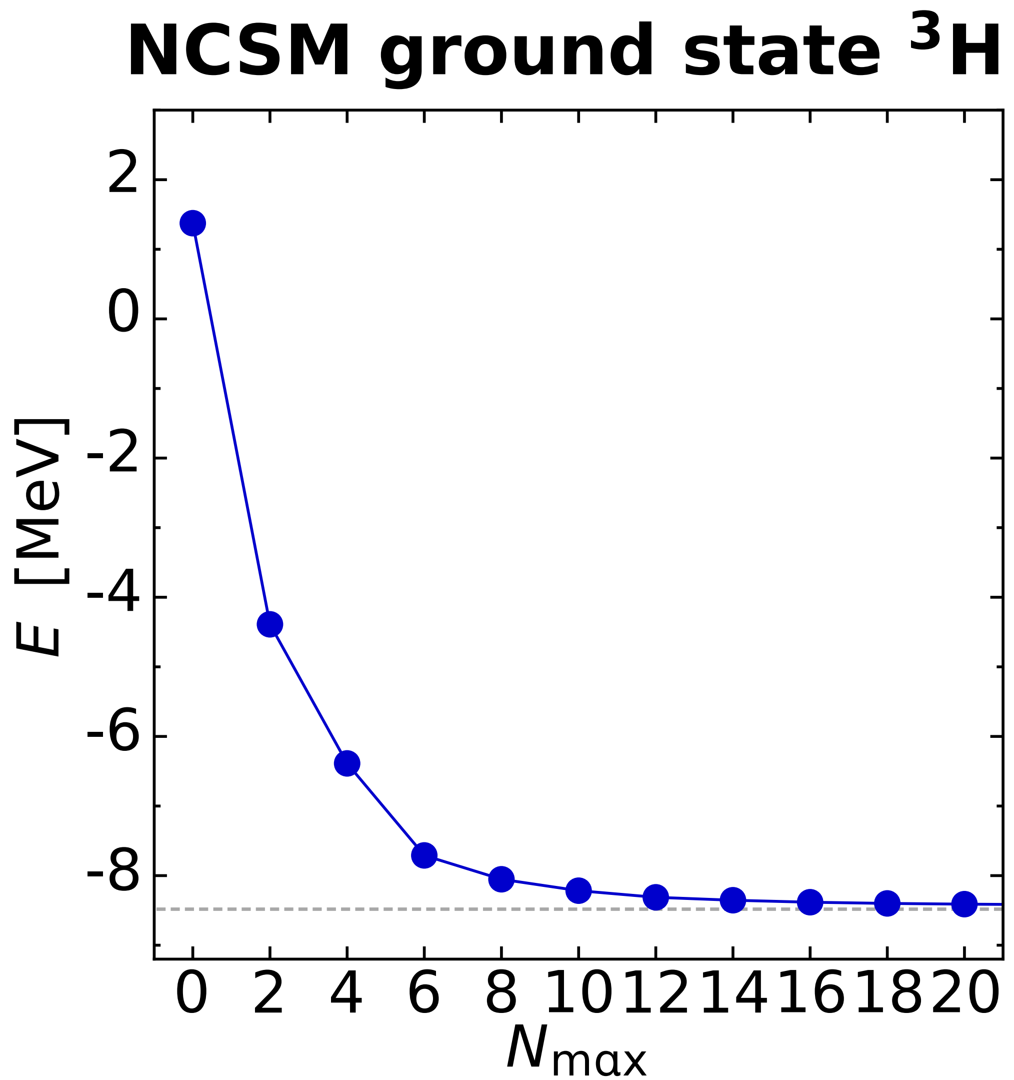
SRG Evolution in Three-Body Space



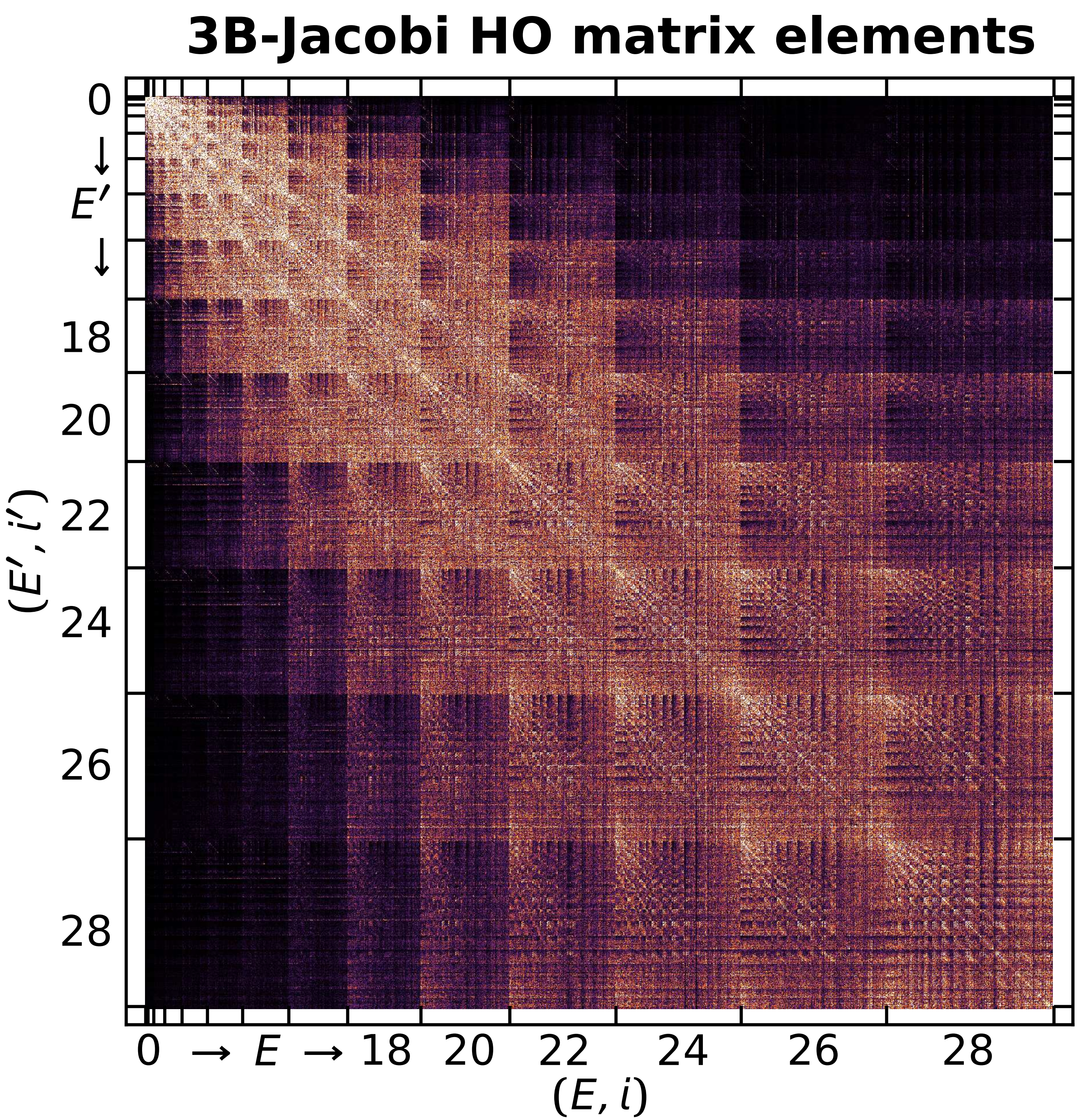
$\alpha = 0.040\,\text{fm}^4$

$\Lambda = 2.24\,\text{fm}^{-1}$

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



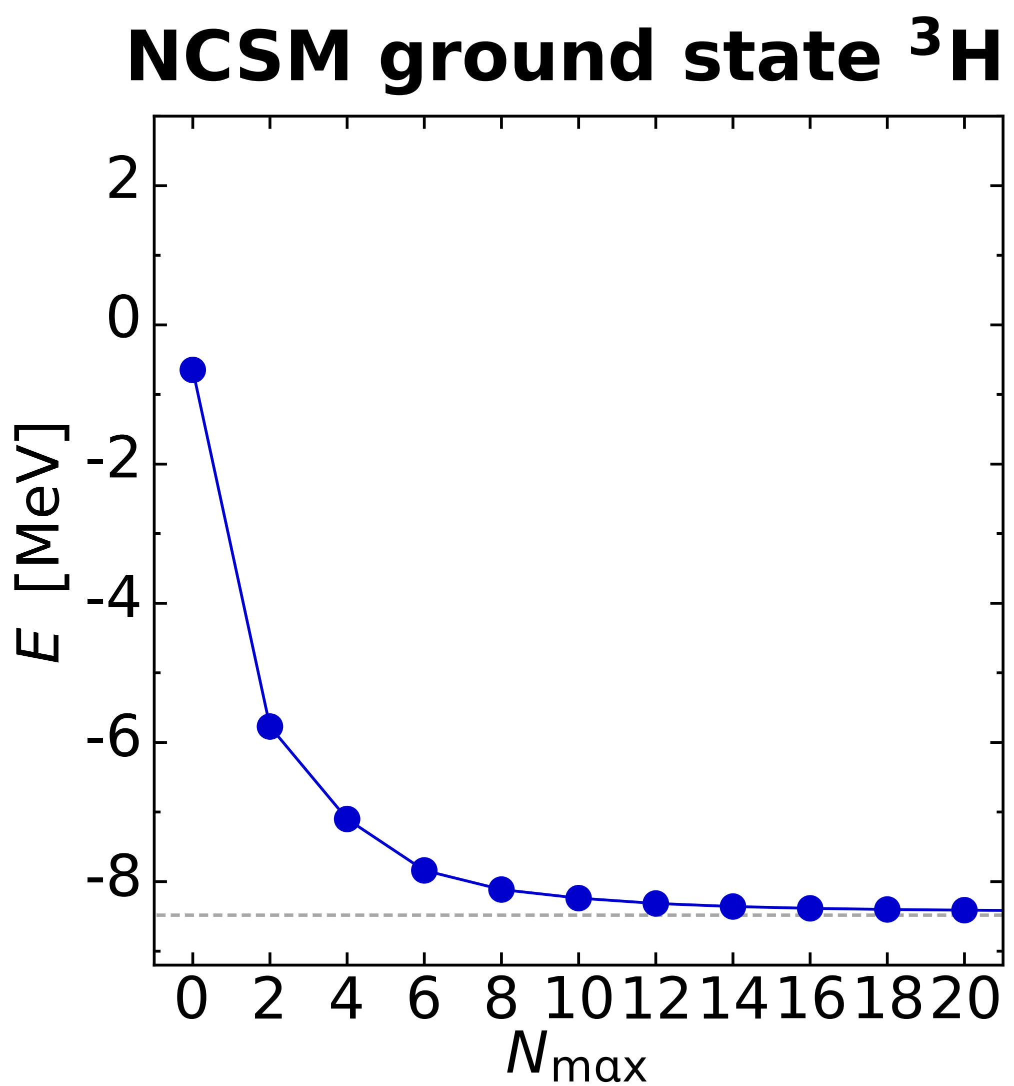
SRG Evolution in Three-Body Space



$\alpha = 0.080\,\text{fm}^4$

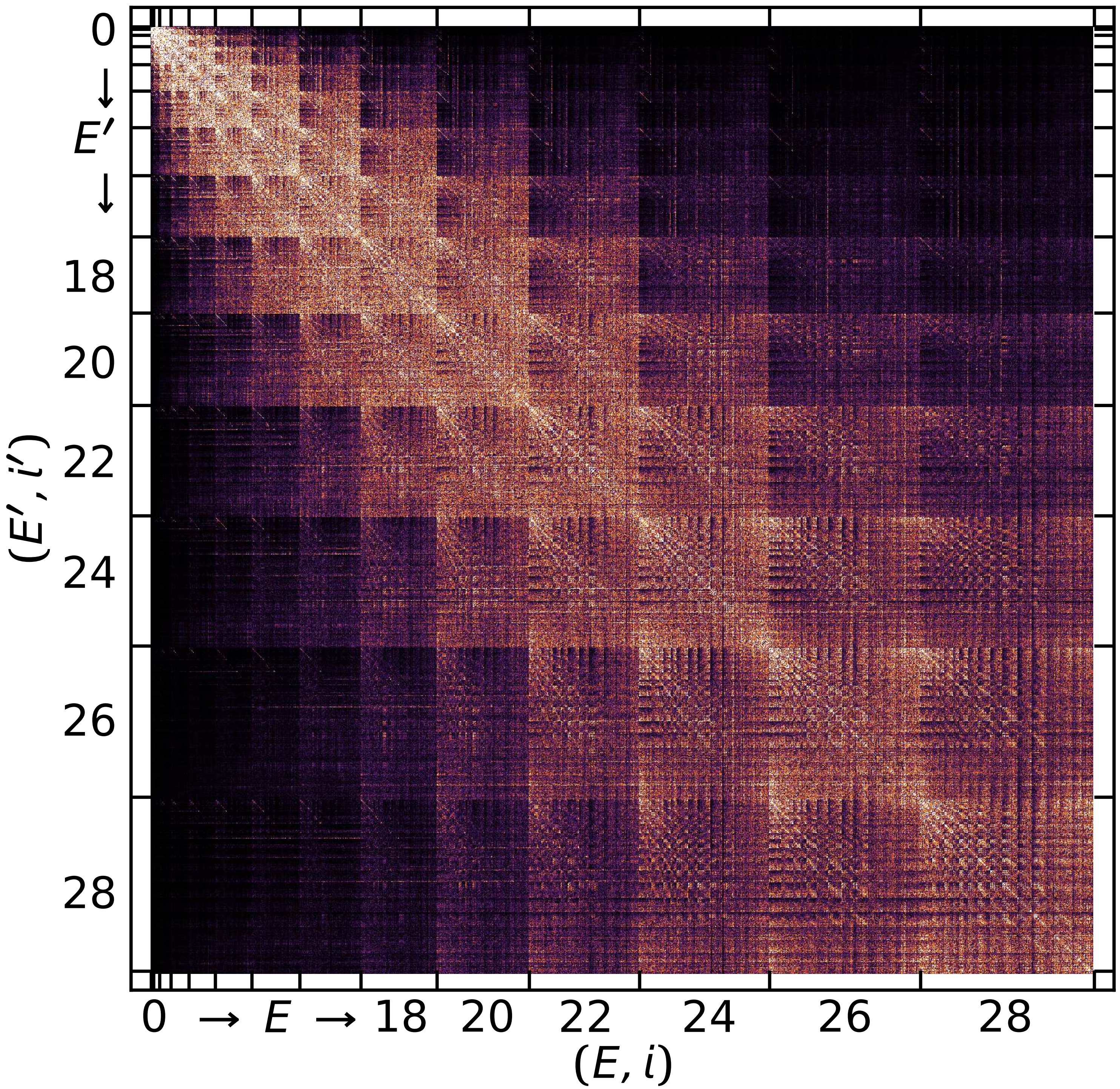
$\Lambda = 1.88\,\text{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

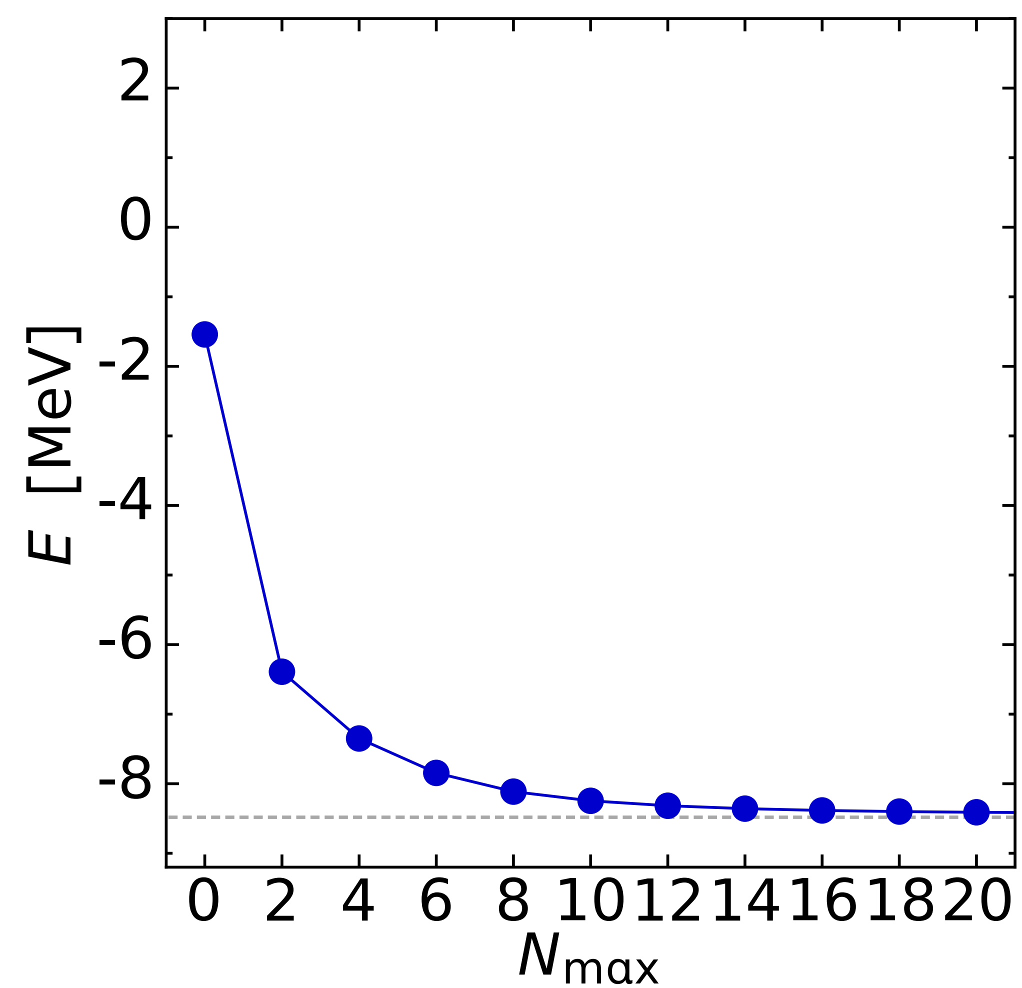


$$\alpha = 0.160\,\text{fm}^4$$

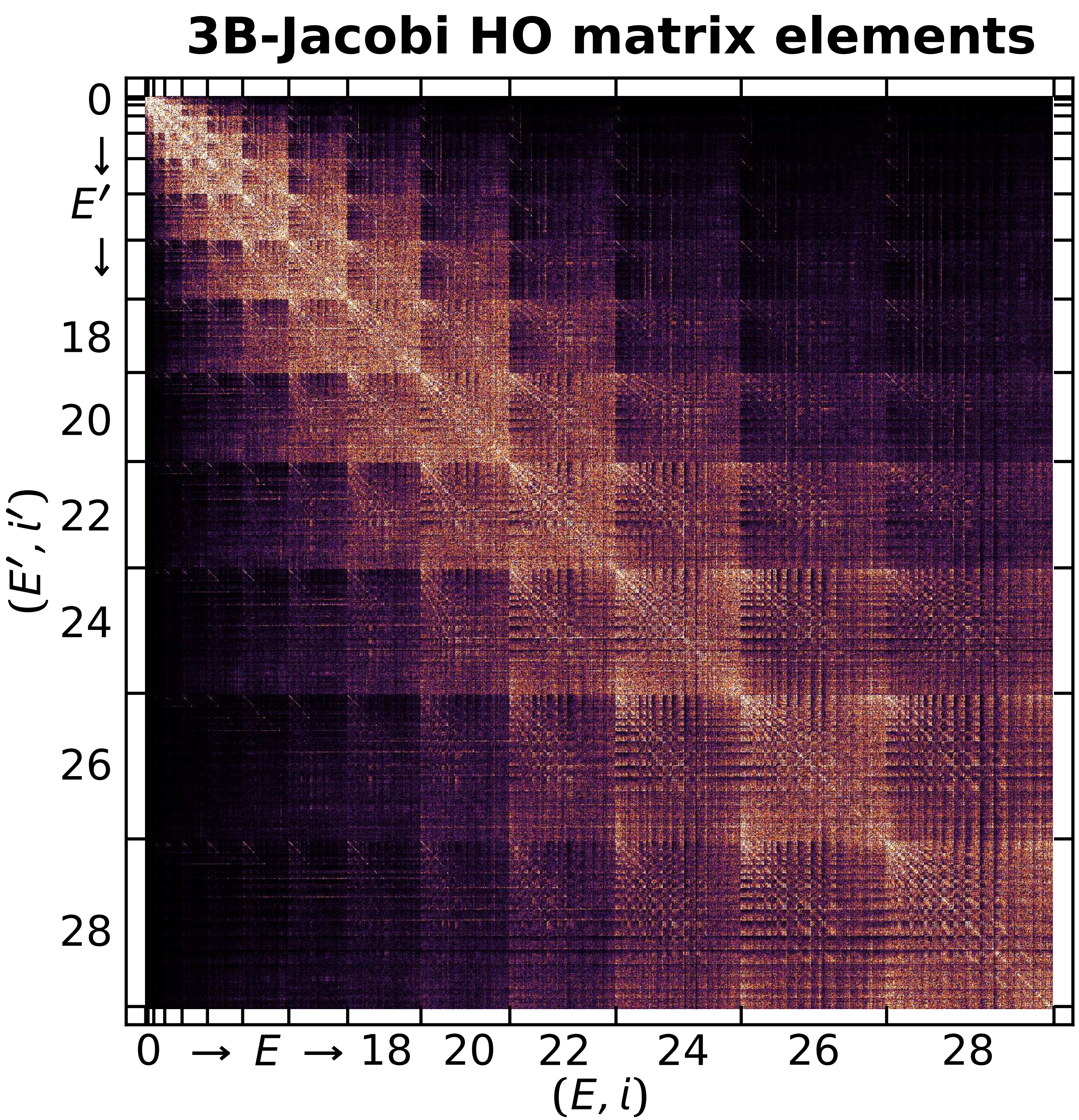
$\Lambda = 1.58\,\text{fm}^{-1}$

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

NCSM ground state ^{3}H



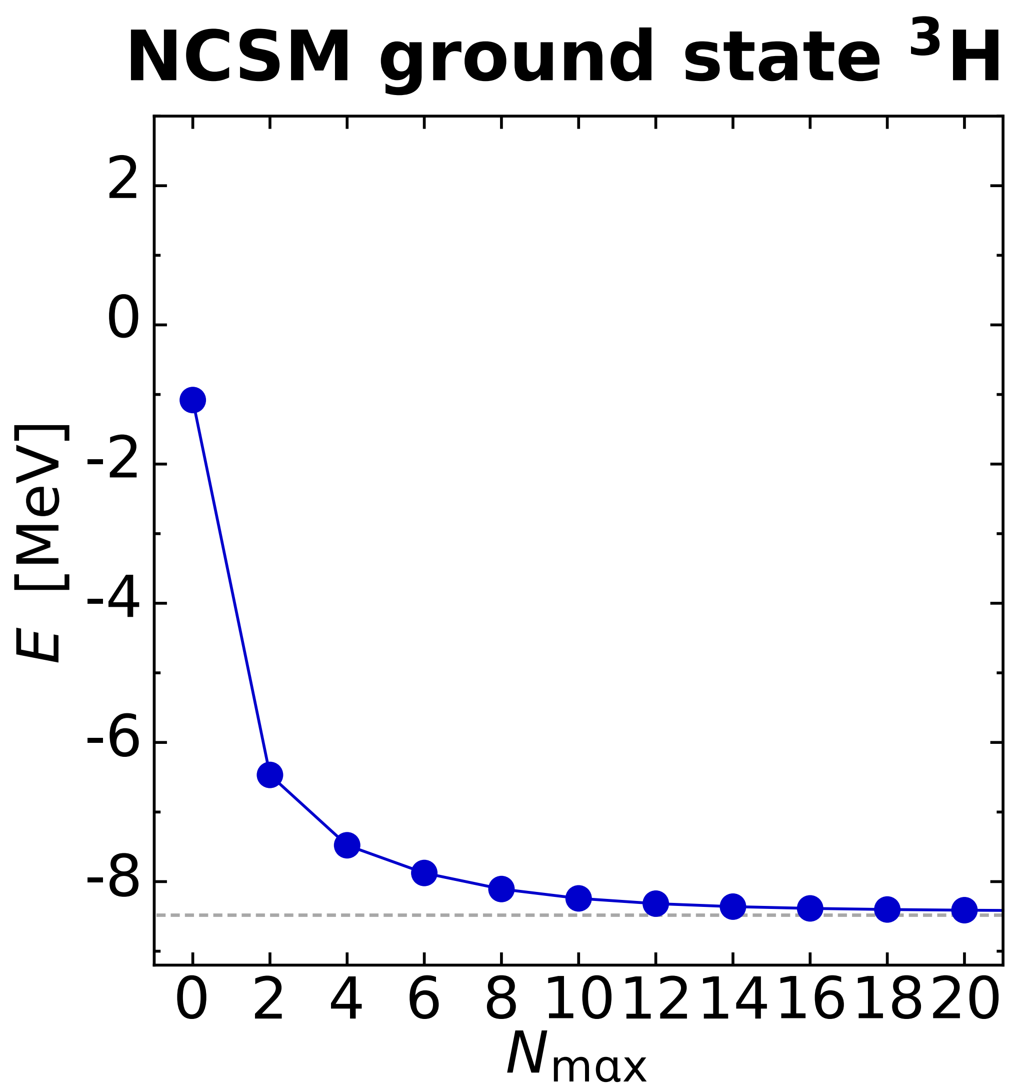
SRG Evolution in Three-Body Space



$\alpha = 0.320\,\mathrm{fm}^4$

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

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



SRG Evolution in A-Body Space

- assume initial Hamiltonian and intrinsic kinetic energy are two-body operators written in second quantization

$$H_0 = \sum \dots a^\dagger a^\dagger a a \,, \qquad T_{int} = T - T_{cm} = \sum \dots a^\dagger a^\dagger a a$$

- perform **single Euler-type evolution step** $\Delta\alpha$ in Fock-space operator form

$$\begin{aligned} H_{\Delta\alpha} &= H_0 + \Delta\alpha \left[\left[T_{int}, H_0 \right], H_0 \right] \\ &= \sum \dots a^\dagger a^\dagger a a + \Delta\alpha \sum \dots \left[\left[a^\dagger a^\dagger a a, a^\dagger a^\dagger a a \right], a^\dagger a^\dagger a a \right] \\ &= \sum \dots a^\dagger a^\dagger a a + \Delta\alpha \sum \dots a^\dagger a^\dagger a^\dagger a^\dagger a a a a + \Delta\alpha \sum \dots a^\dagger a^\dagger a^\dagger a a a + \dots \end{aligned}$$

- SRG evolution **induces many-body contributions** in the Hamiltonian

- induced many-body contributions are the price to pay for the pre-diagonalization of the Hamiltonian

SRG Evolution in A-Body Space

- decompose evolved Hamiltonian into irreducible ***n*-body contributions $H_\alpha^{[n]}$**

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

- **truncation of cluster series** formally destroys unitarity and invariance of energy eigenvalues (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

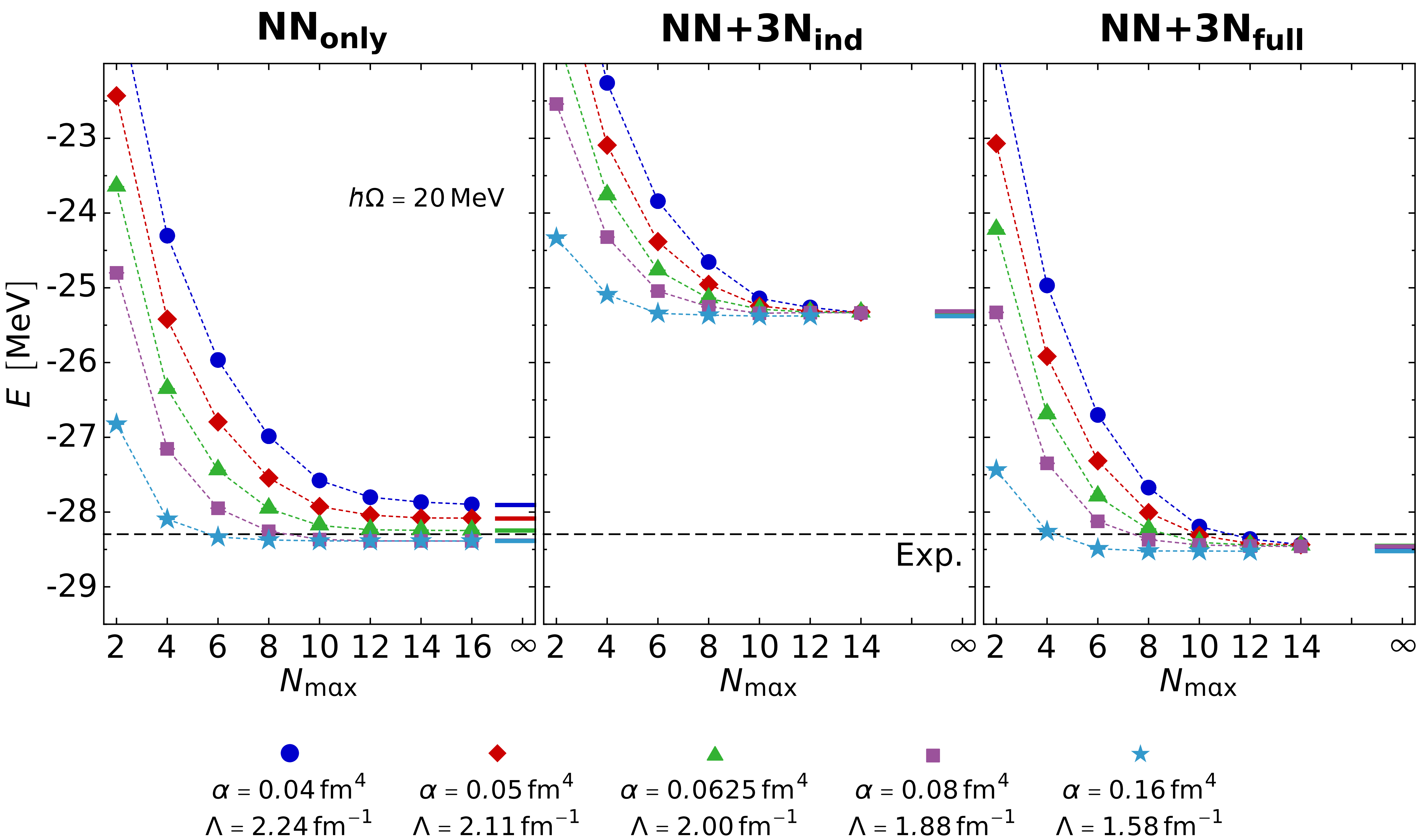
$NN+3N_{ind}$: use initial NN, keep evolved NN+3N

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

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

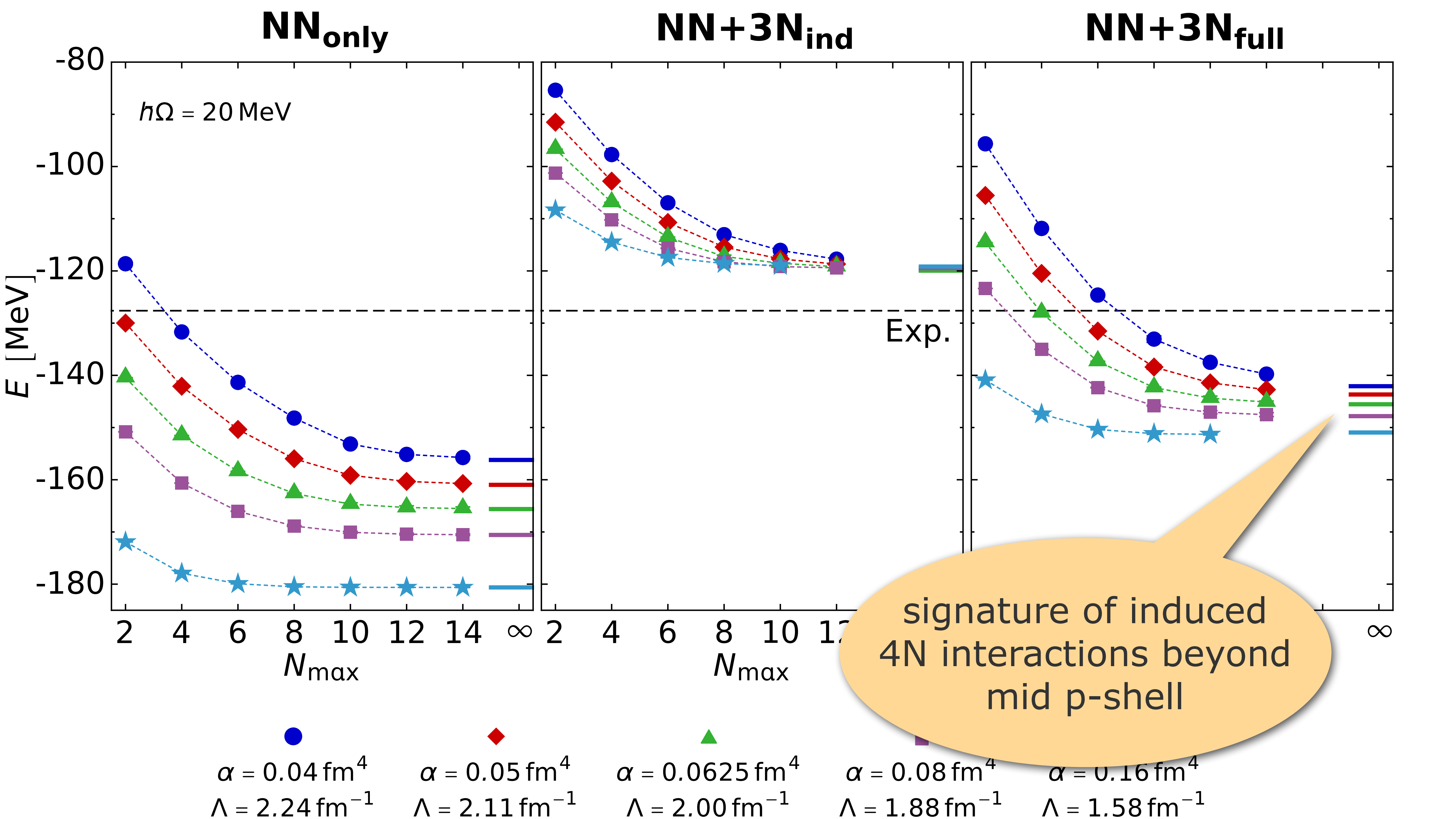
^{4}He: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



^{16}O: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



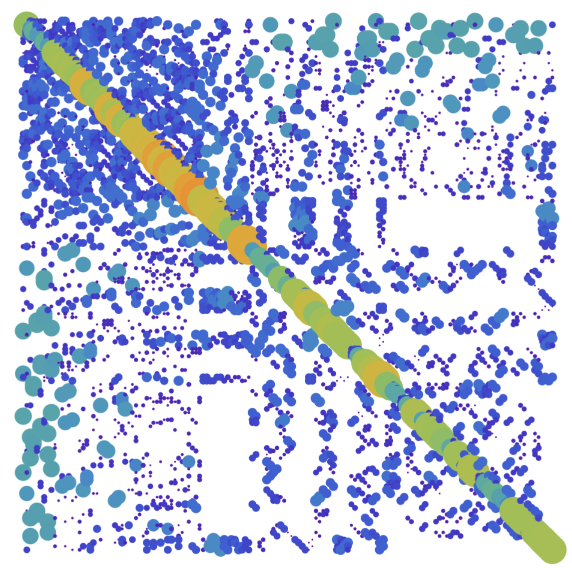
Many-Body Problem

Definition: Ab Initio

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

- numerical treatment with some **truncations or approximations** is inevitable for any nontrivial nuclear structure application
- **challenges for ab initio calculations** are to
  - control the truncation effects
  - quantify the resulting uncertainties
  - reduce them to an acceptable level
- **convergence** with respect to truncations is important: demonstrate that observables become independent of truncations
- continuous transition from approximation to ab initio calculation...

Configuration Interaction Approaches



$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

Configuration Interaction (CI)

- select a convenient **single-particle basis**

$$|\alpha\rangle = |n\,l\,j\,m\,t\,m_t\rangle$$

- construct **A-body basis** of Slater determinants from all possible combinations of A different single-particle states

$$|\Phi_i\rangle = |\{\alpha_1\alpha_2\ldots\alpha_A\}_i\rangle$$

- convert eigenvalue problem of the Hamiltonian into a **matrix eigenvalue problem** in the Slater determinant representation

$$\mathrm{H_{int}}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \qquad |\Psi_n\rangle = \sum_i C_i^{(n)}\,|\Phi_i\rangle$$

$$\begin{pmatrix} & \vdots & \\ \ldots & \langle\Phi_i|\,\mathrm{H_{int}}\,|\Phi_{i'}\rangle & \ldots \\ & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_i^{(n)} \\ \vdots \end{pmatrix}$$

Model Space Truncations

- have to **introduce truncations** of the single/many-body basis to make the Hamilton matrix **finite and numerically tractable**

  - **full CI**:
    truncate the single-particle basis, e.g., at a maximum single-particle energy

  - **particle-hole truncated CI**:
    truncate single-particle basis and truncate the many-body basis at a maximum n-particle-n-hole excitation level

  - **interacting shell model**:
    truncate single-particle basis and freeze low-lying single-particle states (core)

- in order to qualify as ab initio one has to **demonstrate convergence** with respect to all those truncations

- there is freedom to **optimize the single-particle basis**, instead of HO states one can use single-particle states, e.g., from a Hartree-Fock calculation

Variational Perspective

- solving the eigenvalue problem in a finite model space is **equivalent to a variational calculation** with a trial state

$$|\Psi_n(D)\rangle = \sum_{i=1}^{D} C_i^{(n)} \, |\Phi_i\rangle$$

- formally, the stationarity condition for the energy expectation value directly leads to the matrix eigenvalue problem in the truncated model space

- **Ritz variational principle**: the ground-state energy in a D-dimensional model space is an upper bound for the exact ground-state energy

$$E_0(D) \geq E_0(\text{exact})$$

- **Hylleraas-Undheim theorem**: all states of the spectrum have a monotonously decreasing energy with increasing model space dimension

$$E_n(D) \geq E_n(D+1)$$

Theory Uncertainties

- model-space truncation is the **sole source of uncertainties** in the solution of the many-body problem
- absolute energies are **protected by the variational principle**, i.e., smooth and monotonic dependence on model-space size (not so for other observables)

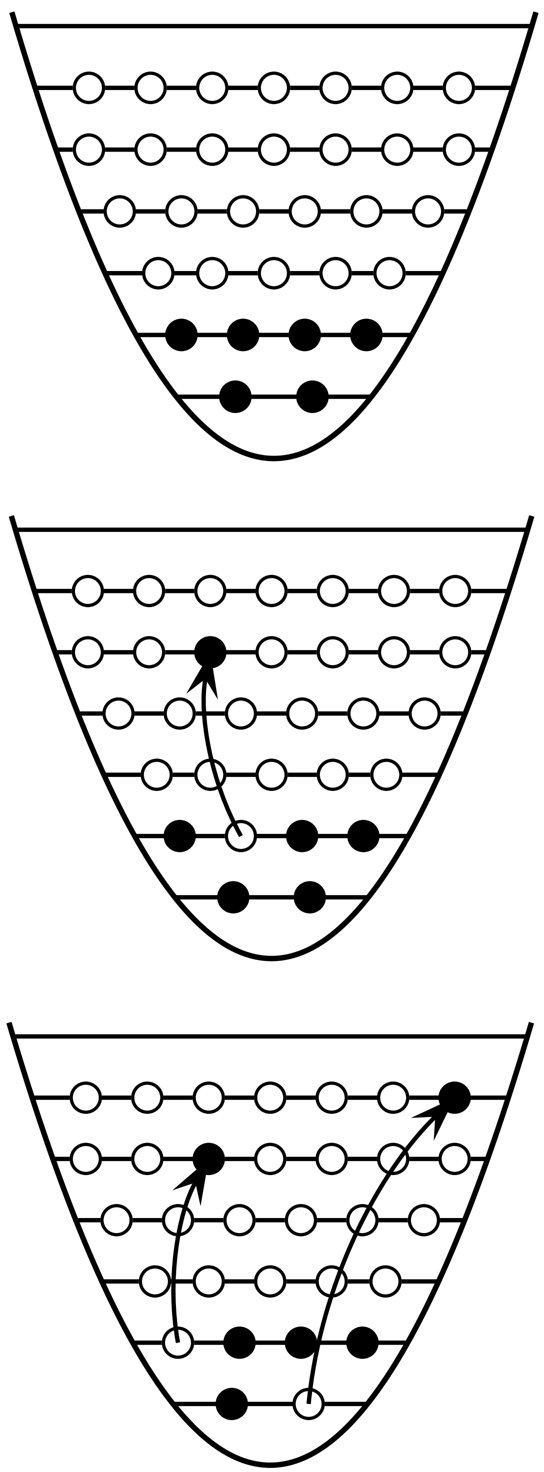
convergence with respect to model-space size is the only thing we have to worry about

- **efficient truncations**: get closer to convergence with smaller model-space dimension, i.e., physics-informed truncation scheme
- **extrapolations**: extrapolate observables to infinite model-space from a sequence of finite-space calculations
- **uncertainty quantification**: extract many-body uncertainty from residual model-space dependence or extrapolation

No-Core Shell Model

No-Core Shell Model (NCSM)

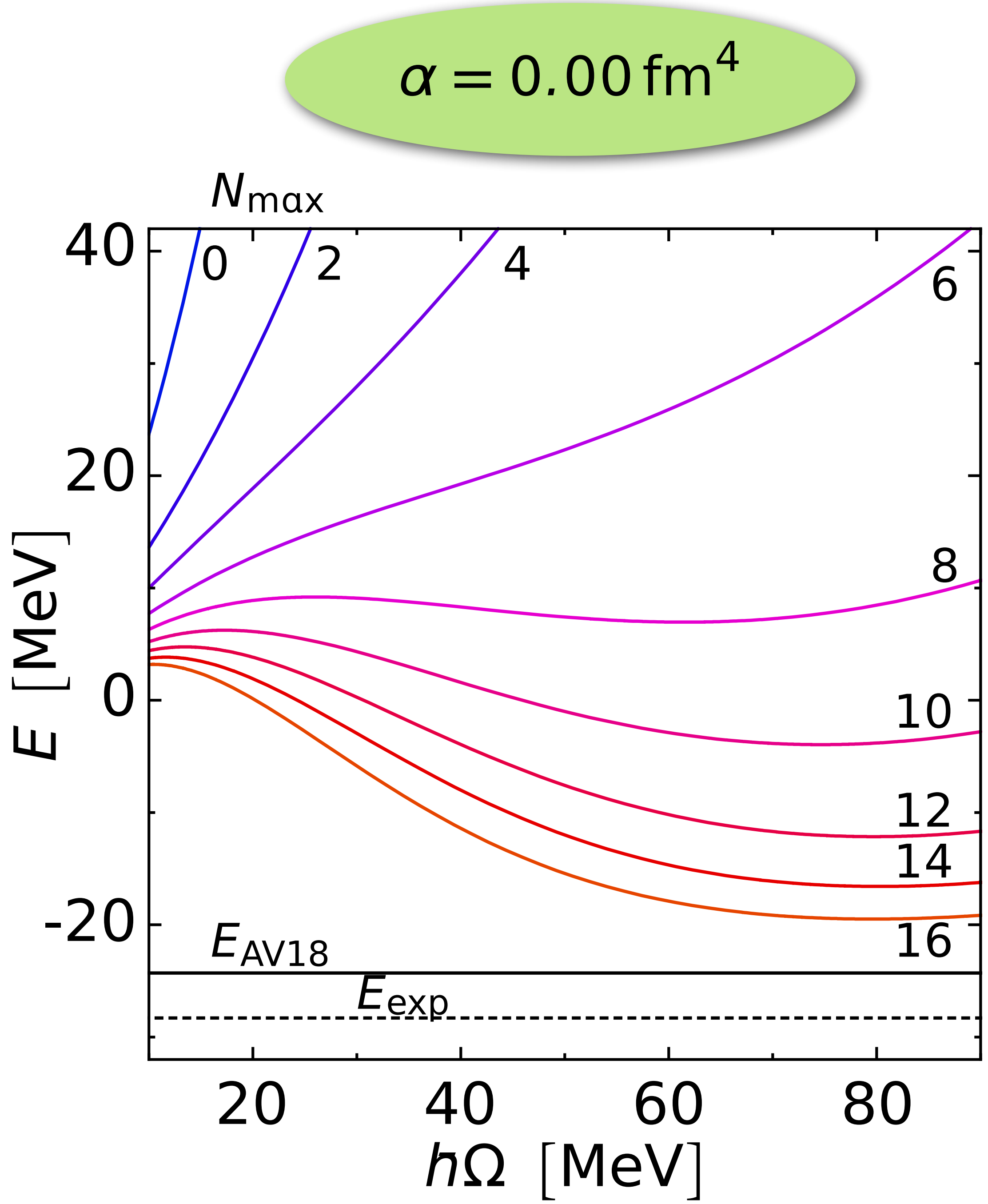
- NCSM is a special case of a CI approach:
  - single-particle basis is a **spherical HO basis**
  - truncation in terms of the total **number of HO excitation quanta $N_{\max}$** in the many-body states

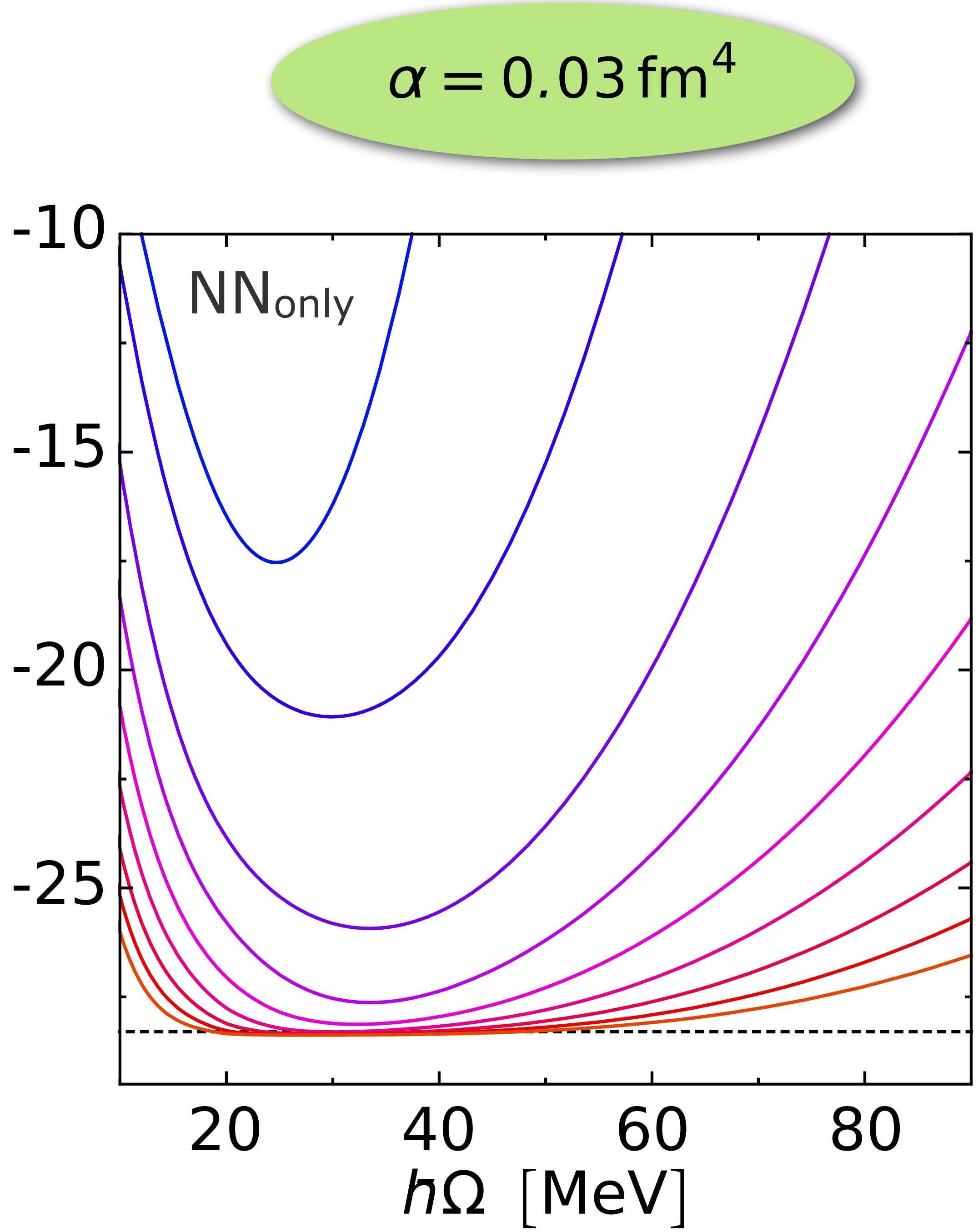


- **specific advantages** of the NCSM:
  - many-body energy truncation (N_{max}) truncation is much **more efficient** than single-particle energy truncation (e_{max})
  - equivalent NCSM formulation in relative Jacobi coordinates for each N_{max} — **Jacobi-NCSM**
  - **explicit separation** of center of mass and intrinsic states possible for each N_{max}

^{4}He: NCSM Convergence

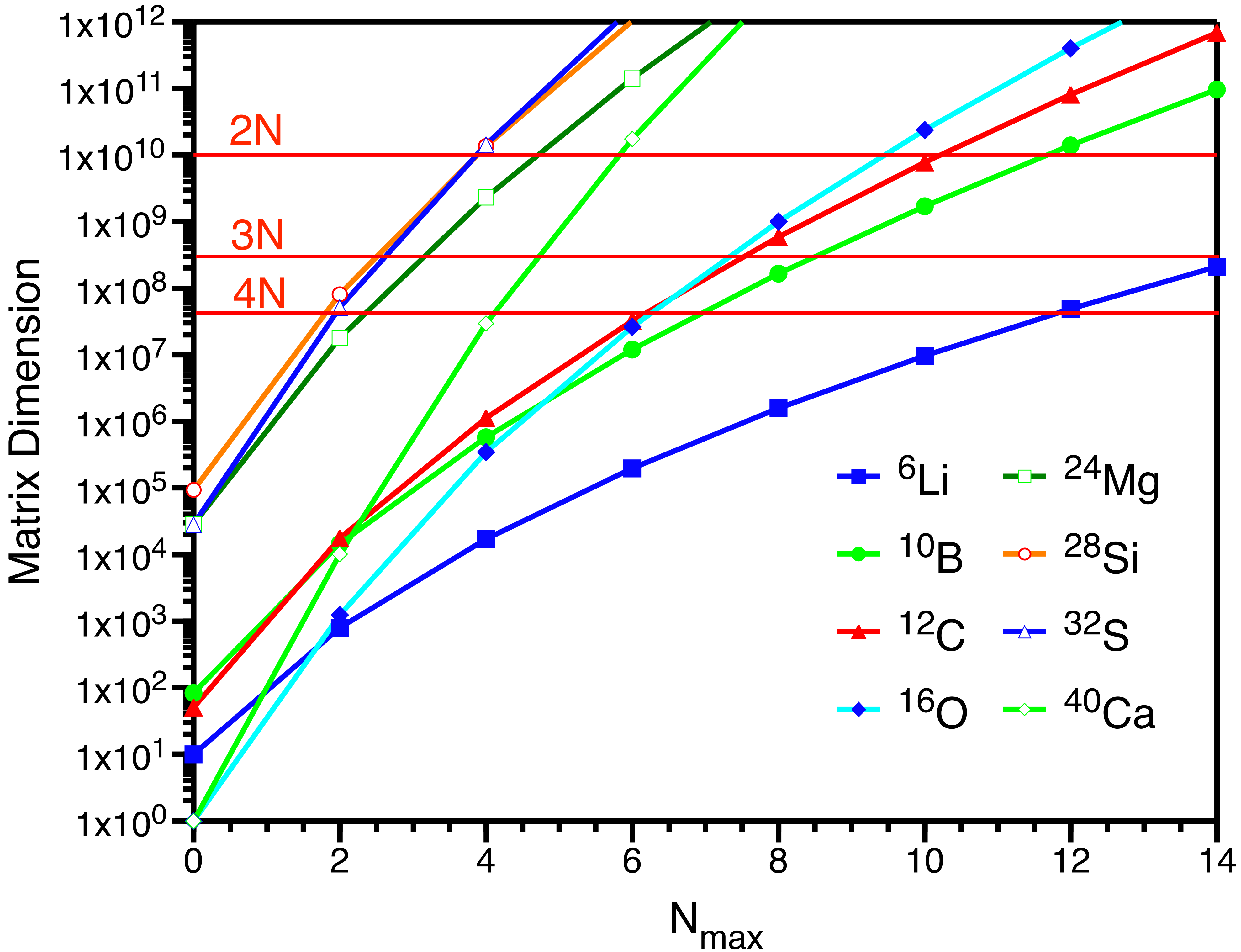
- worst case scenario for NCSM convergence: **Argonne V18 potential**



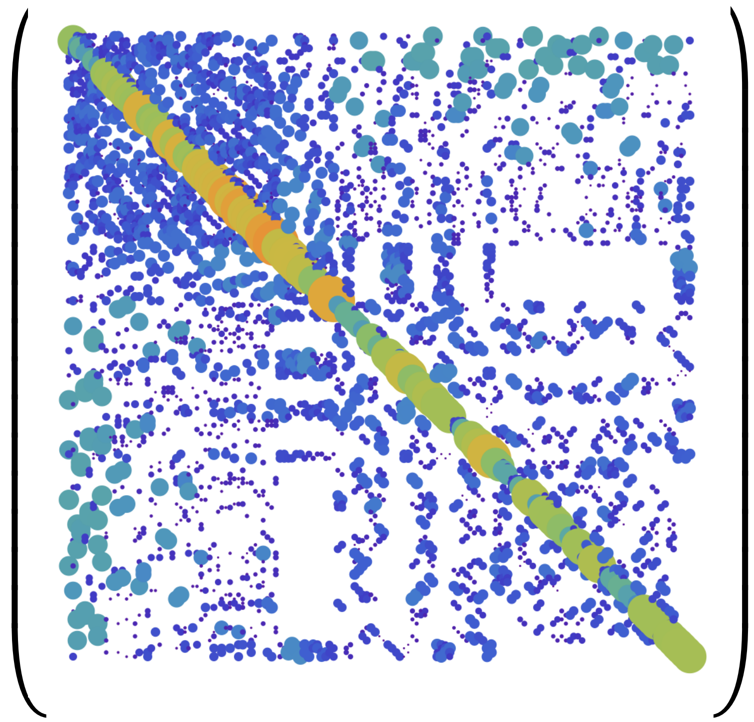


NCSM Basis Dimension

Vary et al.; J. Phys.: Conf. Series 180, 012083 (2009)



Computational Strategy



$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

- **key properties** of the computational problem:
  - only interested in a **few low-lying eigenstates**
  - Hamilton matrix is **very sparse** (typically <0.01% non-zeros)
- **Lanczos-type algorithms** for an iterative solution of the eigenvalue problem
- amount of **fast storage** for non-zero matrix elements & a few eigenvectors sets the limits and drives parallelization strategies

Lanczos Algorithm

- **Lanczos Algorithm**: convert the eigenvalue problem of a huge matrix $\boldsymbol{H}$ in an iterative process to eigenvalue problems of small matrices $\boldsymbol{T_m}$ that converge to the same extremal eigenvalues

$$\boldsymbol{H} = \begin{pmatrix} & & \\ & 10^{10} \times 10^{10} & \\ & & \end{pmatrix}$$

$\vec{v}_0 := \vec{0}$
$\vec{v}_1 :=$ any norm. vector
$\beta_1 := 0$

for $i = 1, m$ **do**

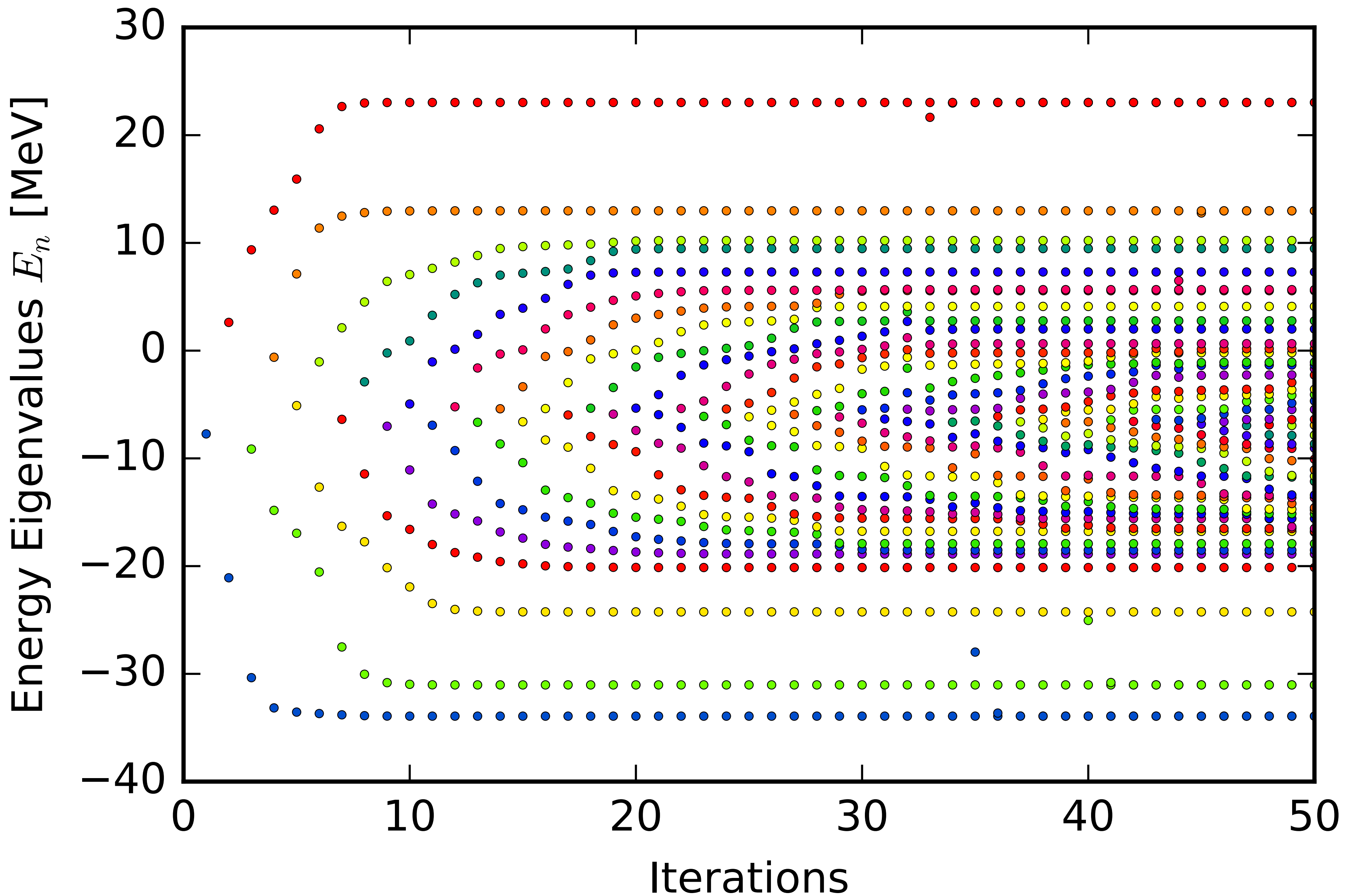
$\quad \vec{w} := \boldsymbol{H} \cdot \vec{v}_i - \beta_i \vec{v}_{i-1}$
$\quad \alpha_i := \vec{w} \cdot \vec{v}_i$
$\quad \vec{w} := \vec{w} - \alpha_i \vec{v}_i$
$\quad \beta_{i+1} := ||\vec{w}||$
$\quad \vec{v}_{i+1} := \vec{w}/\beta_{i+1}$

end for

$$\boldsymbol{T}_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_m \\ & & & \beta_m & \alpha_m \end{pmatrix}$$

Lanczos Algorithm

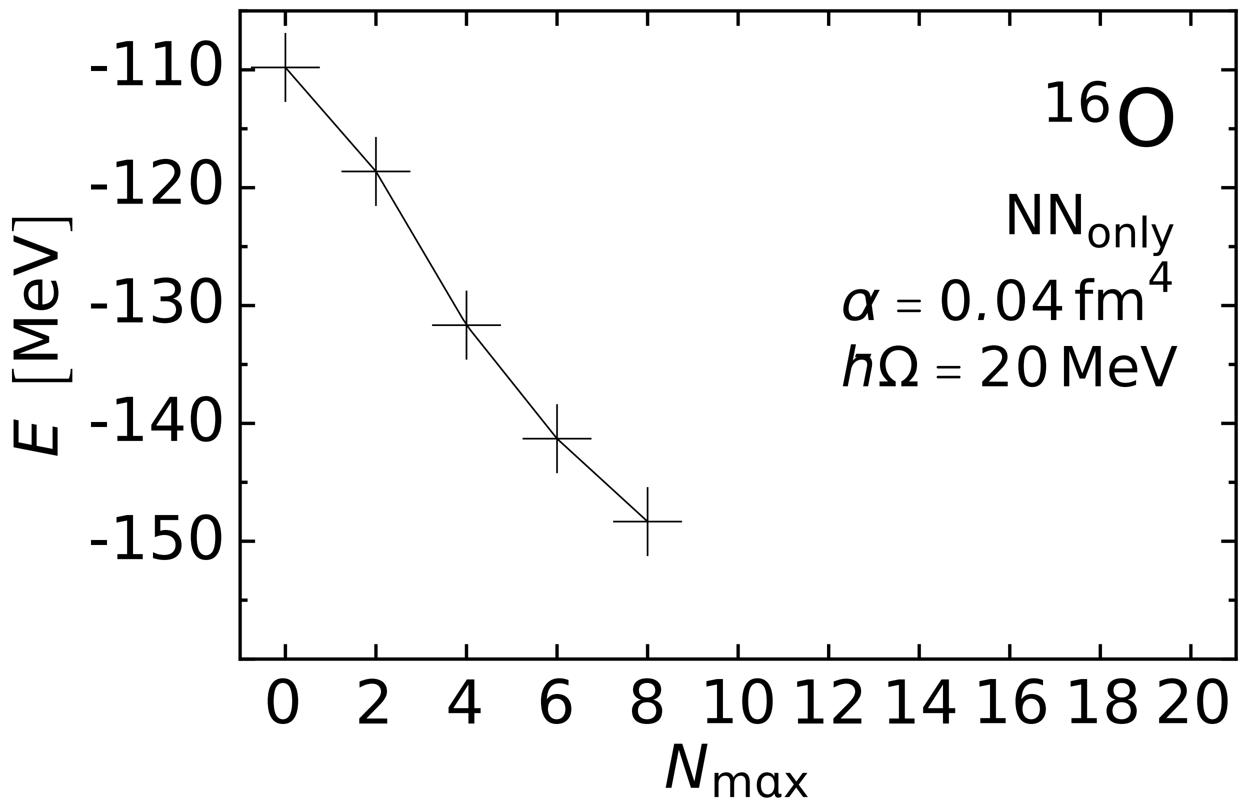
- **Lanczos Algorithm**: convert the eigenvalue problem of a huge matrix $\boldsymbol{H}$ in an iterative process to an eigenvalue problem of small matrices $\boldsymbol{T_m}$ which converge to the same extremal eigenvalues



Importance Truncation

Importance Truncation

- **converged NCSM** calculations limited to lower & mid p-shell nuclei
- example: full N_{max}=10 calculation for ^{16}O would be very difficult, basis dimension $D > 10^{10}$

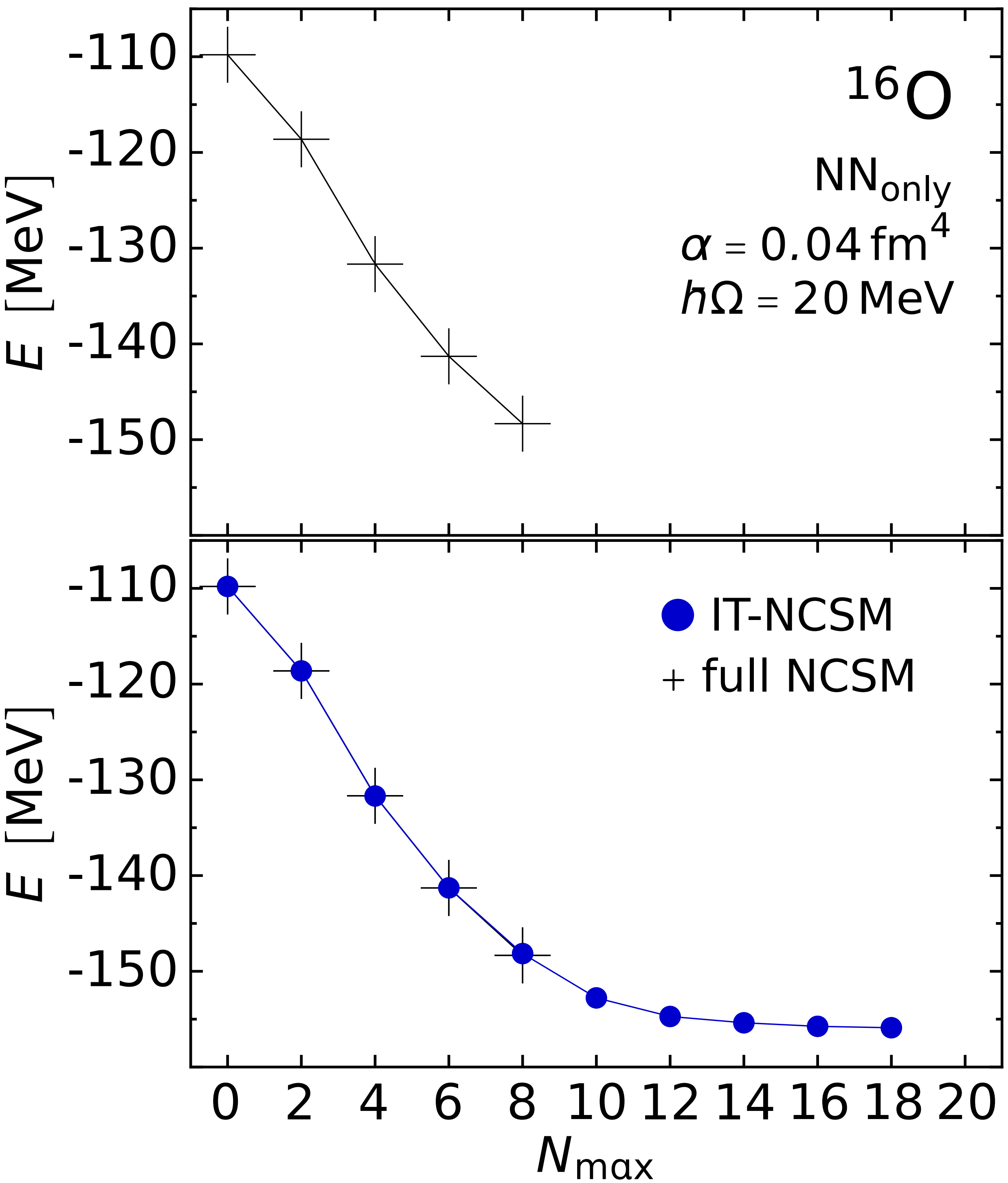


Importance Truncation

- **converged NCSM** calculations limited to lower & mid p-shell nuclei
- example: full N_{max}=10 calculation for ^{16}O would be very difficult, basis dimension D > 10^{10}

Importance Truncation

reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



Importance Truncation

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

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

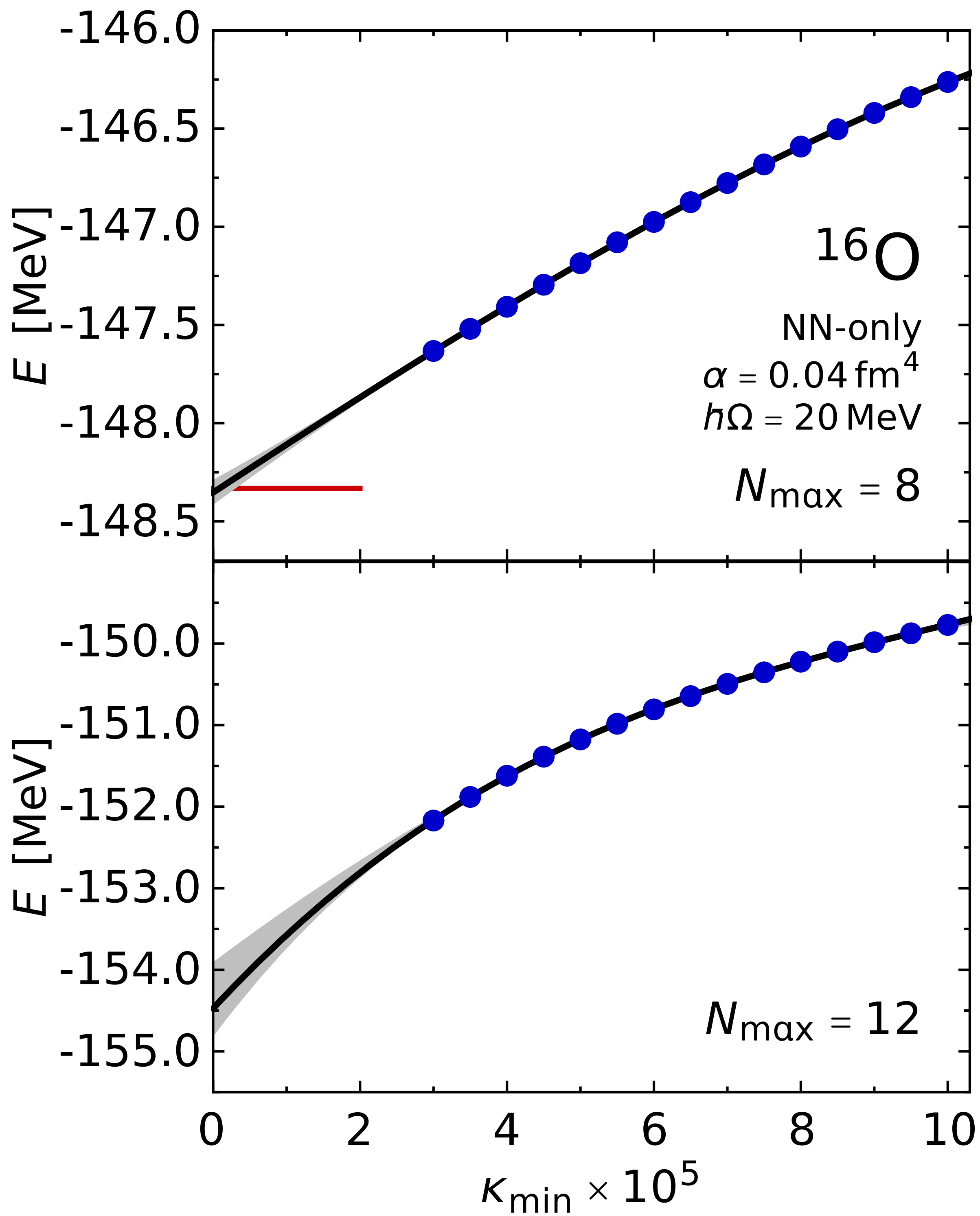
- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

$$\kappa_{\nu} = -\frac{\langle \Phi_{\nu} | \mathrm{H} | \Psi_{\text{ref}} \rangle}{\Delta\epsilon_{\nu}}$$

- construct **importance-truncated space** $\mathcal{M}(\kappa_{\text{min}})$ from all basis states with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$

- **solve eigenvalue problem** in importance truncated space $\mathcal{M}_{\text{IT}}(\kappa_{\text{min}})$ and obtain improved approximation of target state

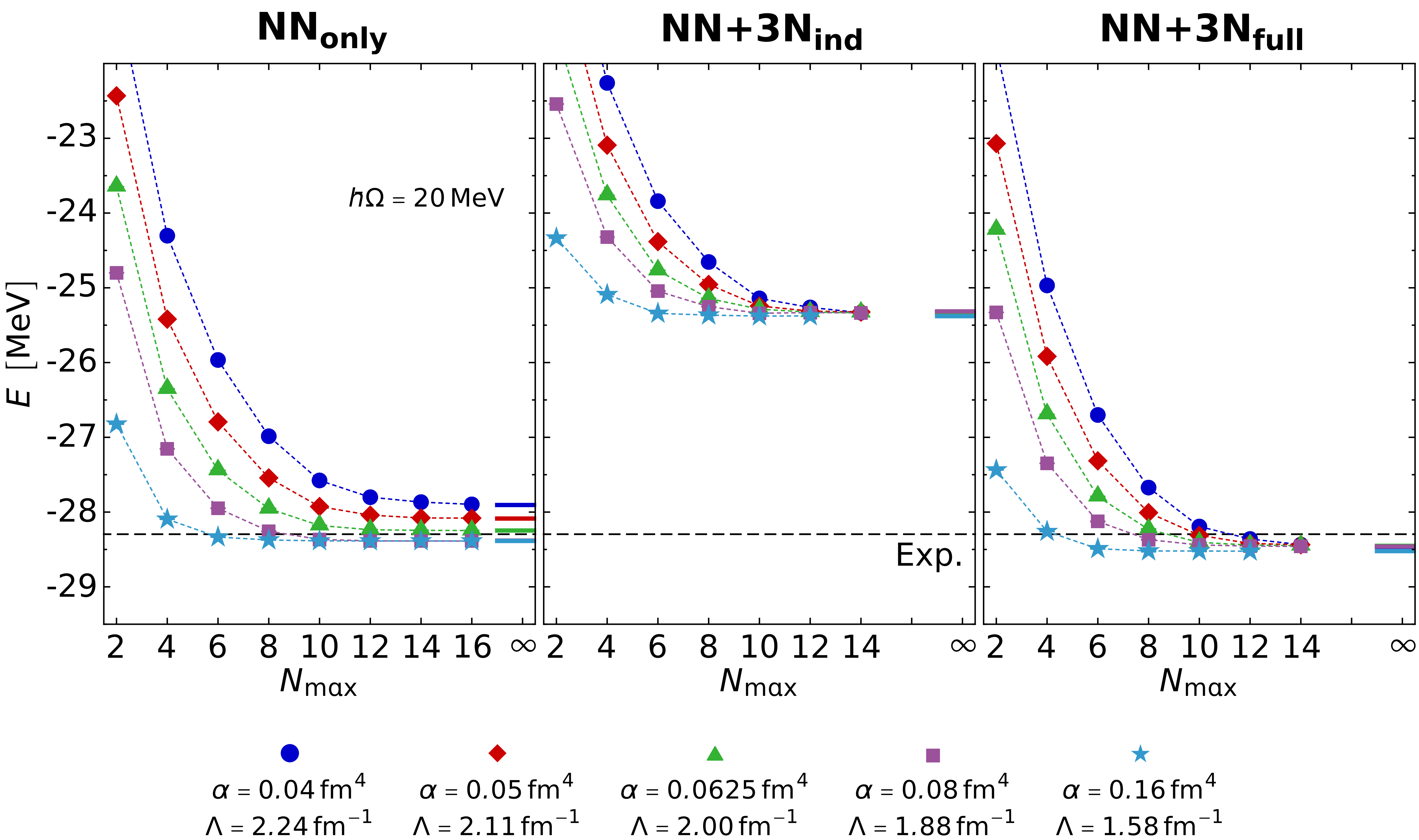
Threshold Extrapolation



- repeat calculations for a **sequence of importance thresholds** κ_{min}
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{min} \to 0$ of observables to account for effect of excluded configurations
- **uncertainty quantification** via set of extrapolations

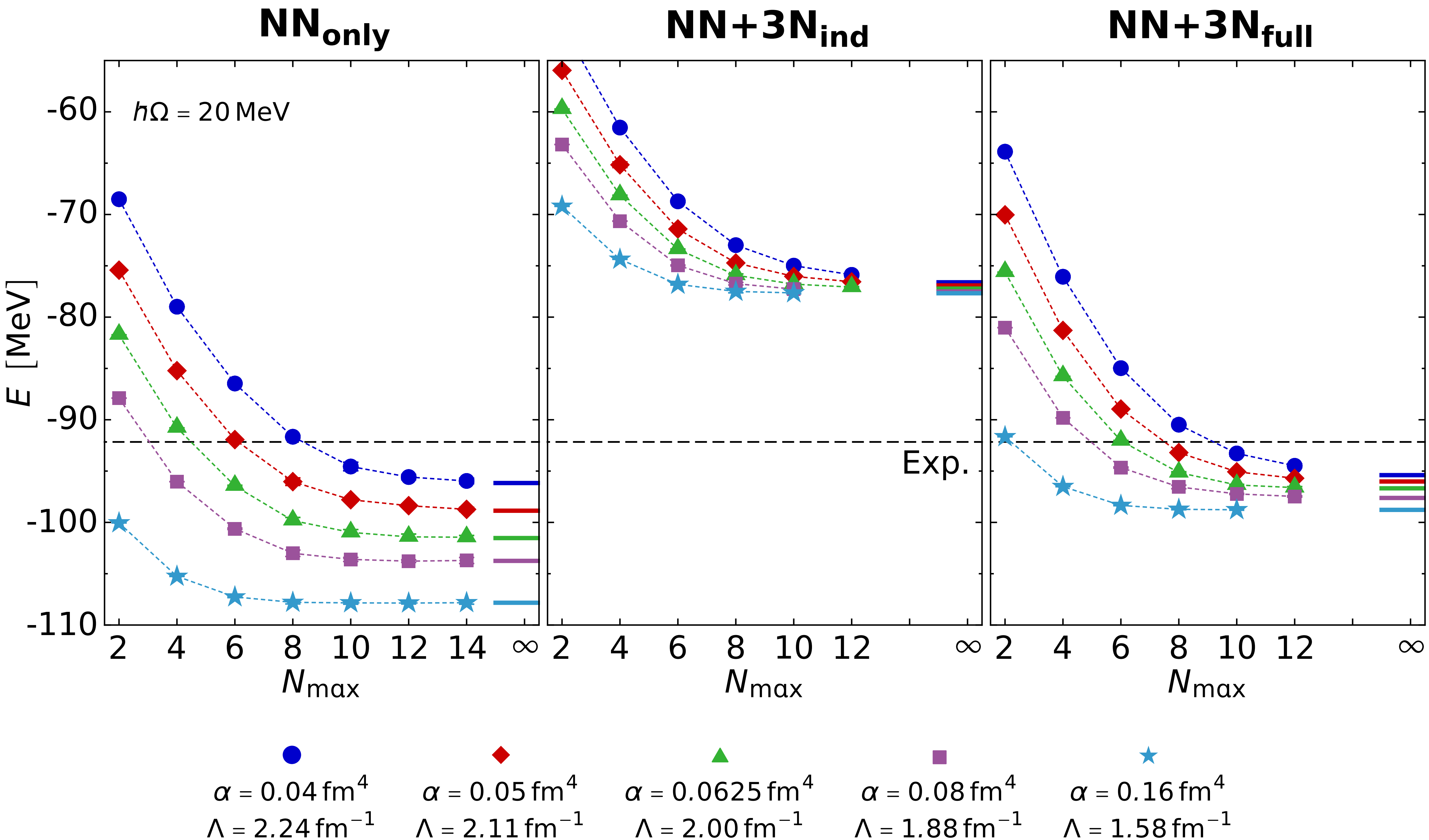
^{4}He: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



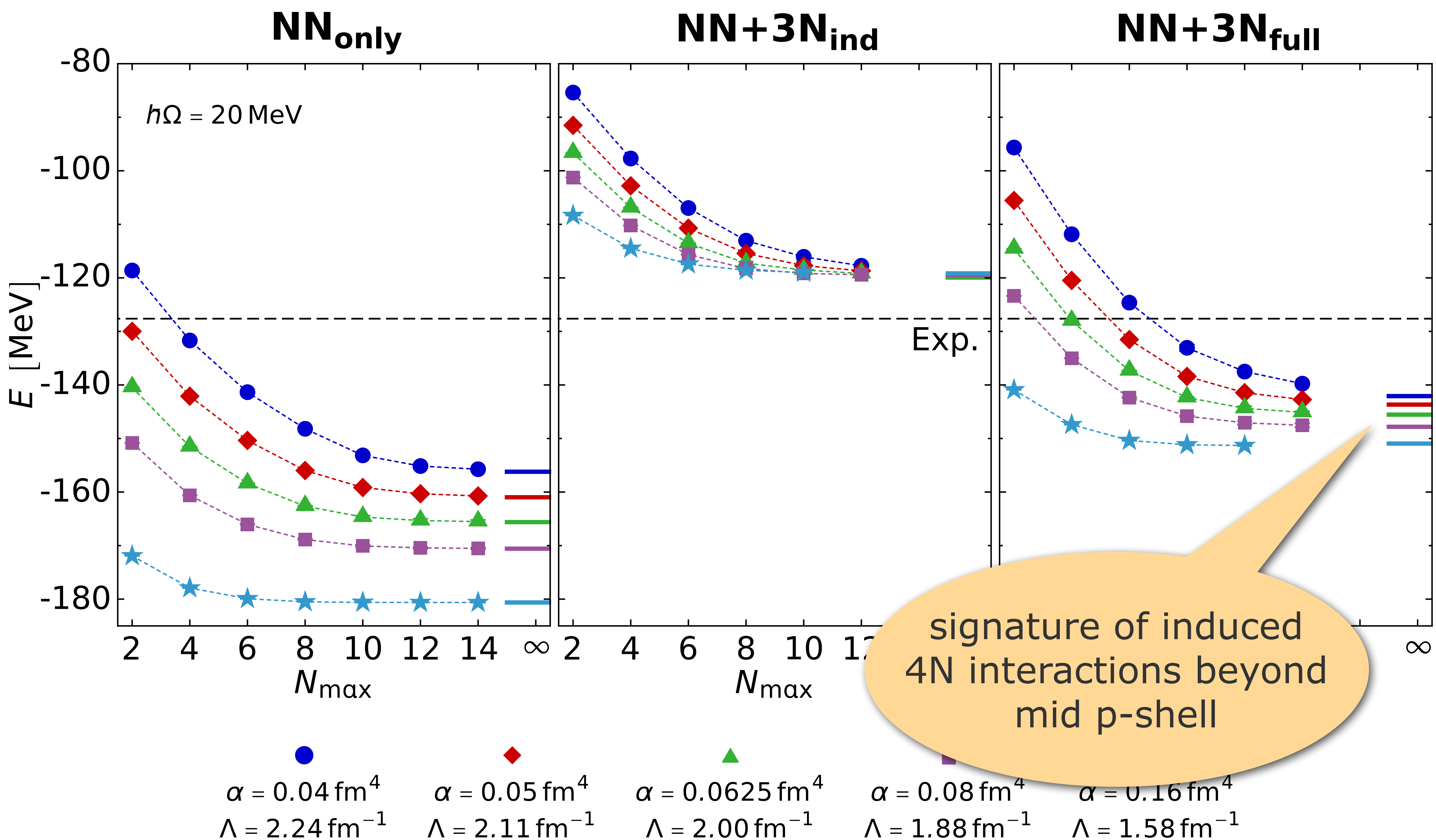
^{12}C: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



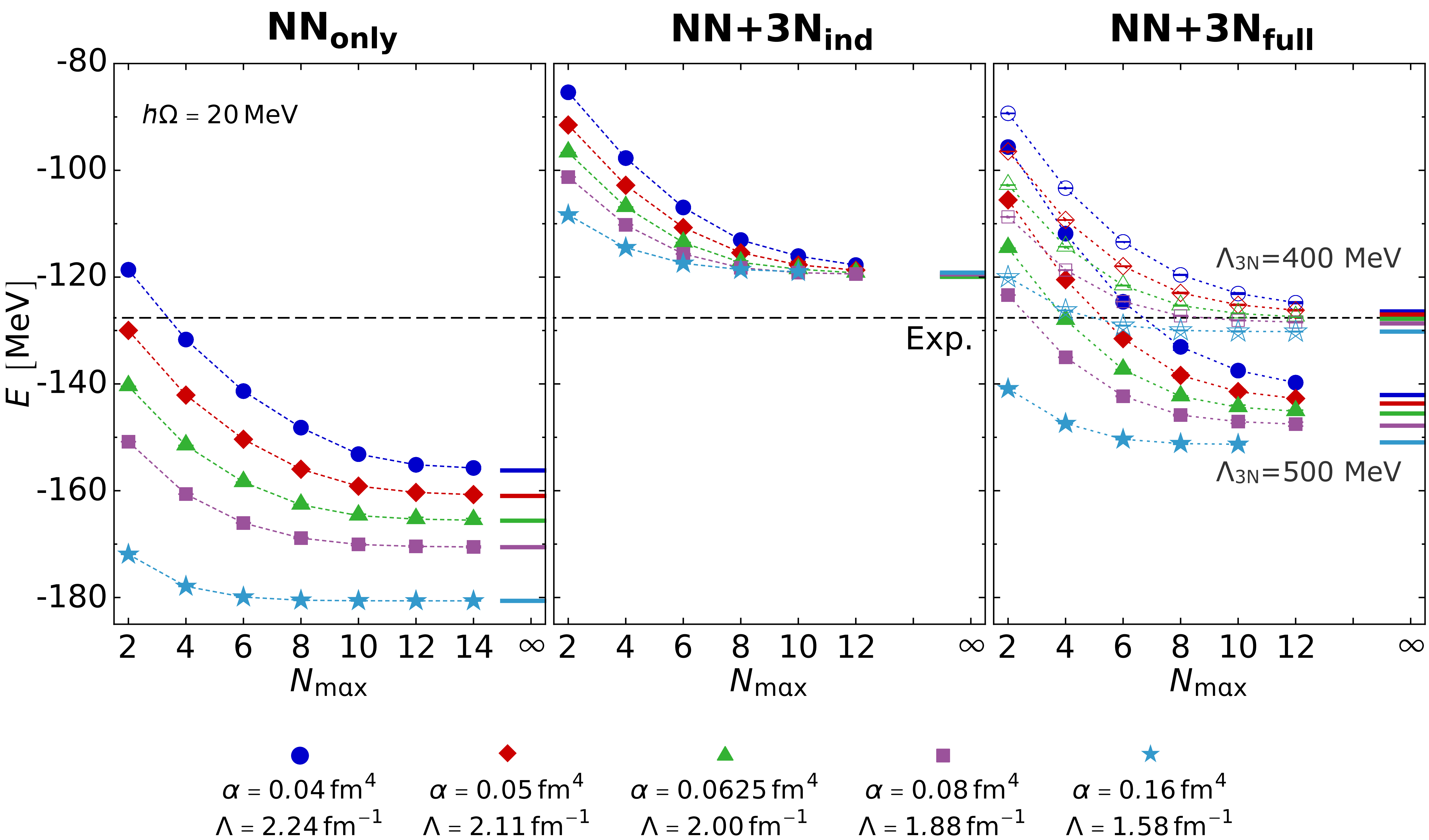
^{16}O: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)

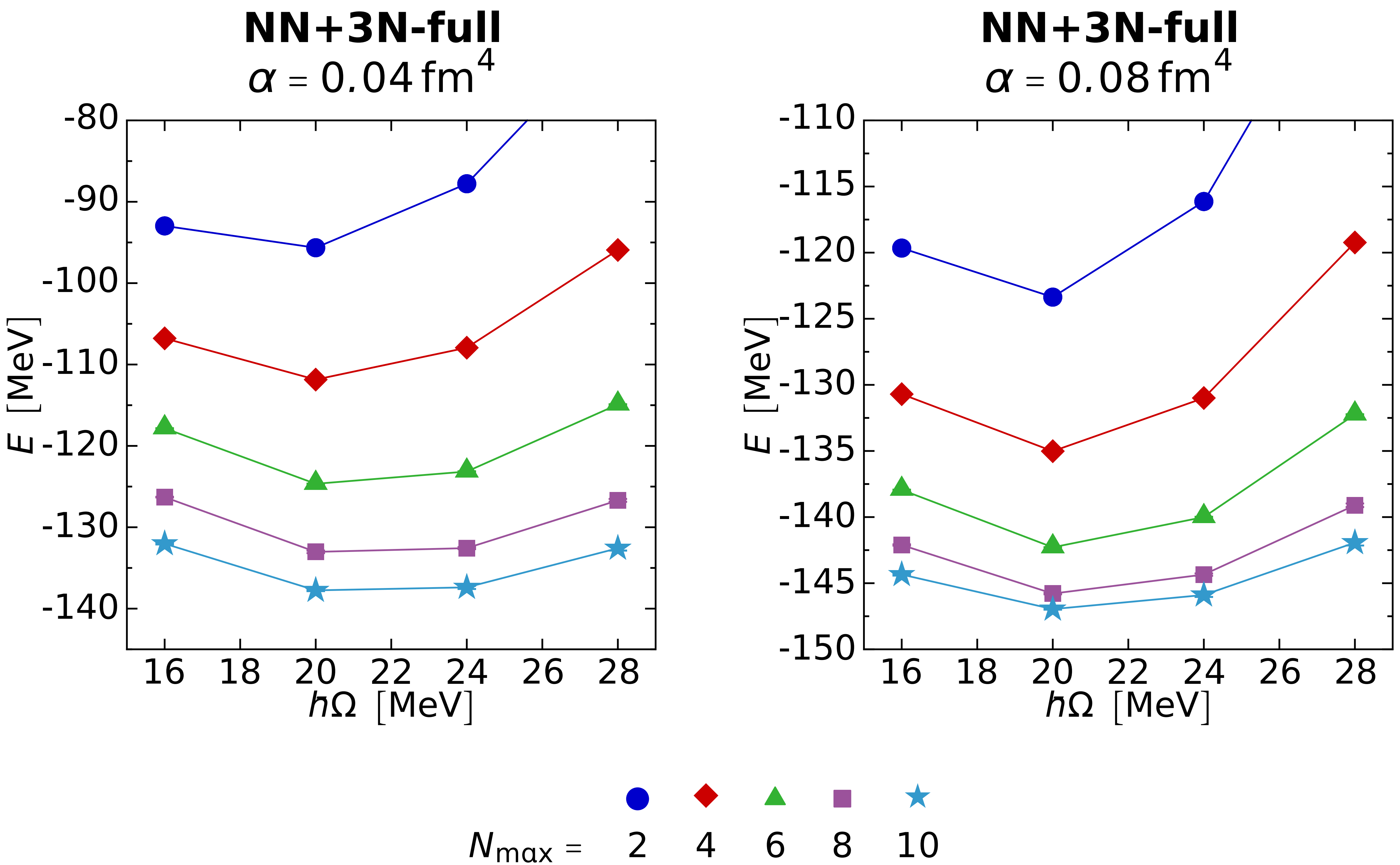


^{16}O: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)

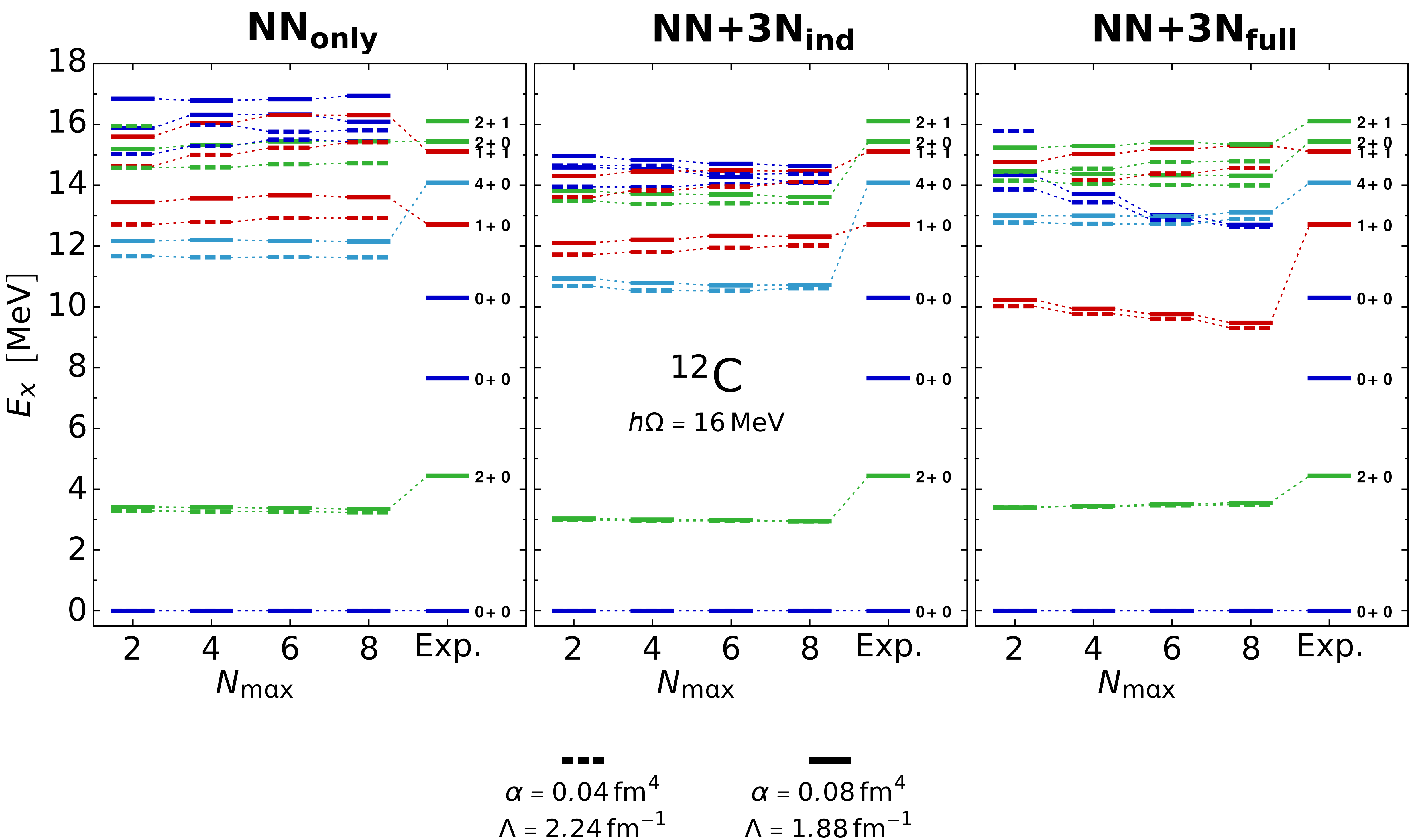


^{16}O: Frequency Dependence



^{12}C: Excitation Spectrum

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



From Dripline to Dripline

Oxygen Isotopes

- **oxygen isotopic chain** has received significant attention and documents the **rapid progress** over the past years

Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL 105, 032501 (2010)

- 2010: **shell-model calculations** with 3N effects highlighting the role of 3N interaction for drip line physics

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, PRL 108, 242501 (2012)

- 2012: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

Hergert, Binder, Calci, Langhammer, Roth, PRL 110, 242501 (2013)

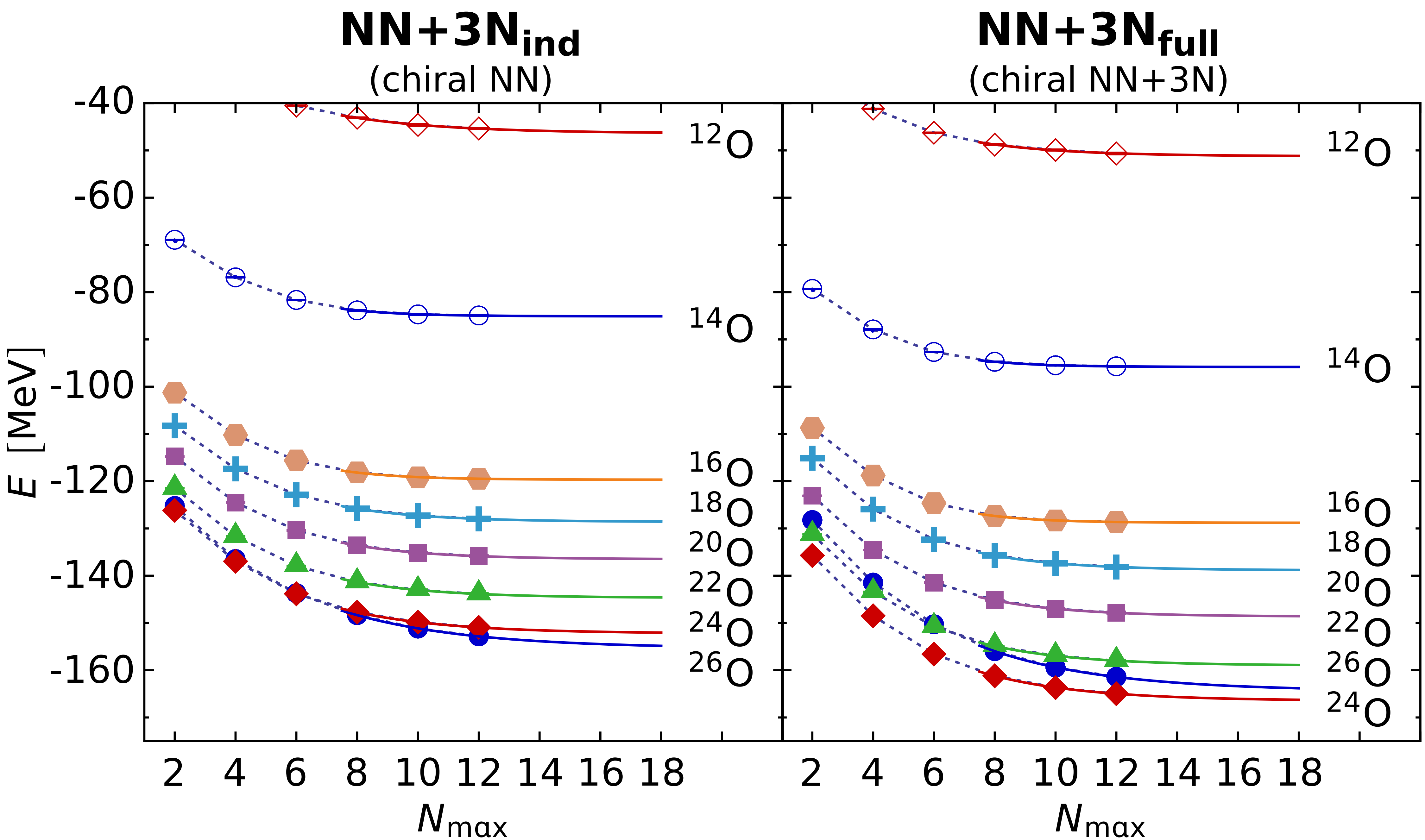
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

Cipollone, Barbieri, Navrátil, PRL 111, 062501 (2013)
Bogner, Hergert, Holt, Schwenk, Binder, Calci, Langhammer, Roth, PRL 113, 142501 (2014)
Jansen, Engel, Hagen, Navratil, Signoracci, PRL 113, 142502 (2014)

- since: self-consistent Green's function, shell model with valence-space interactions from in-medium SRG or Lee-Suzuki,...

Ground States of Oxygen Isotopes

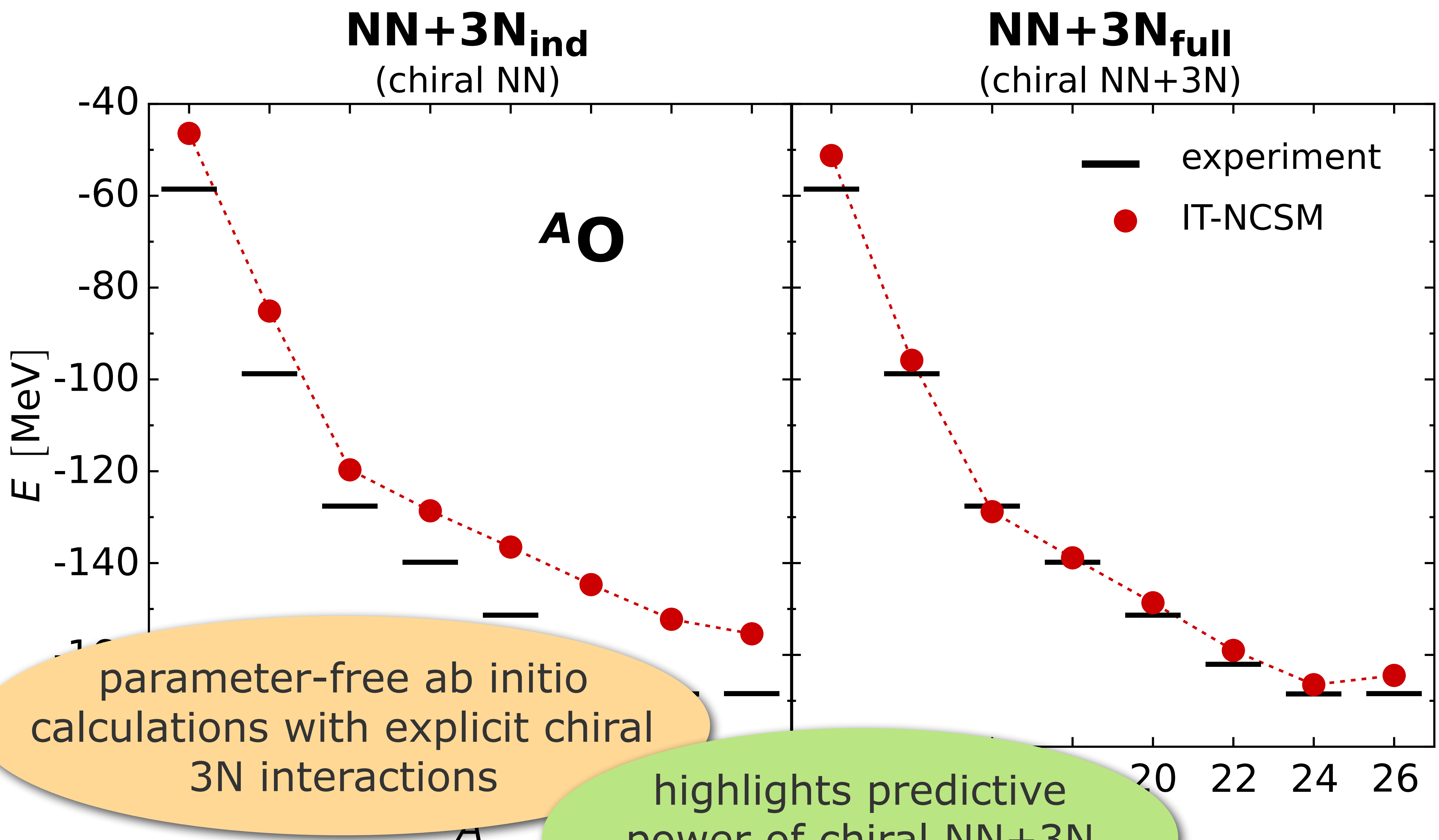
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)



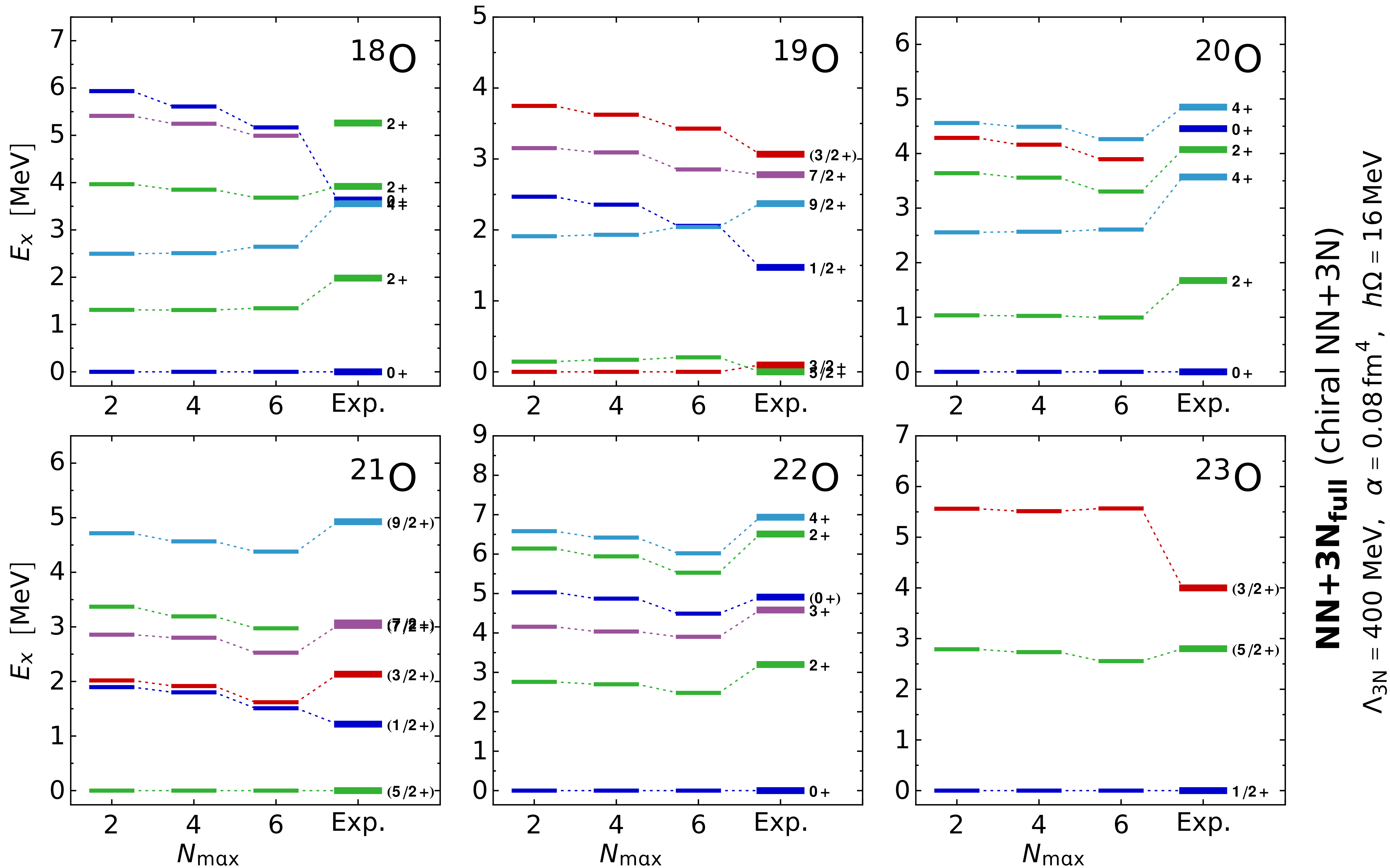
parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

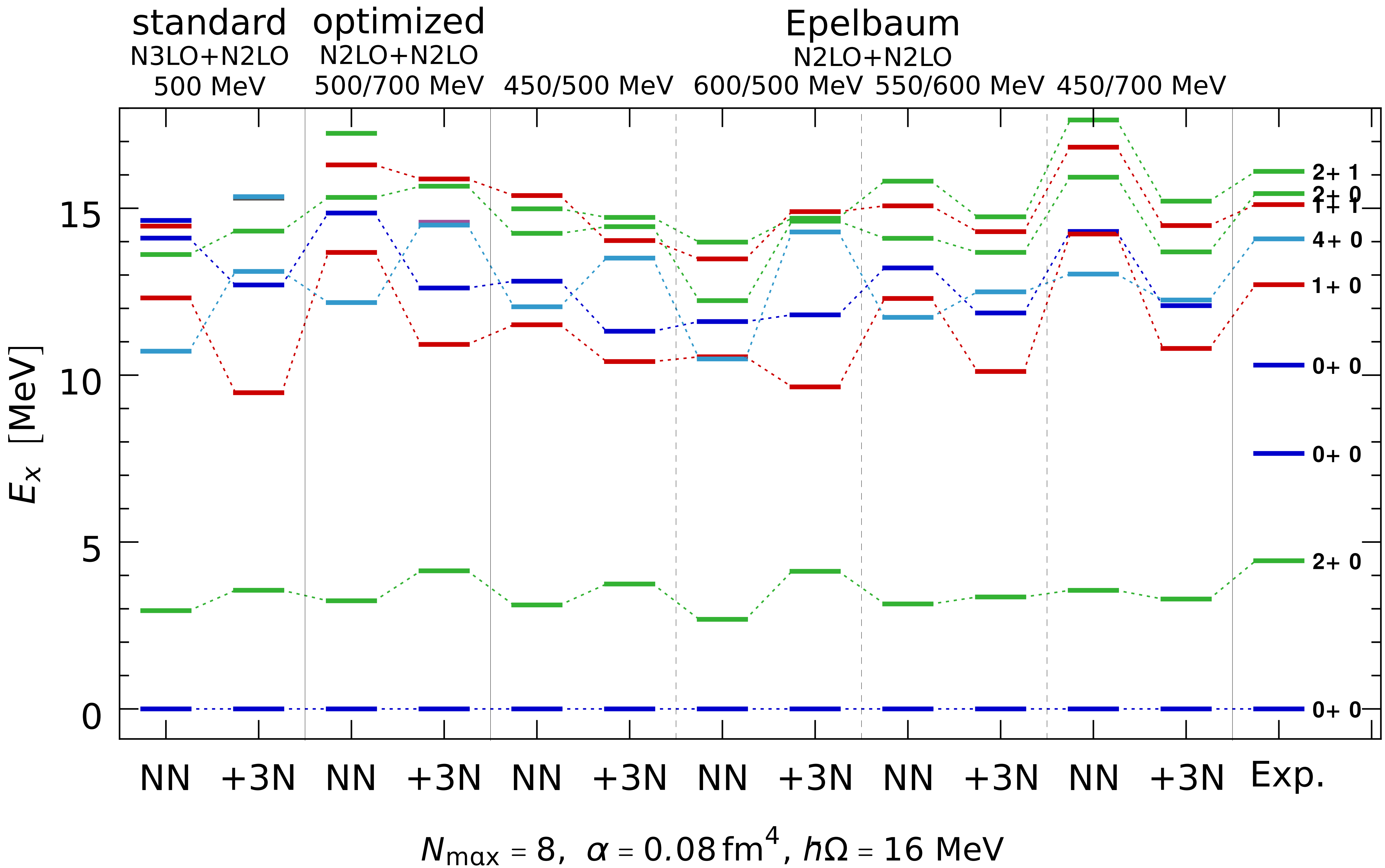
Λ_{3N} = 400 MeV, α = ... ptimal $\hbar\Omega$

Spectra of Oxygen Isotopes

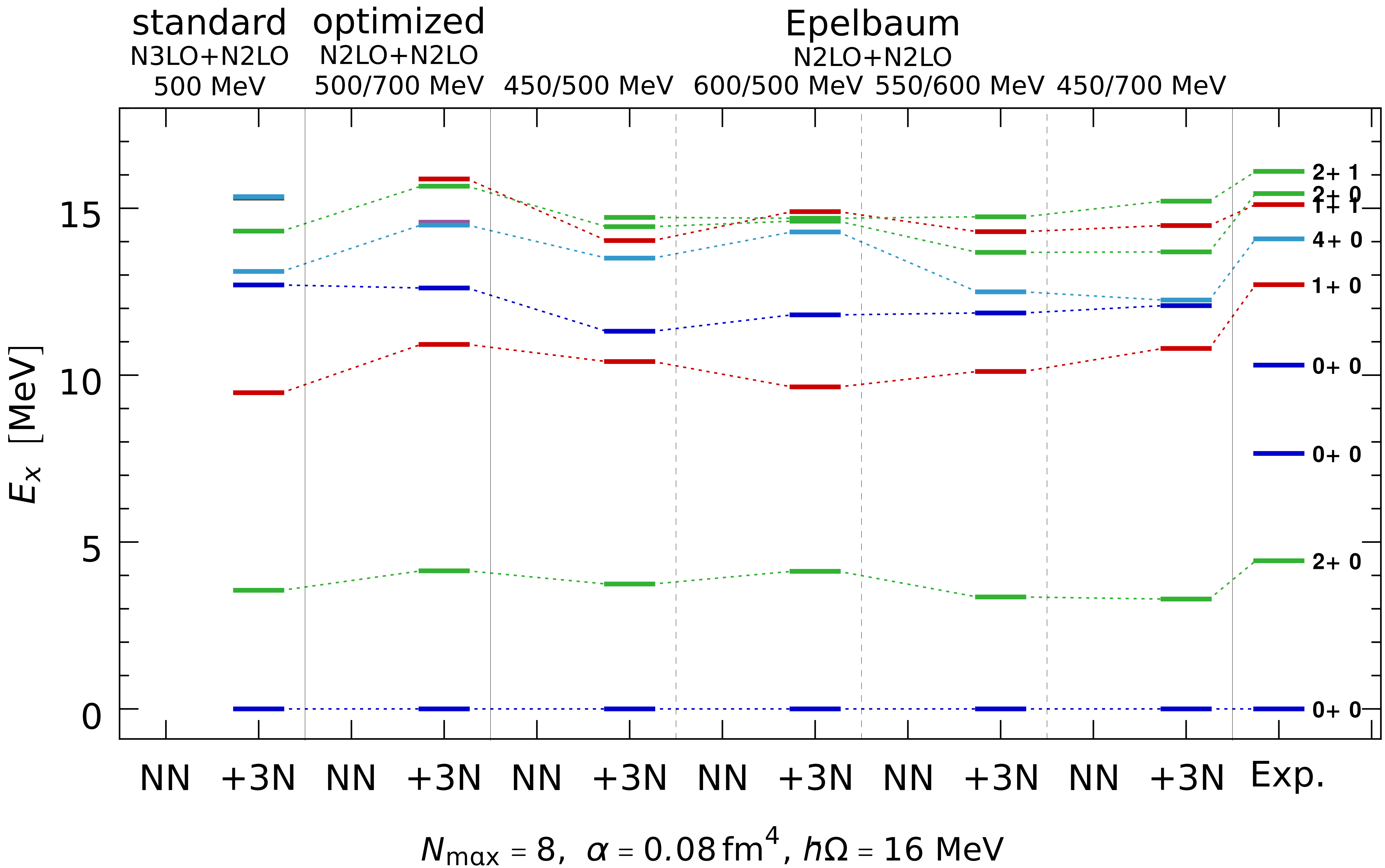
Hergert et al., PRL 110, 242501 (2013) & in prep.



^{12}C: Testing Chiral Hamiltonians



^{12}C: Testing Chiral Hamiltonians



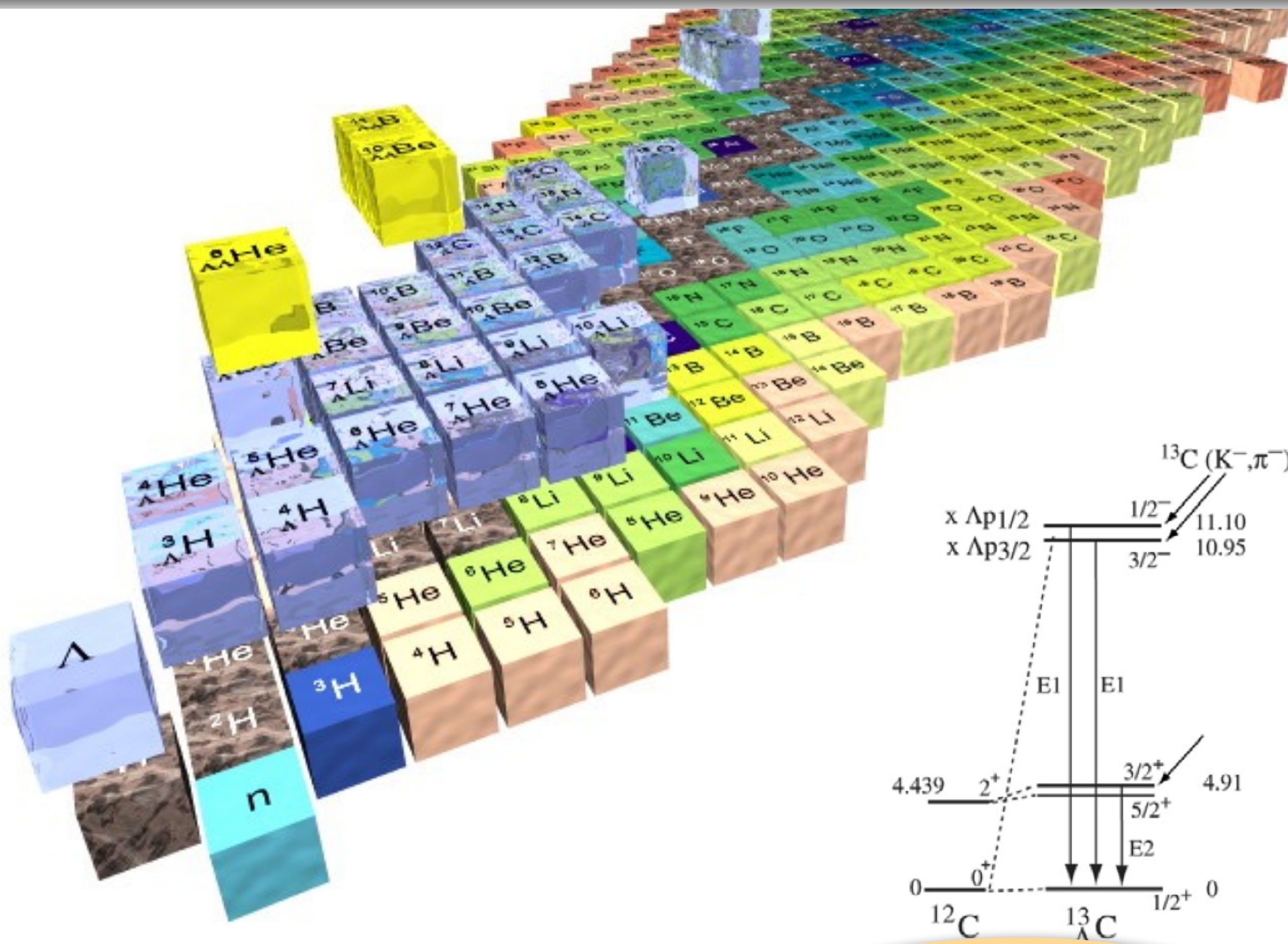
The NCSM Family

- **NCSM**
  HO Slater determinant basis with N_{max} truncation
- **Jacobi NCSM**
  relative-coordinate Jacobi HO basis with N_{max} truncation
- **Importance Truncated NCSM**
  HO Slater determinant basis with N_{max} and importance truncation
- **Symmetry Adapted NCSM**
  group-theoretical basis with SU(3) deformation quantum numbers & truncations
- **Gamow NCSM/CI**
  Slater determinant basis including Gamow single-particle resonance states
- **NCSM with Continuum**
  NCSM for sub-clusters with explicit RGM treatment of relative motion

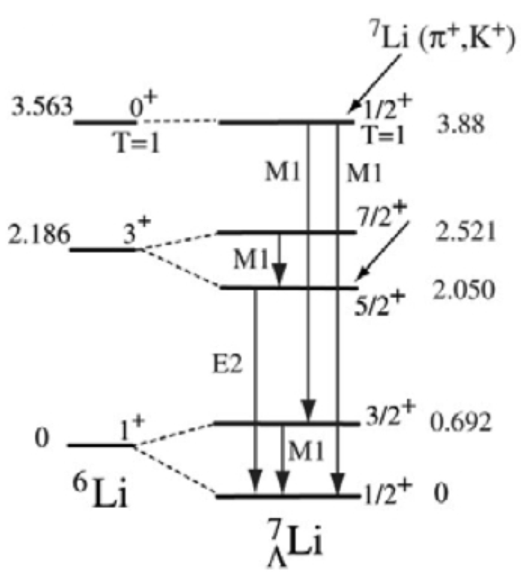
Hypernuclei

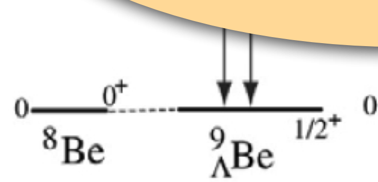
$N_f = 2 \rightarrow N_f = 3$

Ab Initio Hypernuclear Structure



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

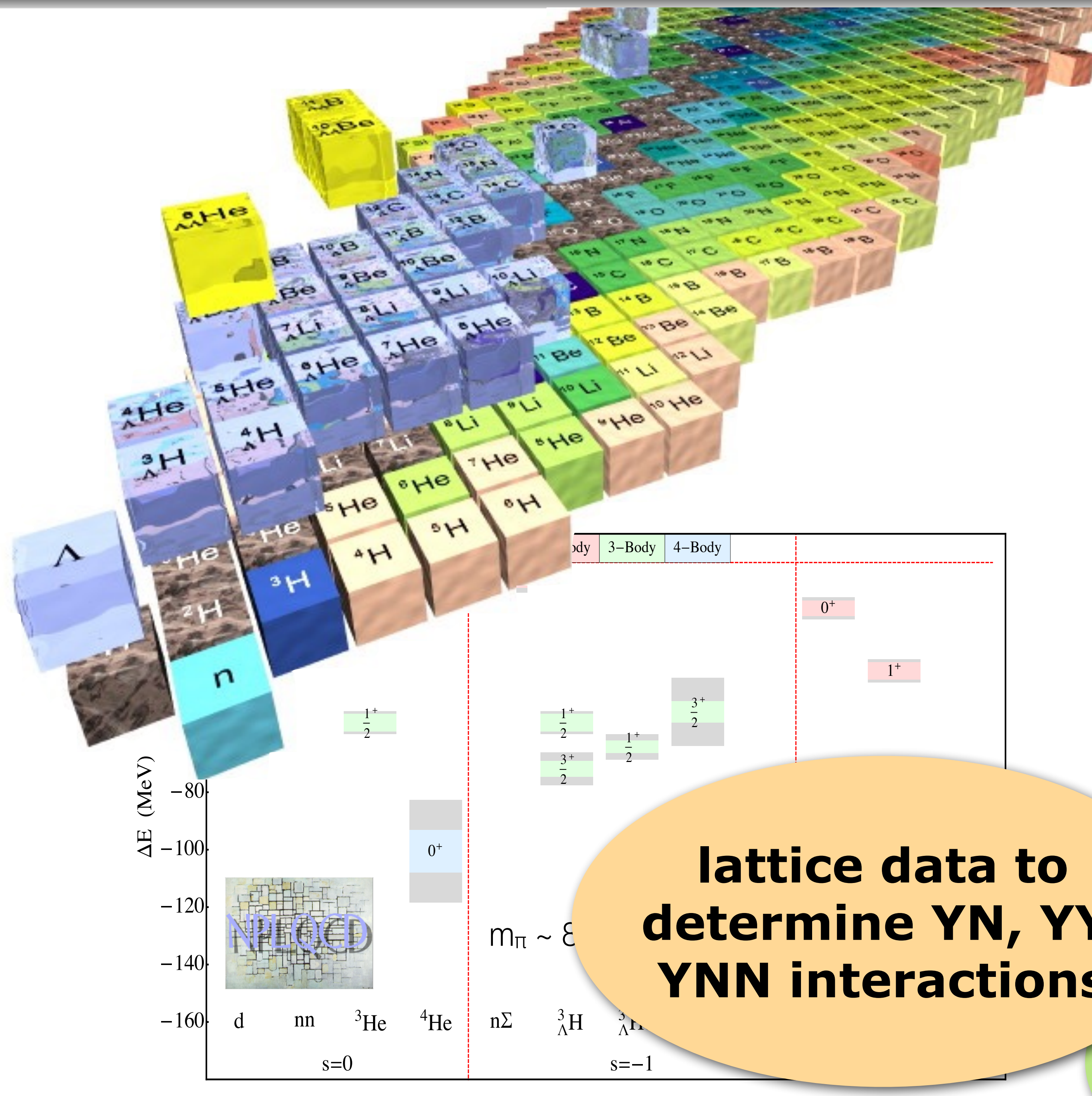




constrain YN interactions with hypernuclear spectroscopy

time to transfer ab initio toolbox to hypernuclei

Ab Initio Hypernuclear Structure



- Lattice QCD can be a game changer in hypernuclear physics
- extract YN & YY phase shifts from Lattice QCD, possibly also YNN
- compute light hypernuclei directly on the lattice

lattice data to determine YN, YY, YNN interactions

structure theory for consistency check and access to heavier hypernuclei

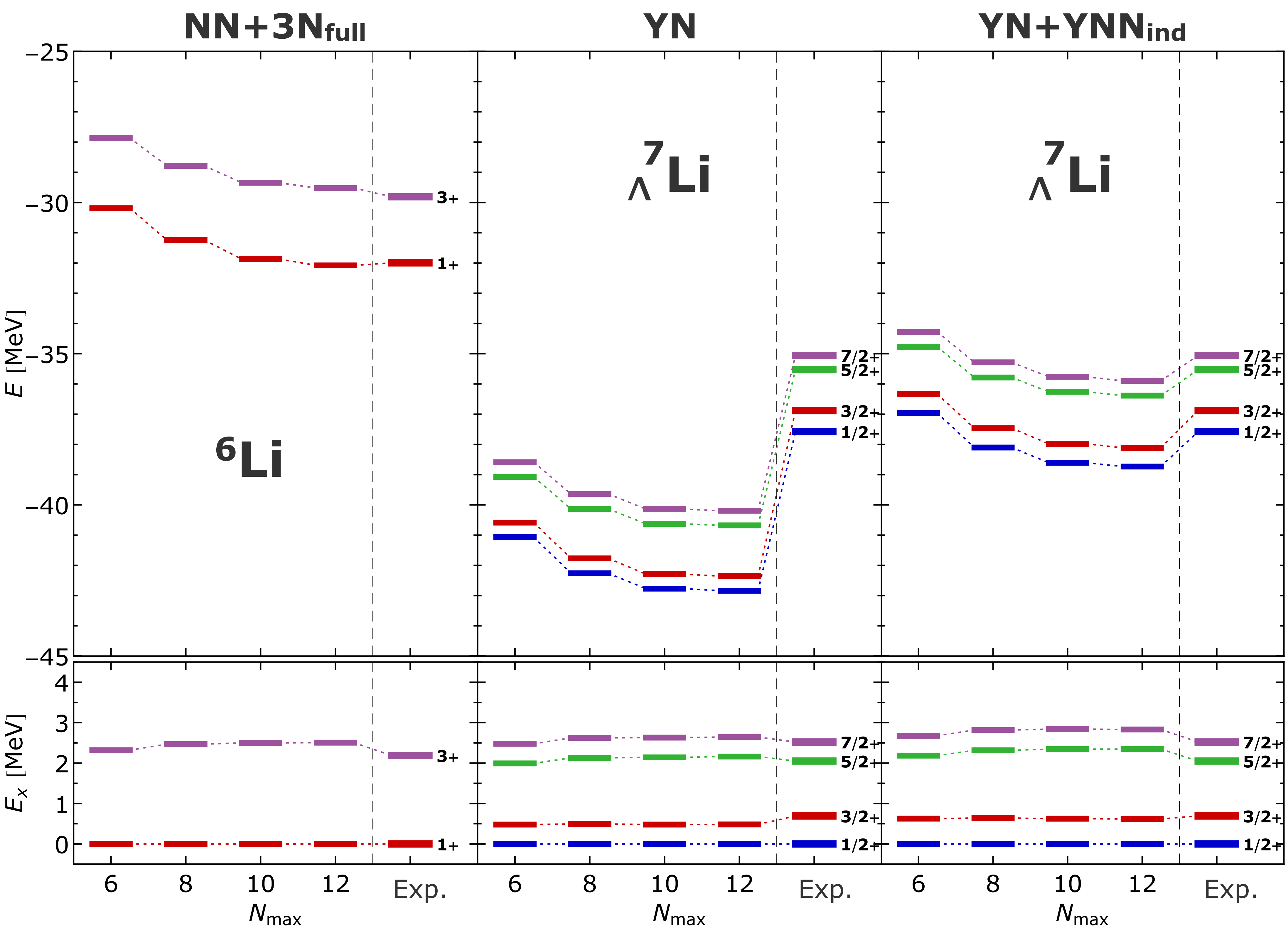
Ab Initio Toolbox for Hypernuclei

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 ΛΣ-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: ${}^{7}_{\Lambda}\mathrm{Li}$

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



IT-NCSM

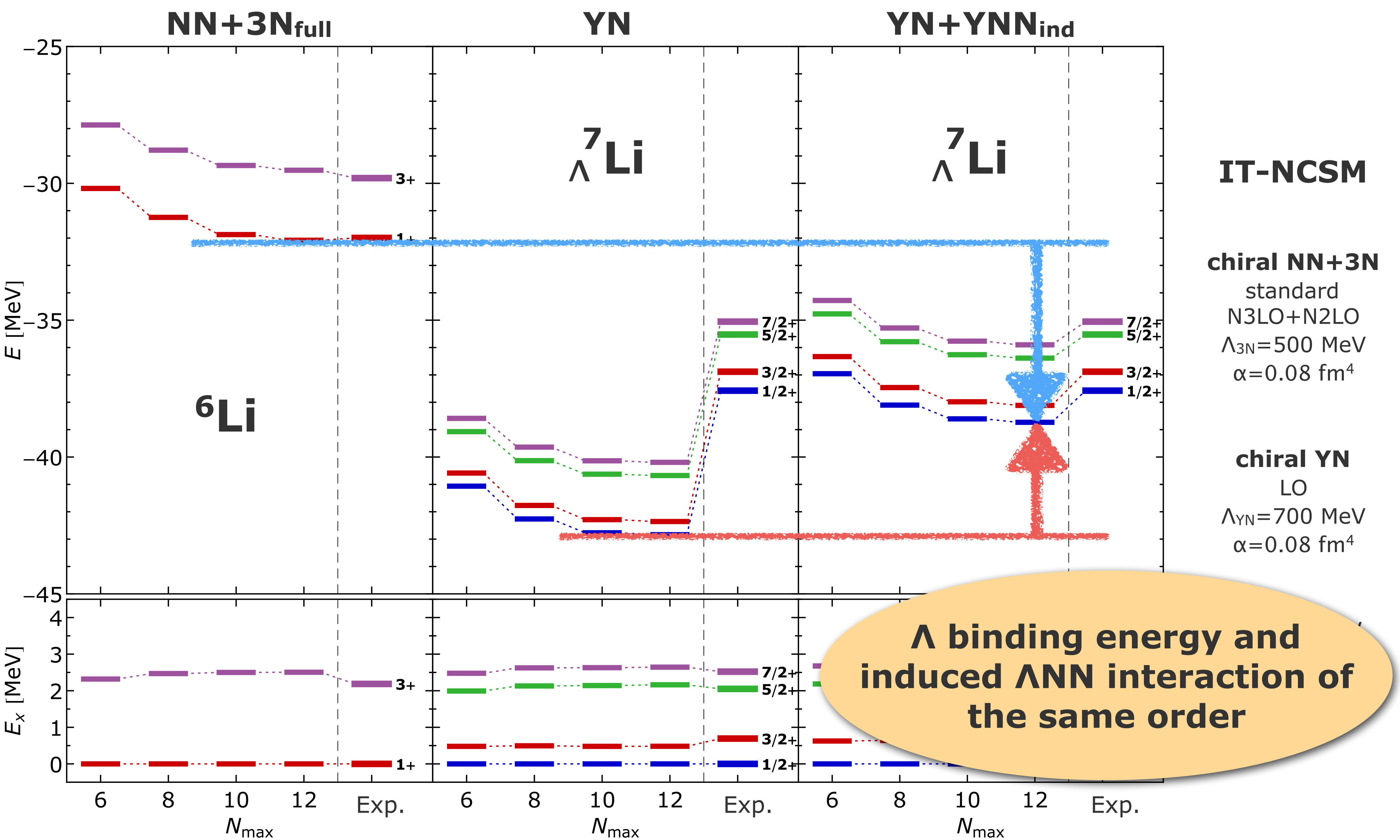
chiral NN+3N
standard
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm^4

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm^4

ħΩ=20 MeV

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

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



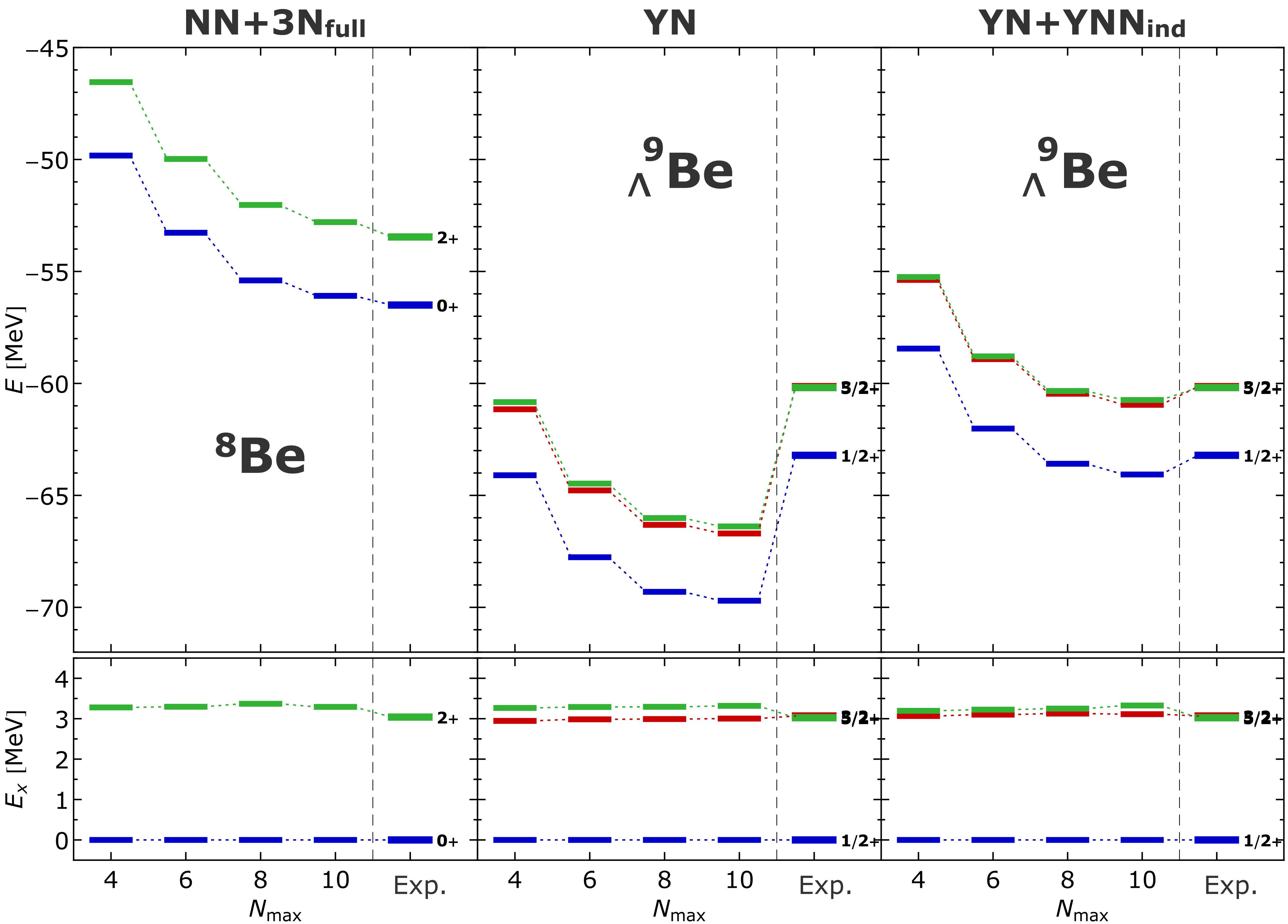
IT-NCSM

chiral NN+3N
standard
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm^4

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm^4

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

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



IT-NCSM

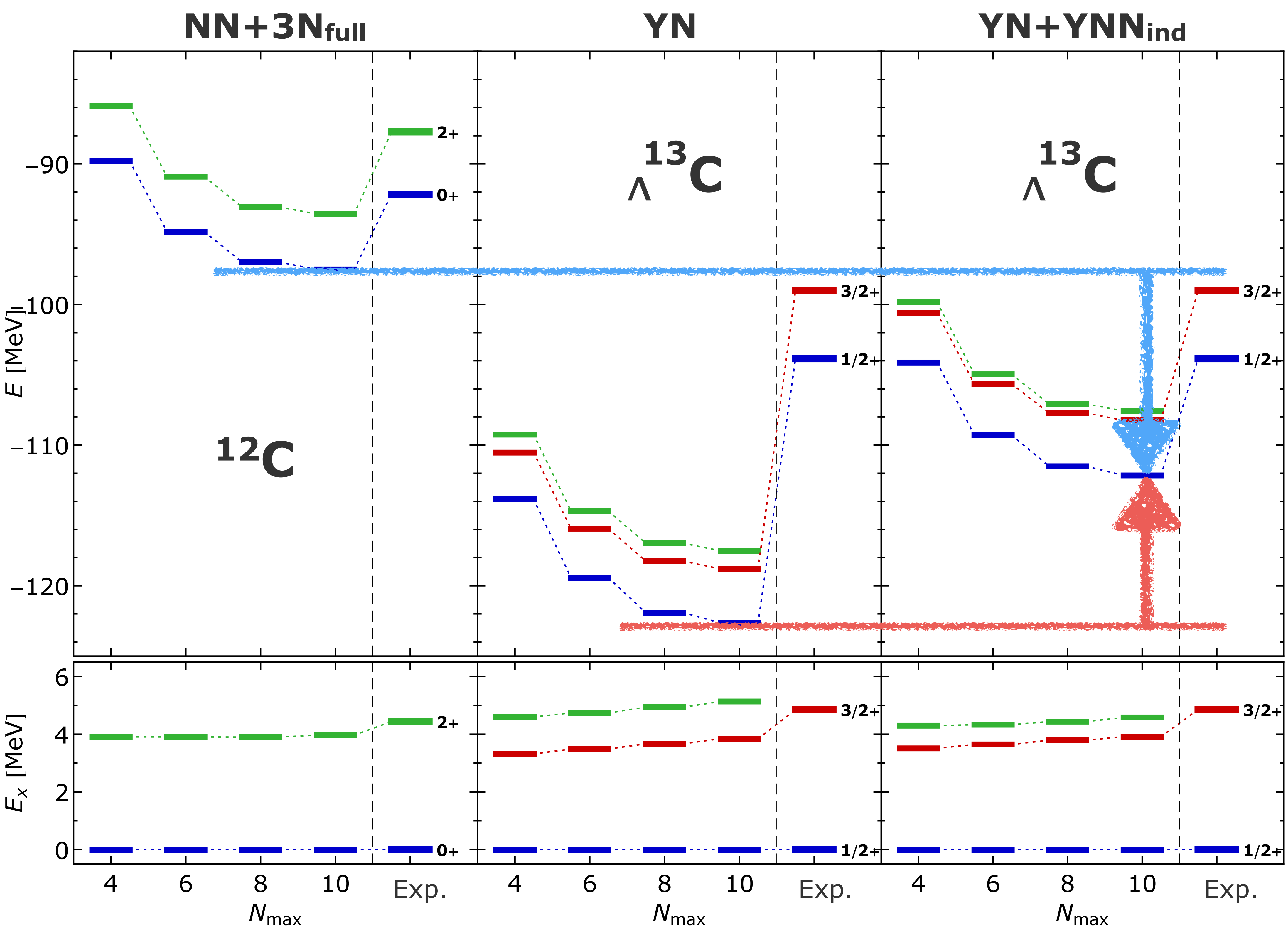
chiral NN+3N
standard
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm^4

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm^4

ħΩ=20 MeV

Application: ${}^{13}_{\Lambda}C$

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



IT-NCSM

chiral NN+3N
standard
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm⁴

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm⁴

ħΩ=20 MeV

Overview

- **Lecture 1: Hamiltonian**

  Prelude • Nuclear Hamiltonian • Matrix Elements • Two-Body Problem • Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**

  Similarity Renormalization Group • Many-Body Problem • Configuration Interaction • No-Core Shell Model • Hypernuclei

- **Lecture 3: Beyond Light Nuclei**

  Normal Ordering • Coupled-Cluster Theory • In-Medium Similarity Renormalization Group

- **Hands-On: Do-It-Yourself NCSM**

  Three-Body Problem • Numerical SRG Evolution • NCSM Eigenvalue Problem • Lanczos Algorithm