Ab Initio Calculations of Nuclear Structure

Lecture 2: Light Nuclei

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Overview

- **Lecture 1: Hamiltonian**

  Prelude • Many-Body Quantum Mechanics • 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 • Basis Optimization

- **Lecture 3: Medium-Mass Nuclei**

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

- **Project: Do-It-Yourself NCSM**

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

- **Lecture 4: Precision, Uncertainties, and Applications**

  Chiral Interactions for Precision Calculations • Uncertainty Quantification • Applications to Nuclei and Hypernuclei

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

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

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

- we thus obtain for the derivative of the transformed Hamiltonian

$$\begin{aligned} \frac{d}{d\alpha} \mathrm{H}_\alpha &= \eta_\alpha \mathrm{H}_\alpha - \mathrm{H}_\alpha \eta_\alpha \\ &= \left[\eta_\alpha, \mathrm{H}_\alpha \right] \end{aligned}$$

  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

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

- 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 $\quad |Ei J^\pi T\rangle$

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

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle Eij^\pi T|\,\mathrm{H}_\alpha\,|E'i'J^\pi T\rangle = (2\mu)^2 \sum_{E'',i''}^{E_{\mathrm{SRG}}} \sum_{E''',i'''}^{E_{\mathrm{SRG}}} \Big[$$

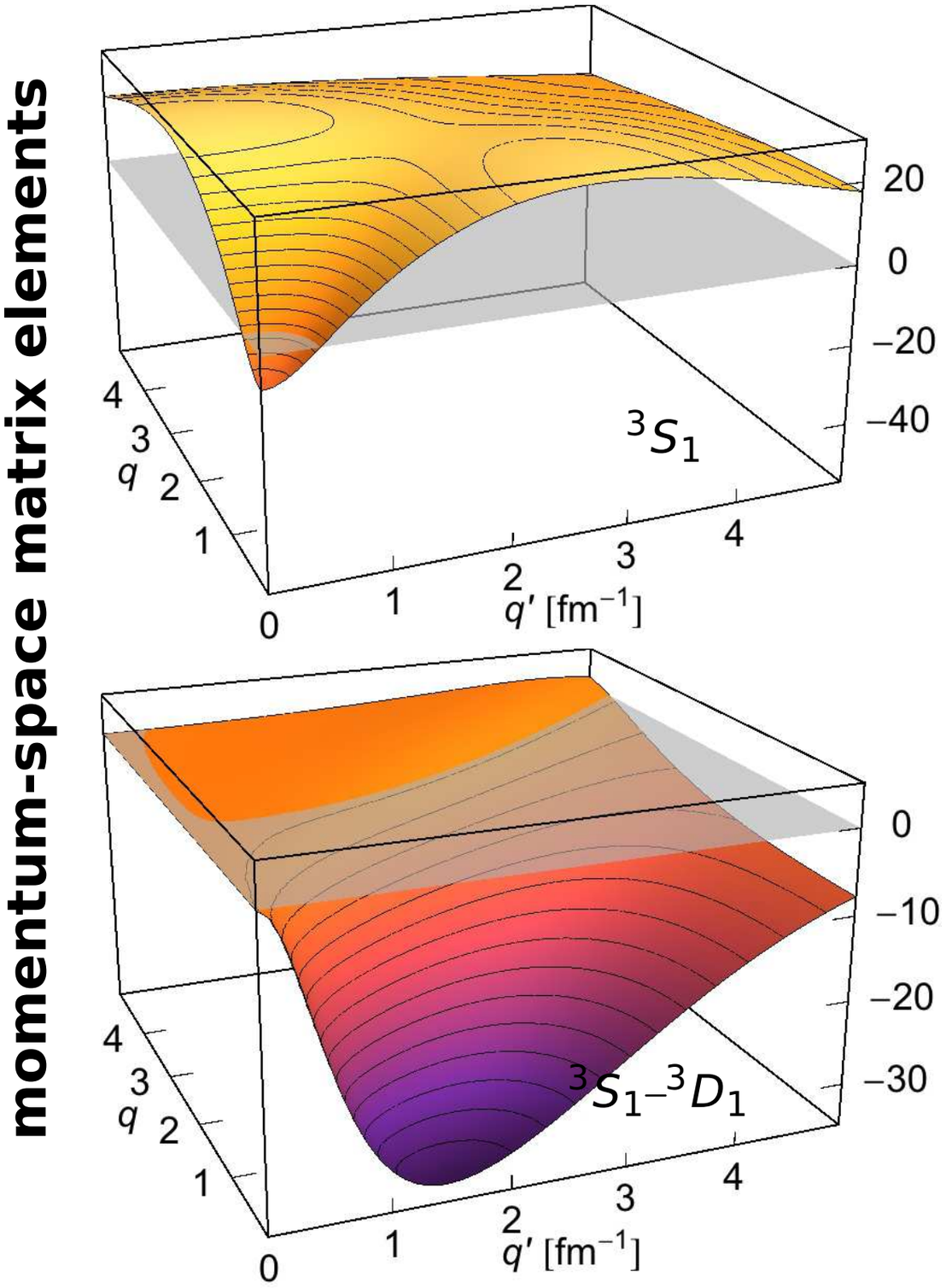
$$\langle Ei\ldots|\,\mathrm{T}_{\mathrm{int}}\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{H}_\alpha\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{H}_\alpha\,|E'i'\ldots\rangle$$

$$-2\langle Ei\ldots|\,\mathrm{H}_\alpha\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{T}_{\mathrm{int}}\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{H}_\alpha\,|E'i'\ldots\rangle$$

$$+\langle Ei\ldots|\,\mathrm{H}_\alpha\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{H}_\alpha\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{T}_{\mathrm{int}}\,|E'i'\ldots\rangle\Big]$$

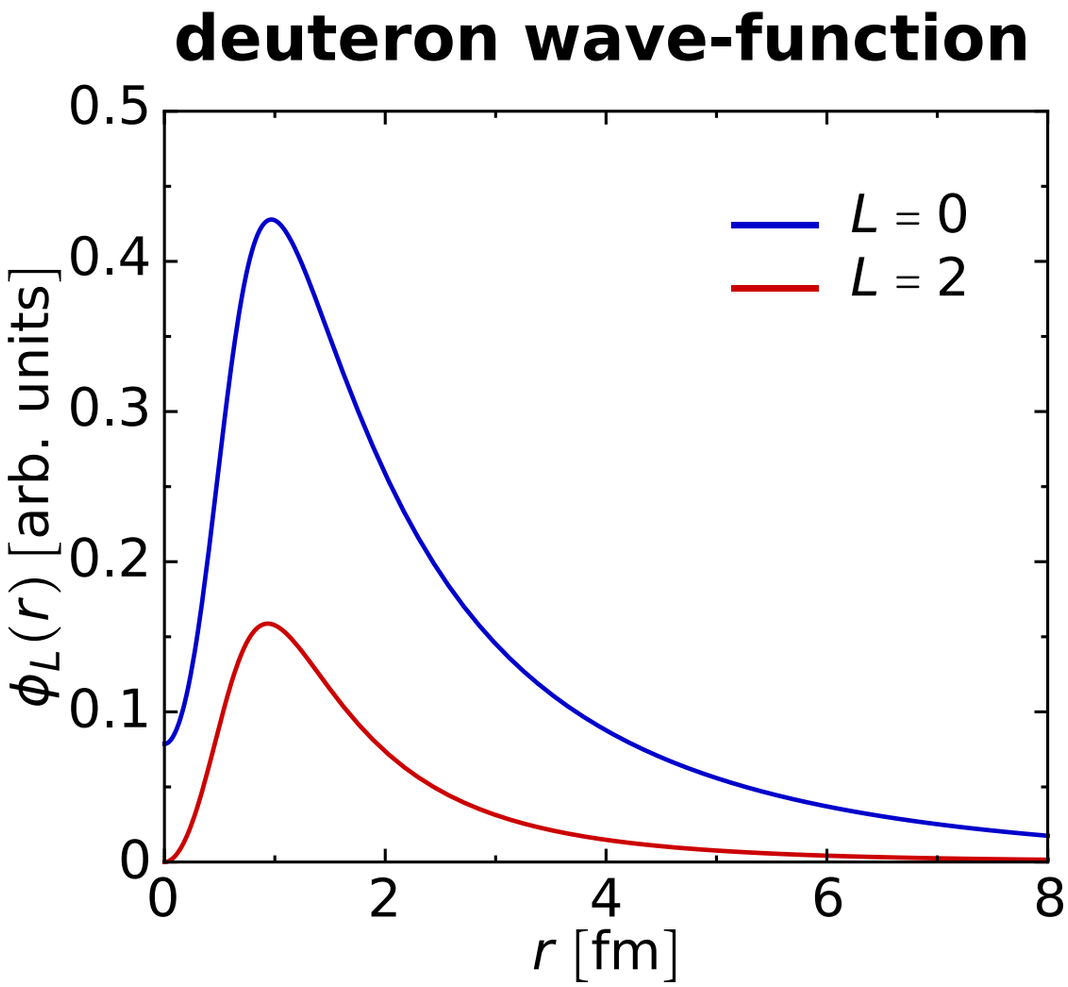
- **note**: when using *n*-body matrix elements, components of the evolved Hamiltonian with particle-rank > *n* are discarded

SRG Evolution in Two-Body Space



Argonne V18

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



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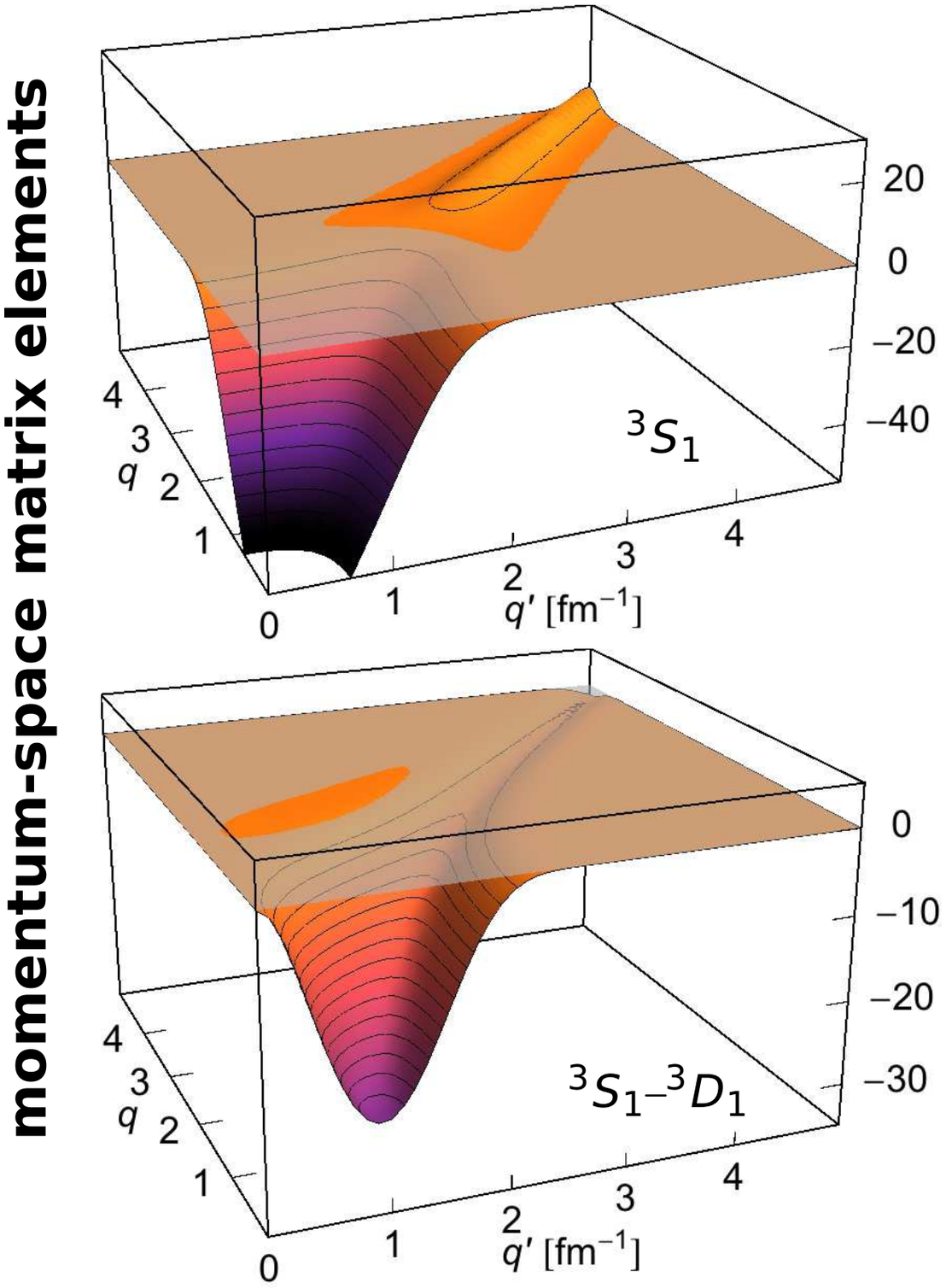
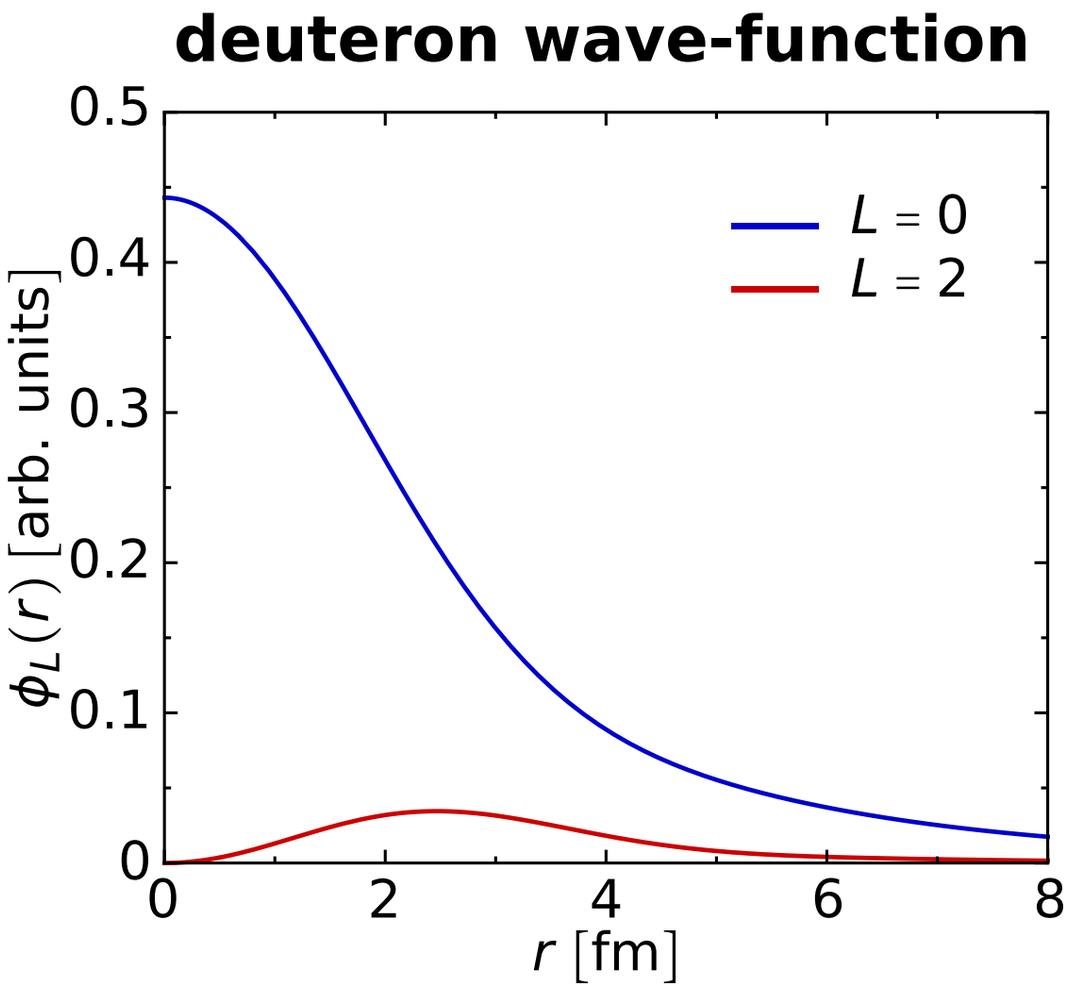


$$\alpha = 0.160\,\mathrm{fm}^4$$

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

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



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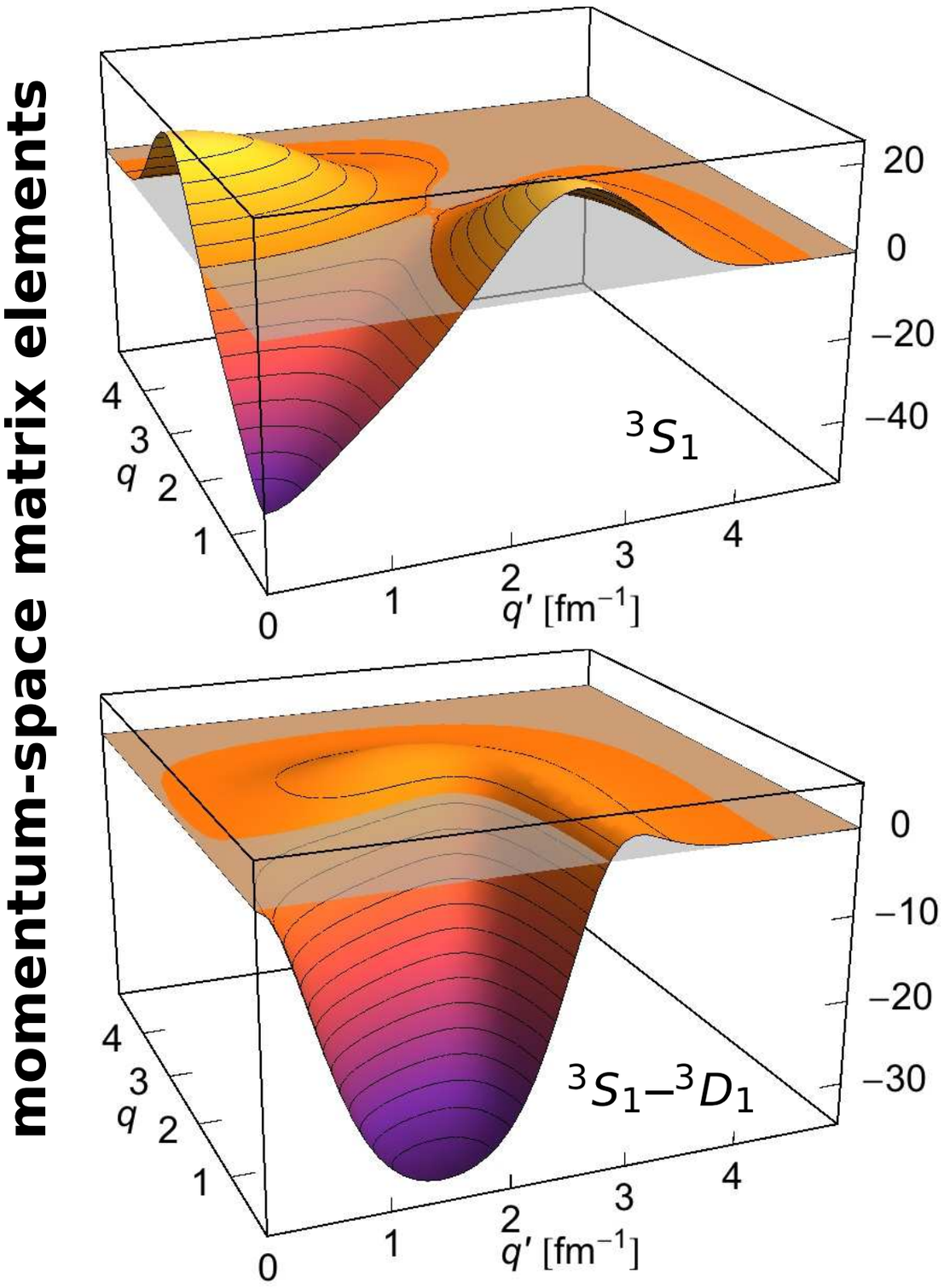
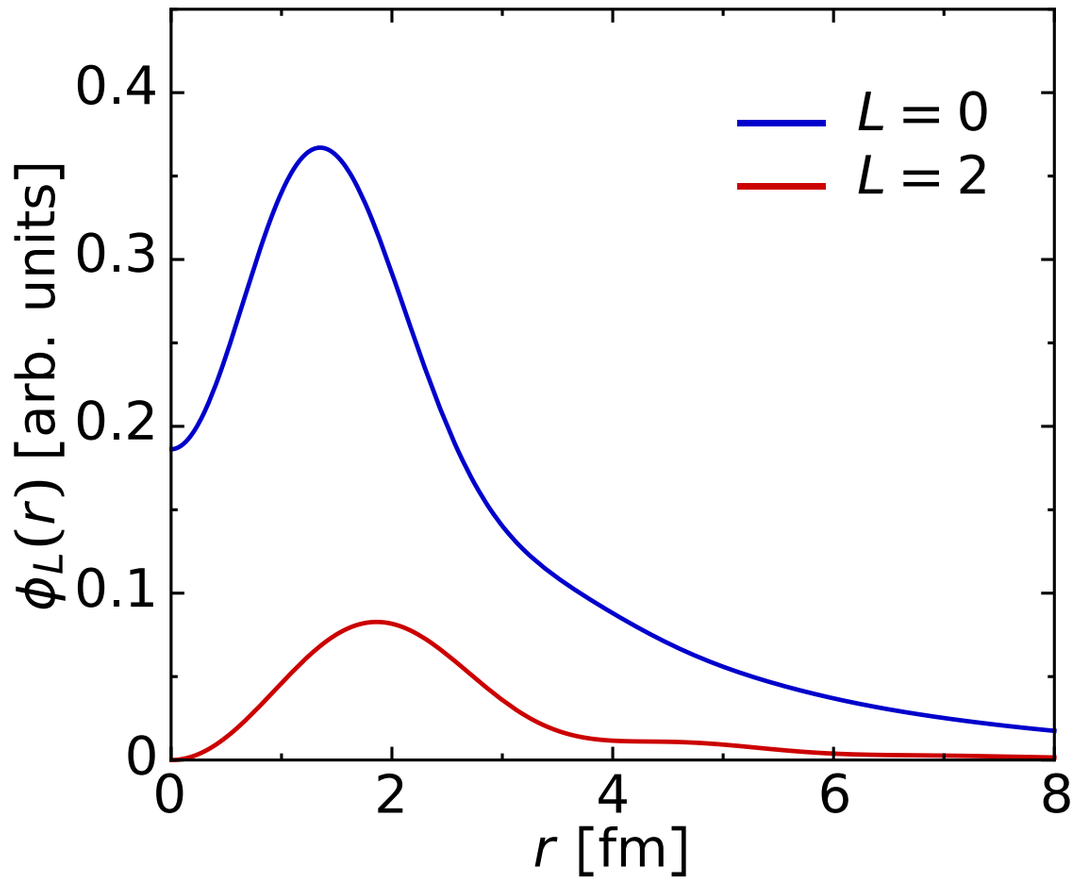


chiral NN

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

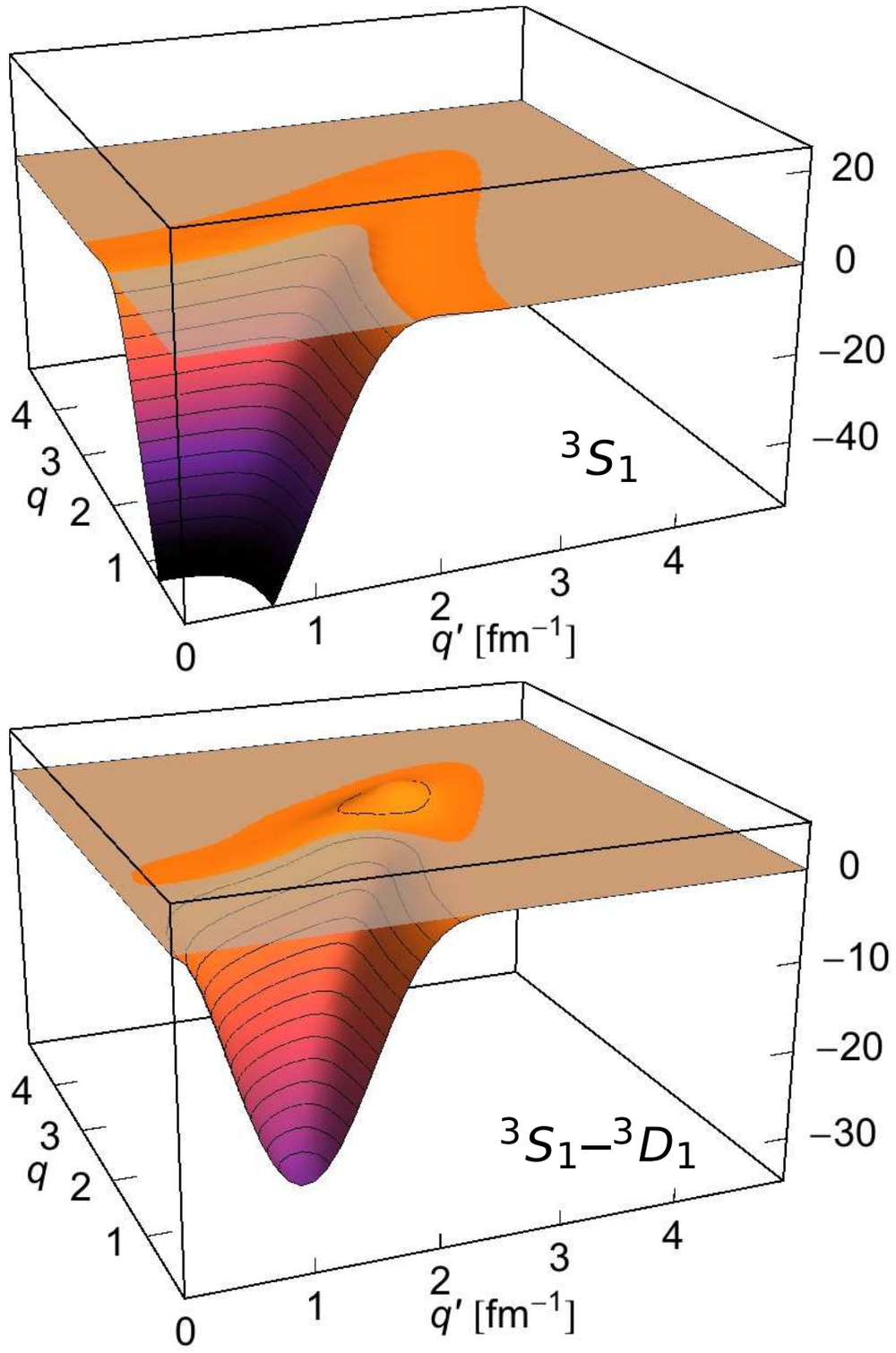
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements



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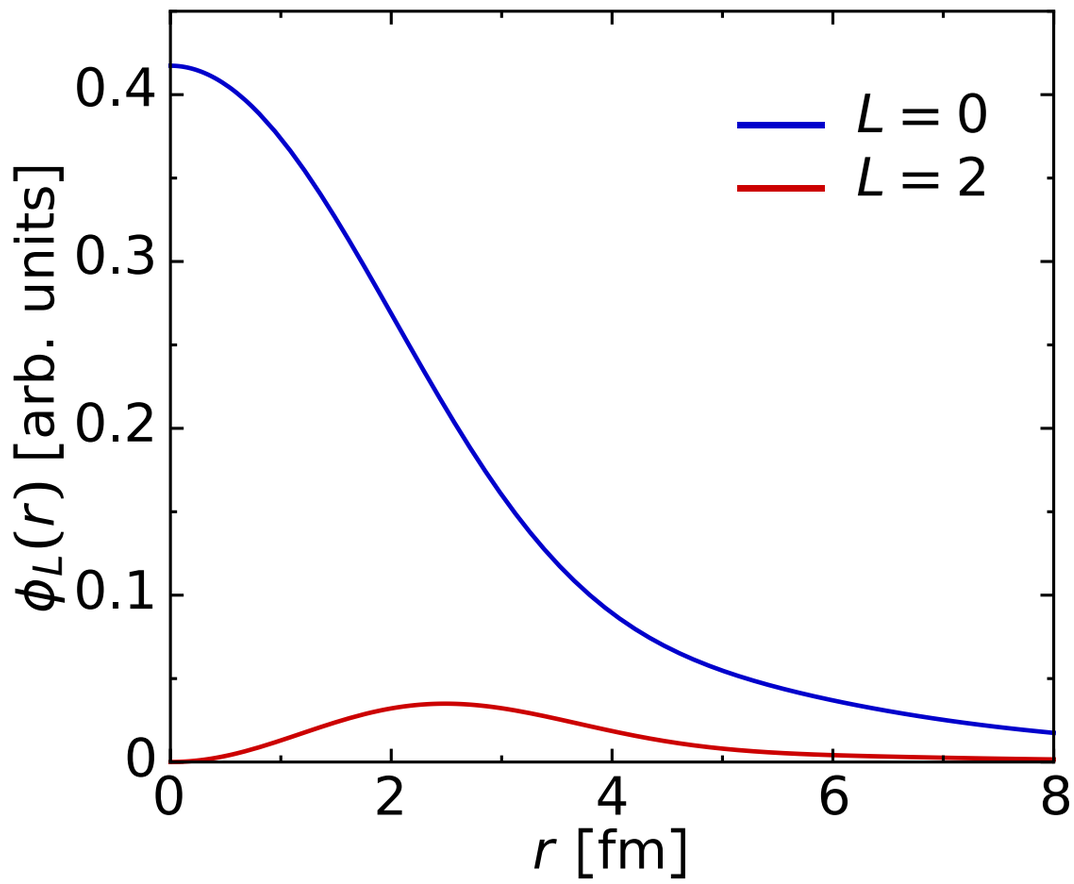
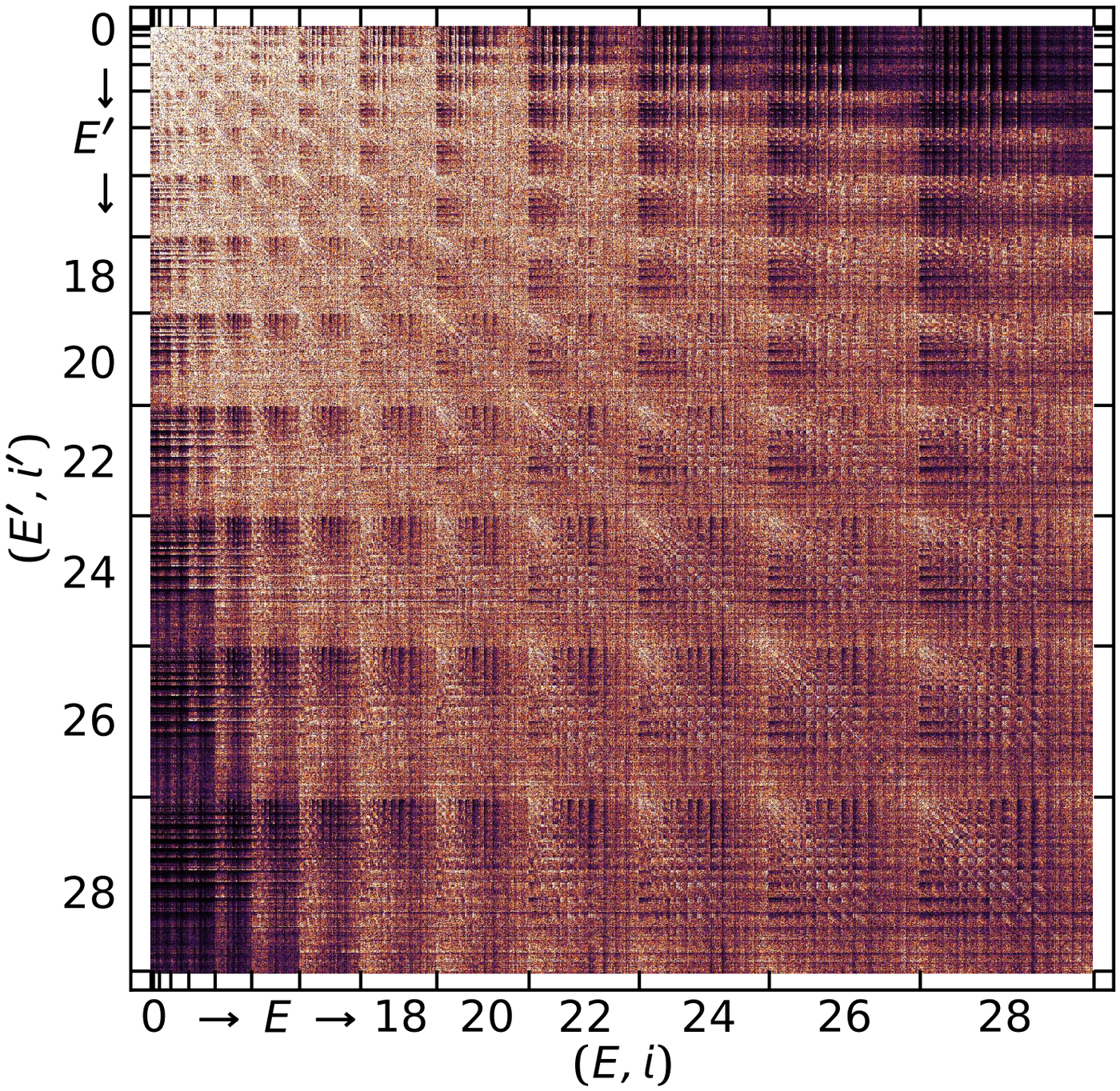


SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

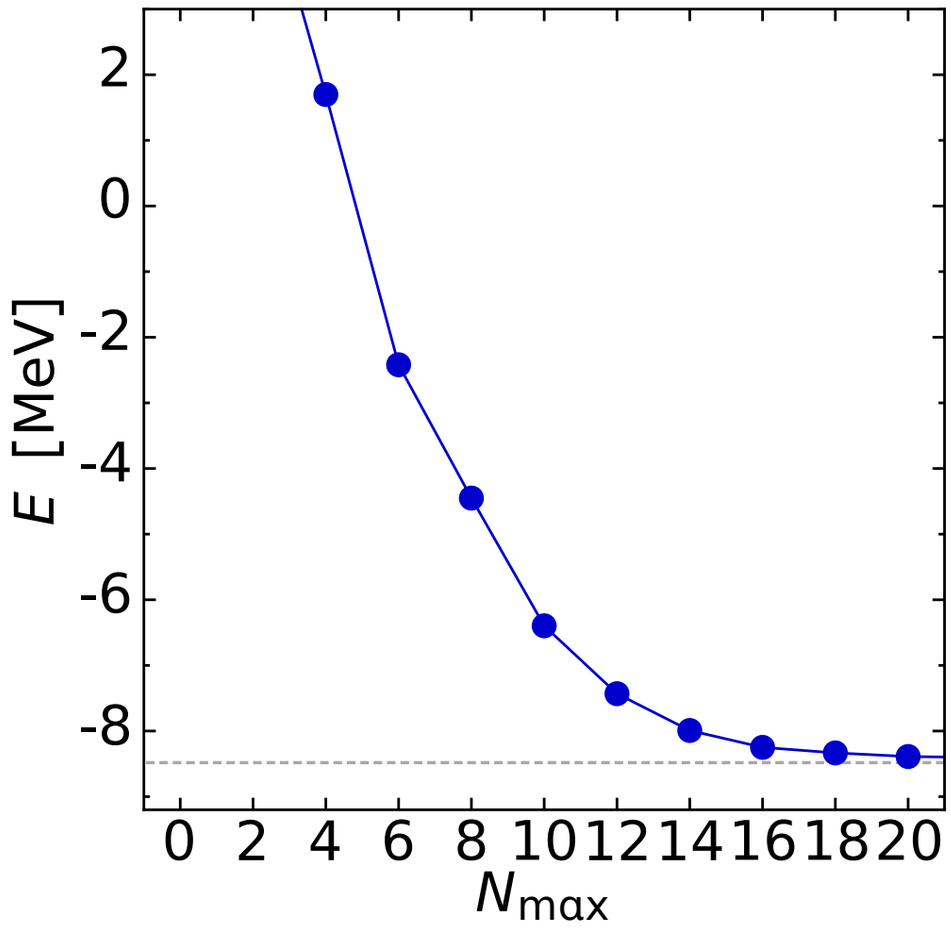


chiral NN+3N

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

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

NCSM ground state ^{3}H



SRG Evolution in Three-Body Space

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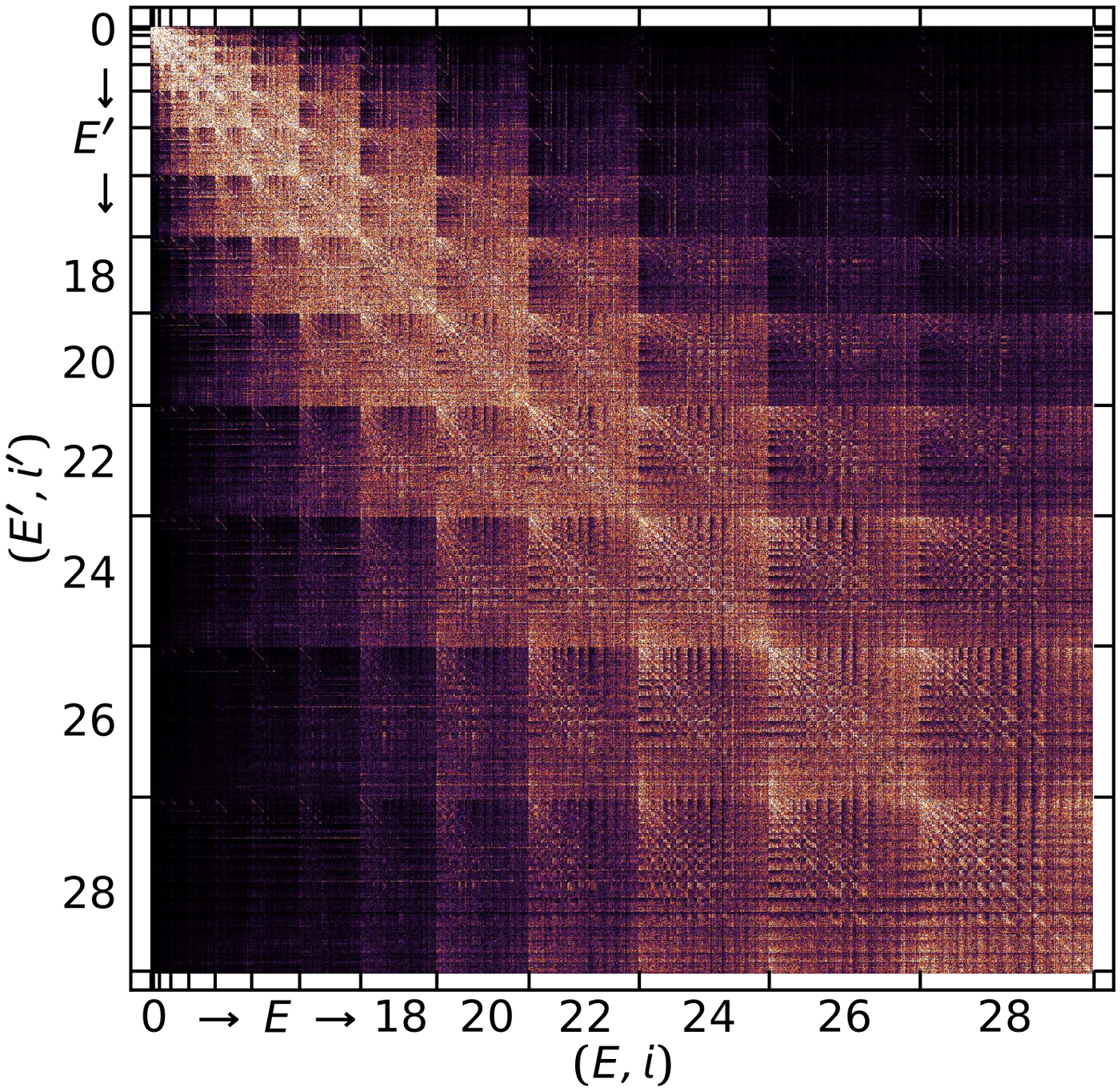

$$\alpha = 0.160\,\mathrm{fm}^4$$

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

NCSM ground state ^{3}H

SRG Evolution in A-Body Space

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

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

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

$$\begin{aligned} H_{\Delta\alpha} &= H_0 + \Delta\alpha \, \big[\big[T_{\rm int}, H_0\big], H_0\big] \\ &= \sum \ldots a^\dagger a^\dagger a a + \Delta\alpha \sum \ldots \big[\big[a^\dagger a^\dagger a a, a^\dagger a^\dagger a a\big], a^\dagger a^\dagger a a\big] \\ &= \sum \ldots a^\dagger a^\dagger a a + \Delta\alpha \sum \ldots a^\dagger a^\dagger a^\dagger a^\dagger a a a a + \Delta\alpha \sum \ldots a^\dagger a^\dagger a^\dagger a a a a + \ldots \end{aligned}$$

- 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

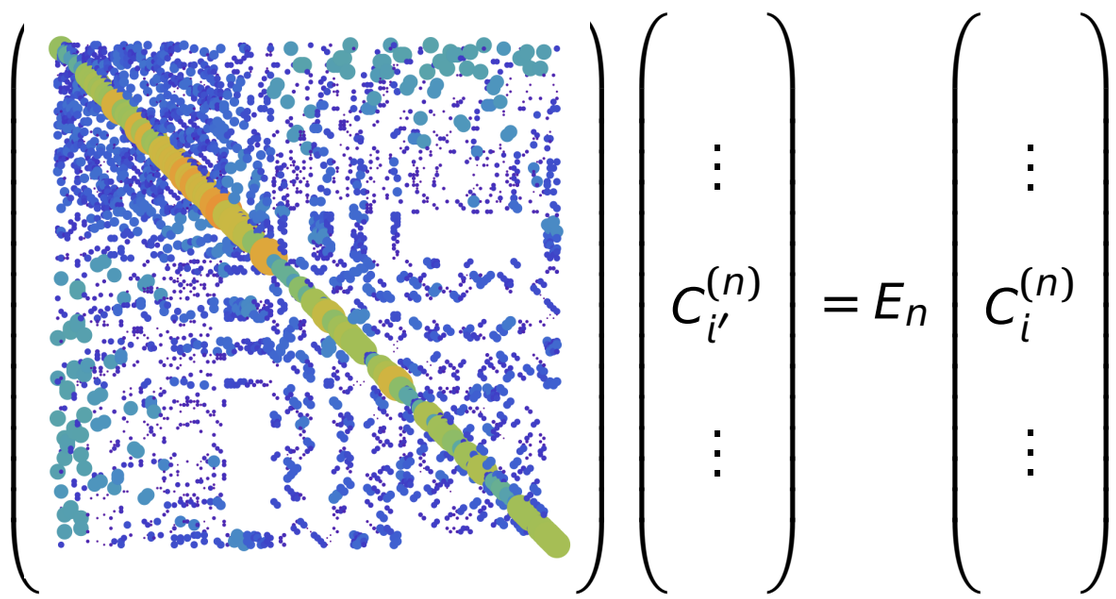
$NN+3N_{ind}$: use initial NN, keep evolved NN+3N

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

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

Many-Body Problem

Configuration Interaction Approaches



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

Configuration Interaction (CI)

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

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

- 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

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

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

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

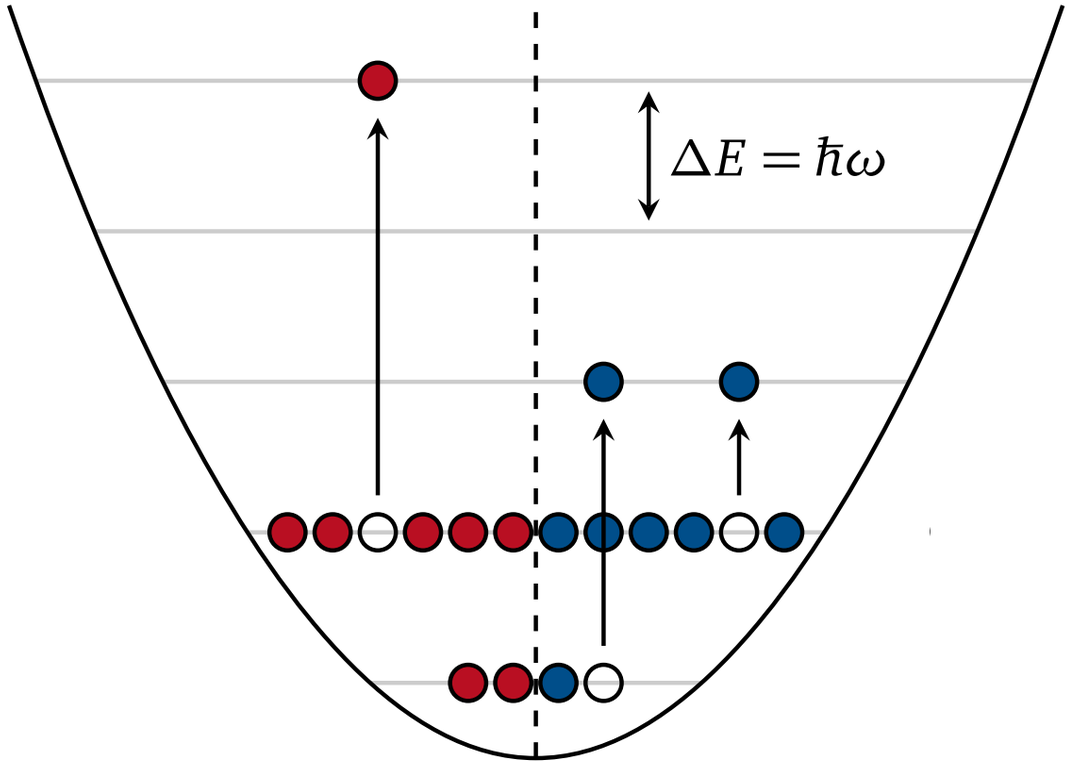
- **extrapolations**: extrapolate observables to infinite model-space from a sequence of finite-space calculations

- **uncertainty quantification**: extract many-body uncertainty from residual model-space dependence or extrapolation

No-Core Shell Model

No-Core Shell Model (NCSM)

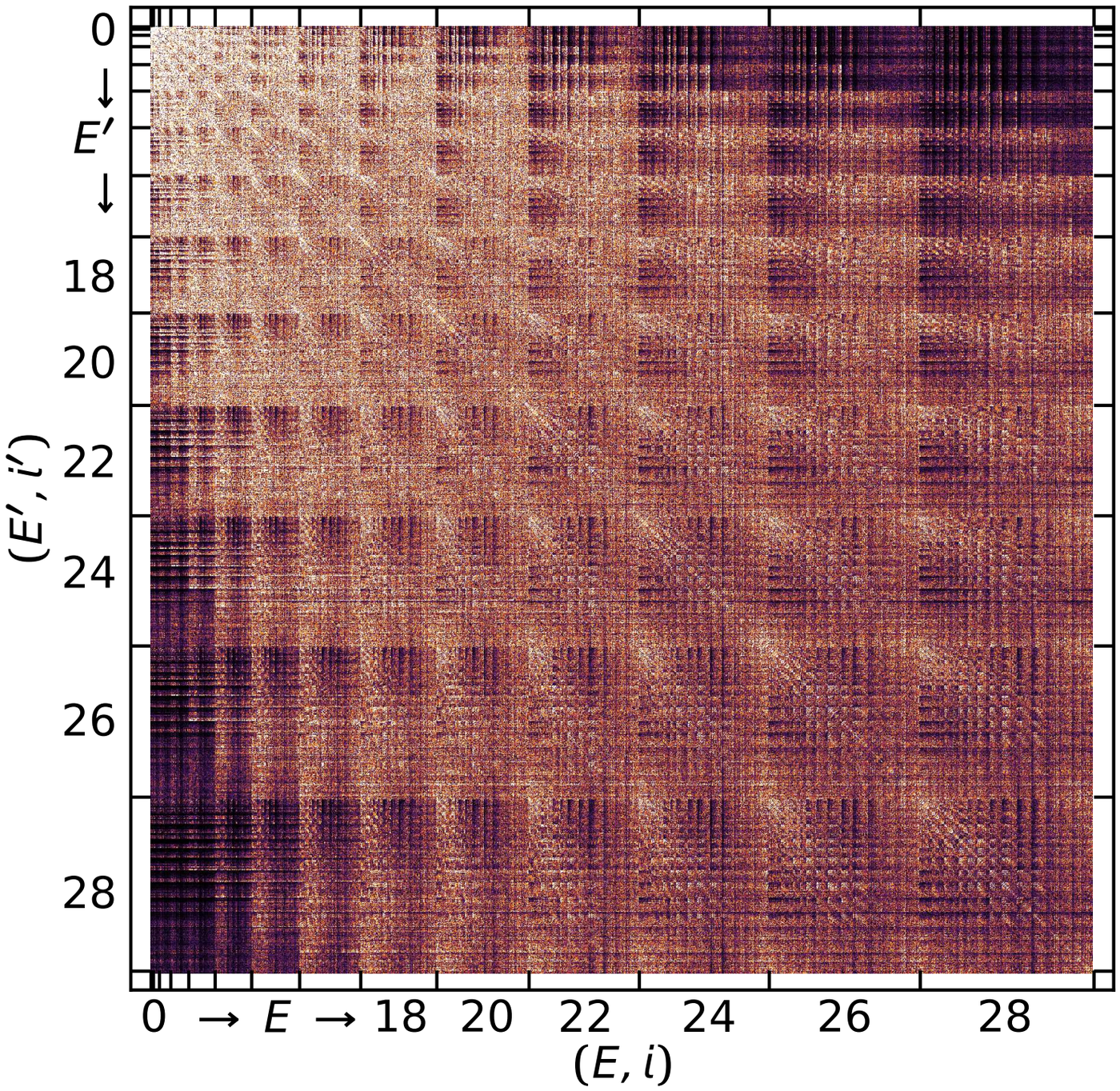
- special case of a CI approach:
  - single-particle basis is a **spherical HO basis**
  - truncation in terms of the total **number of HO excitation quanta** N_{max} in the many-body states



- **technical advantages** of the NCSM:
  - many-body energy truncation (N_{max}) truncation is much **more efficient** than single-particle energy truncation (e_{max}, cf. FCI)
  - equivalent NCSM formulation in **relative / Jacobi coordinates** for each N_{max}
  - **explicit separation** of center of mass and intrinsic motion for each N_{max}

NCSM Model-Space Convergence

3B-Jacobi HO matrix elements



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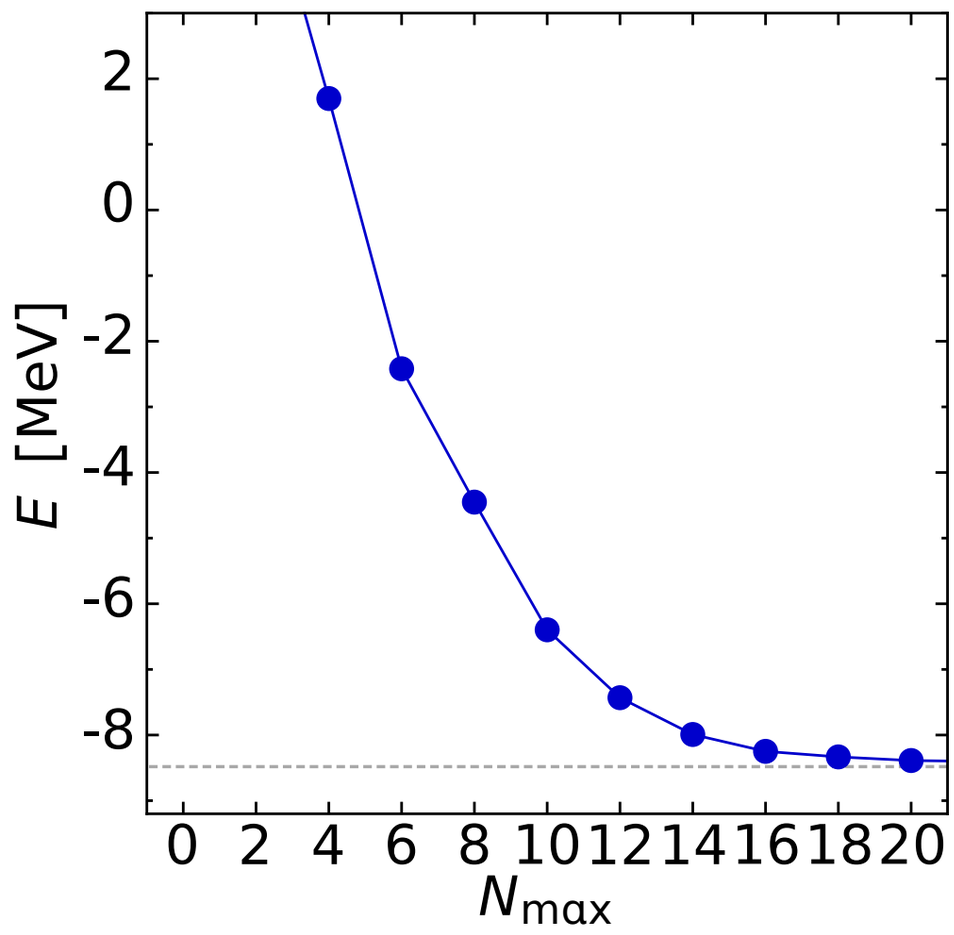
NCSM ground state ^{3}H



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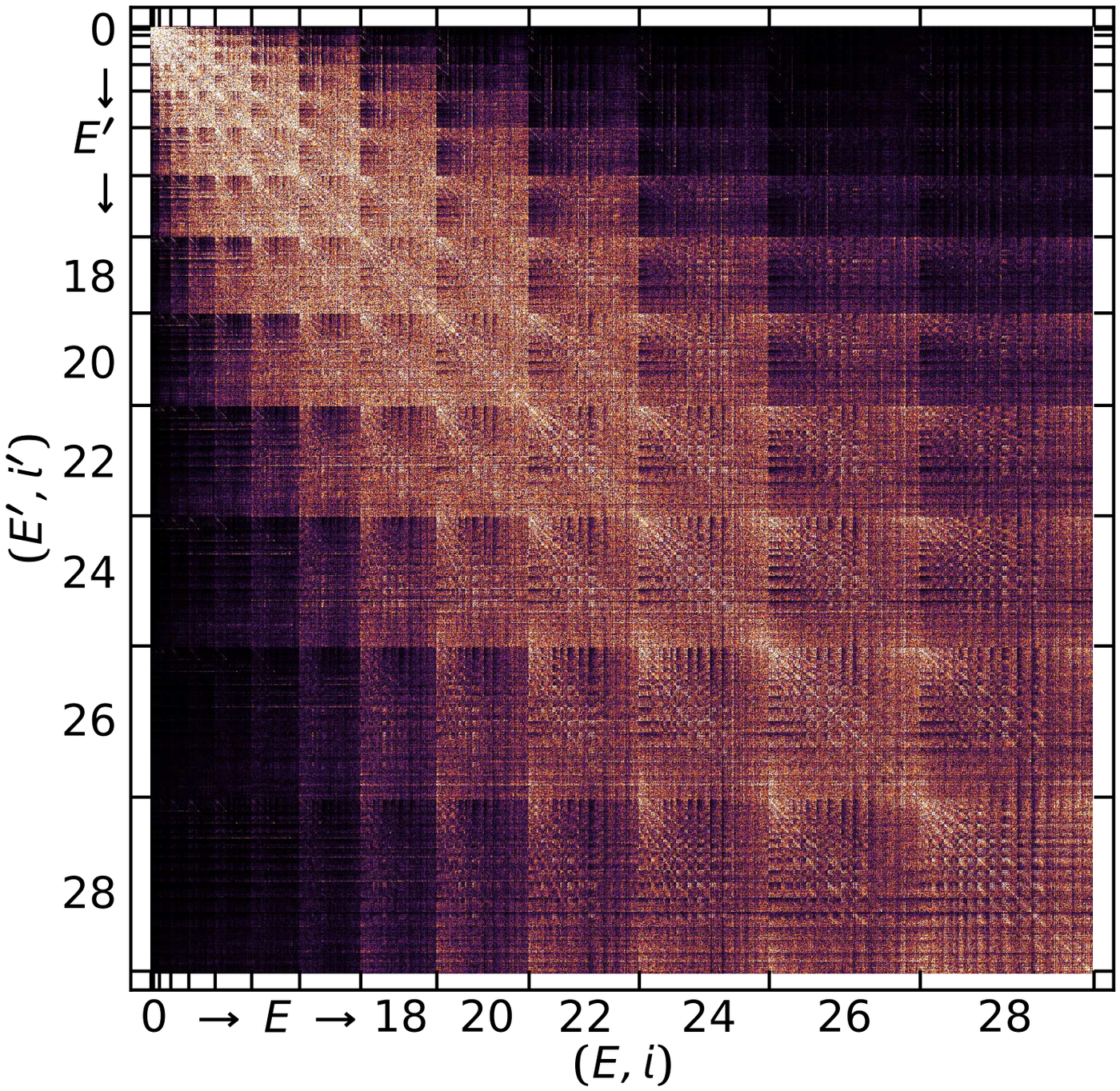


$$\alpha = 0.080\,\mathrm{fm}^4$$

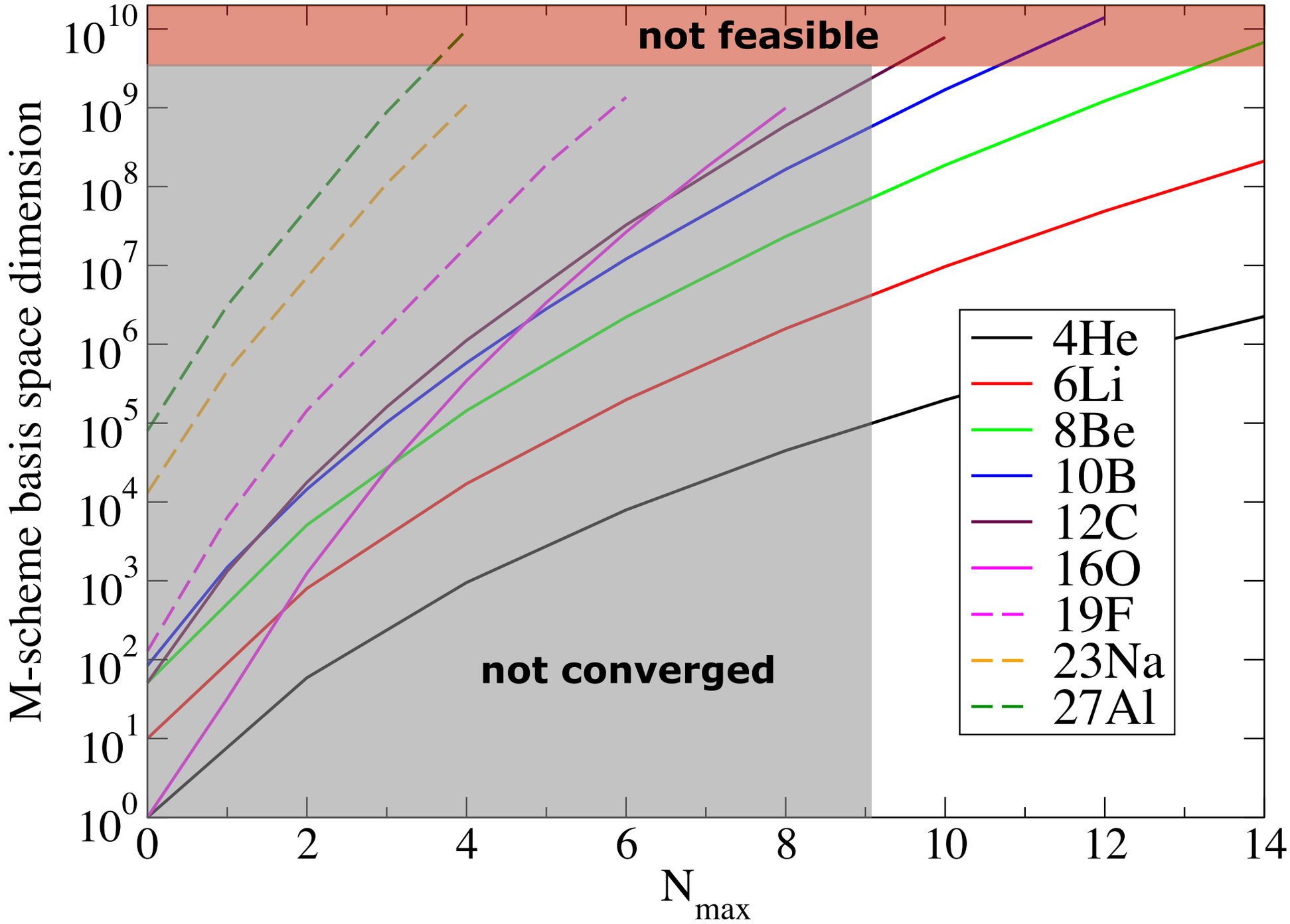
$\Lambda = 1.88\,\mathrm{fm}^{-1}$

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

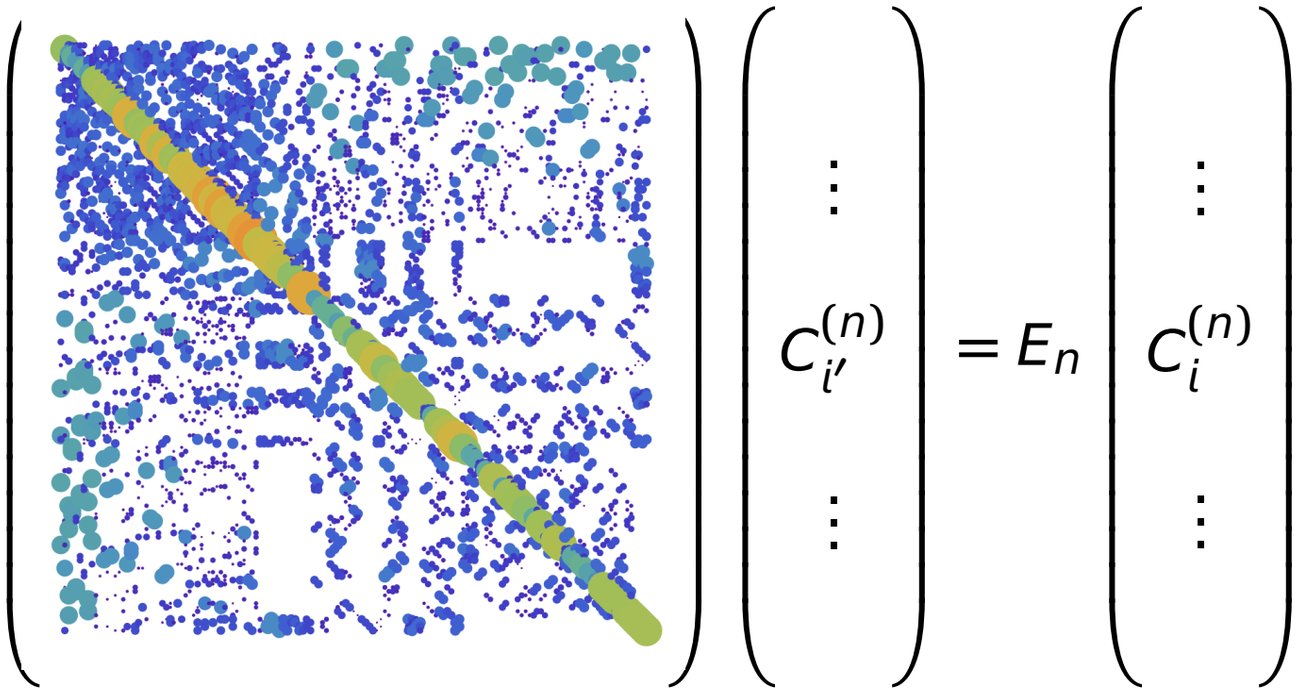
NCSM ground state ^{3}H

NCSM Basis Dimension

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



Computational Strategy



- **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**

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

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

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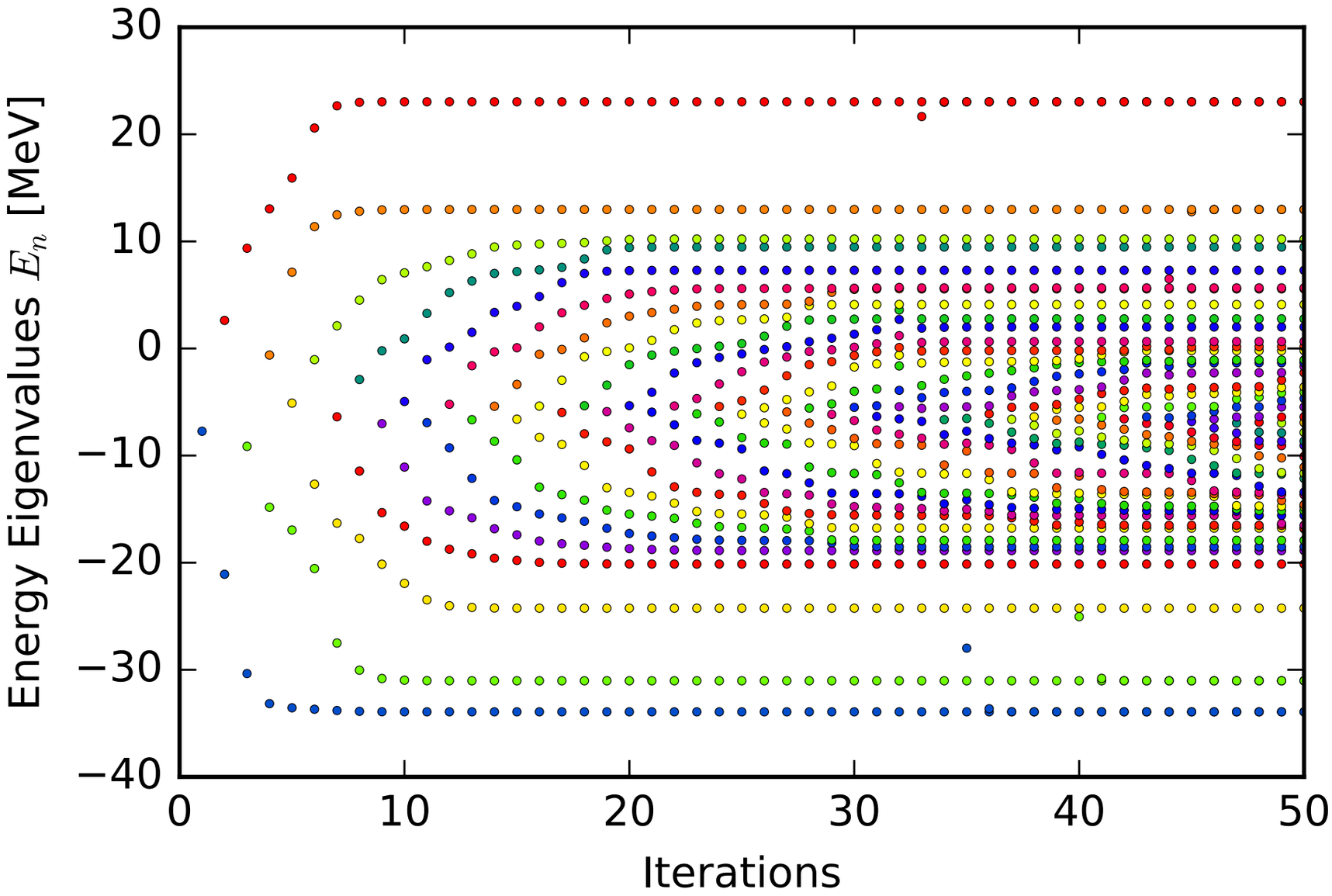
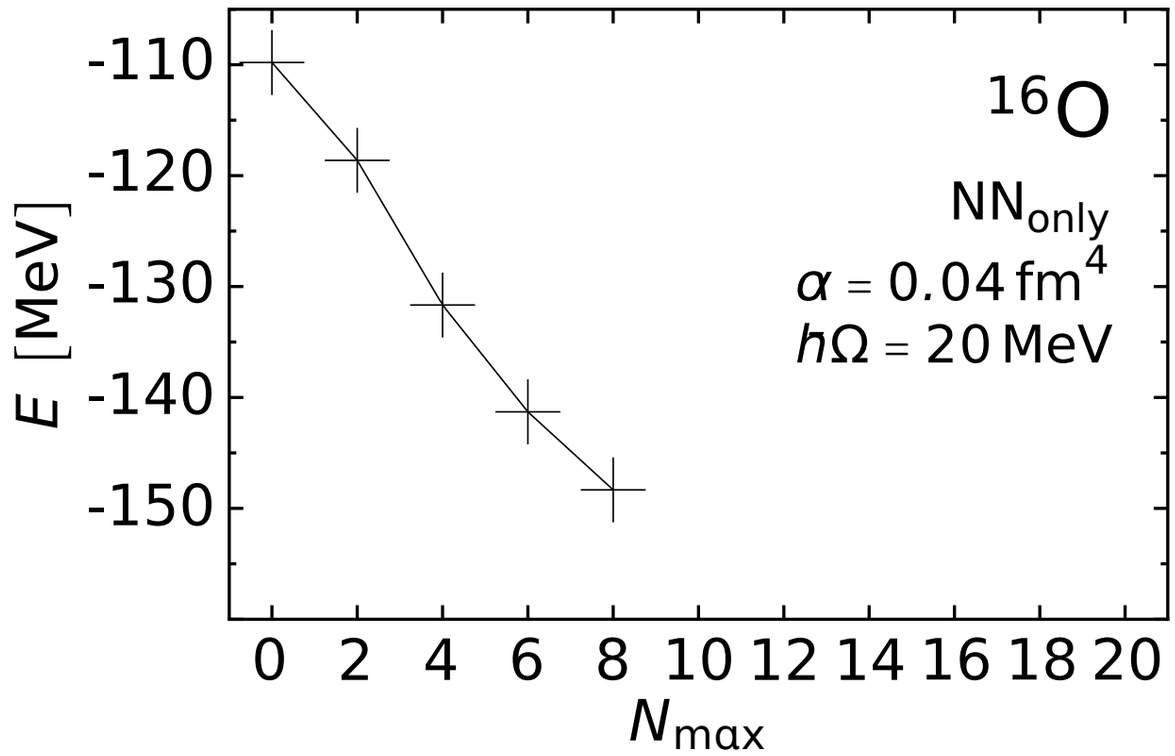


Importance Truncation

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

Roth, PRC 79, 064324 (2009)

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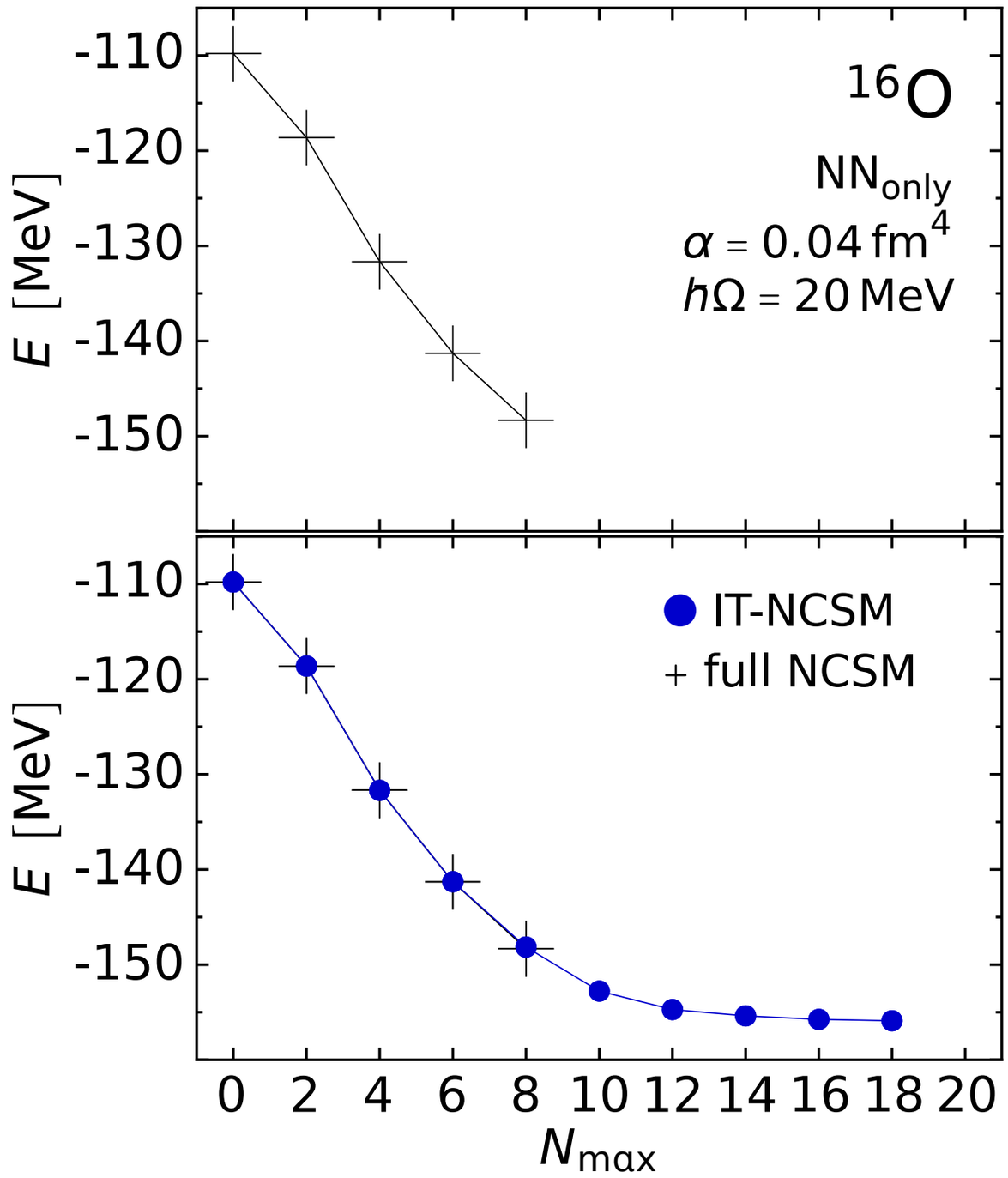
Importance Truncation

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



Importance Truncation

Roth, PRC 79, 064324 (2009)

- **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

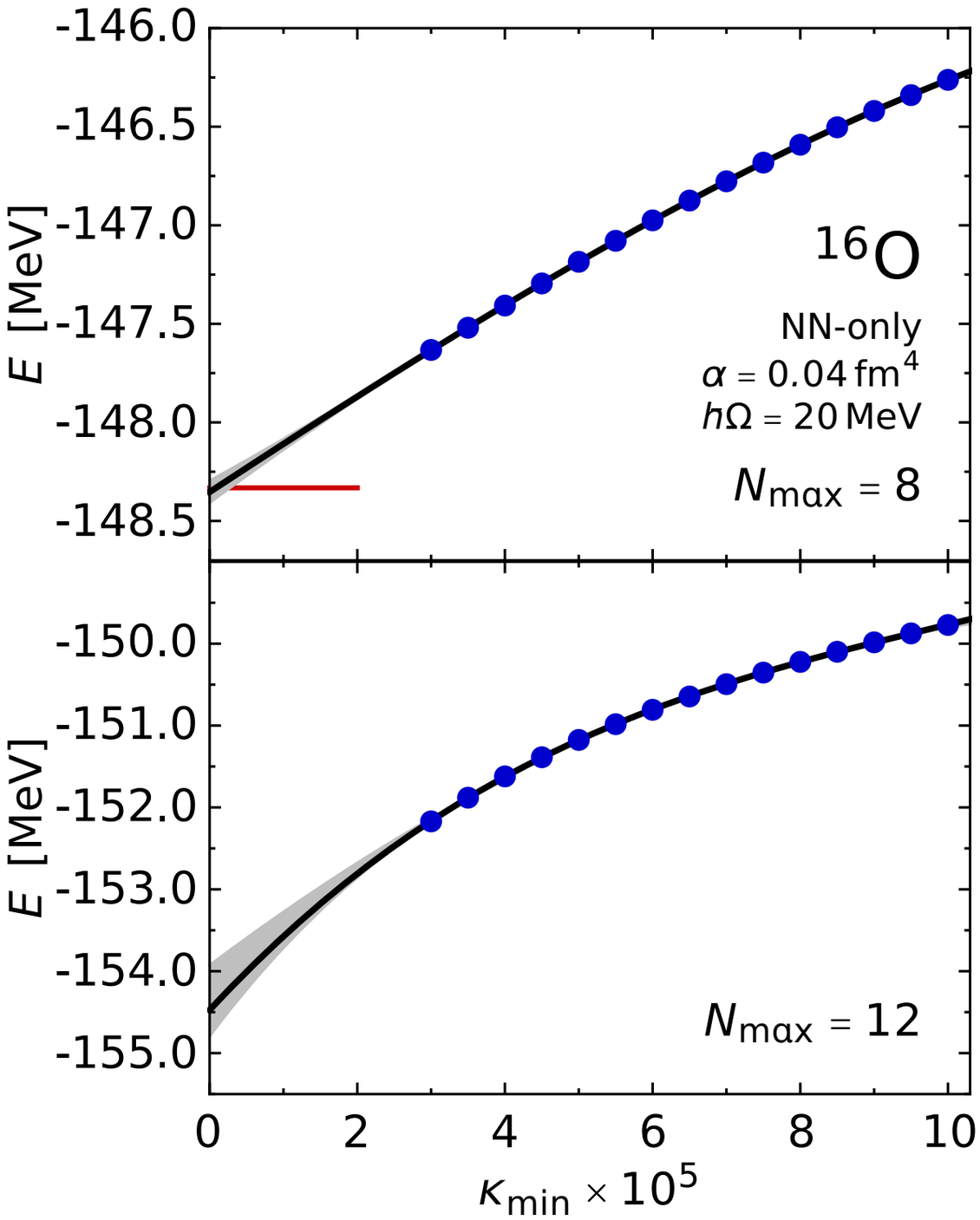
$$\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\Delta\epsilon_\nu}$$

- 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

Roth, PRC 79, 064324 (2009)



- repeat calculations for a **sequence of importance thresholds** $\kappa_{\min}$
- 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

Basis Optimization

Single-Particle Basis

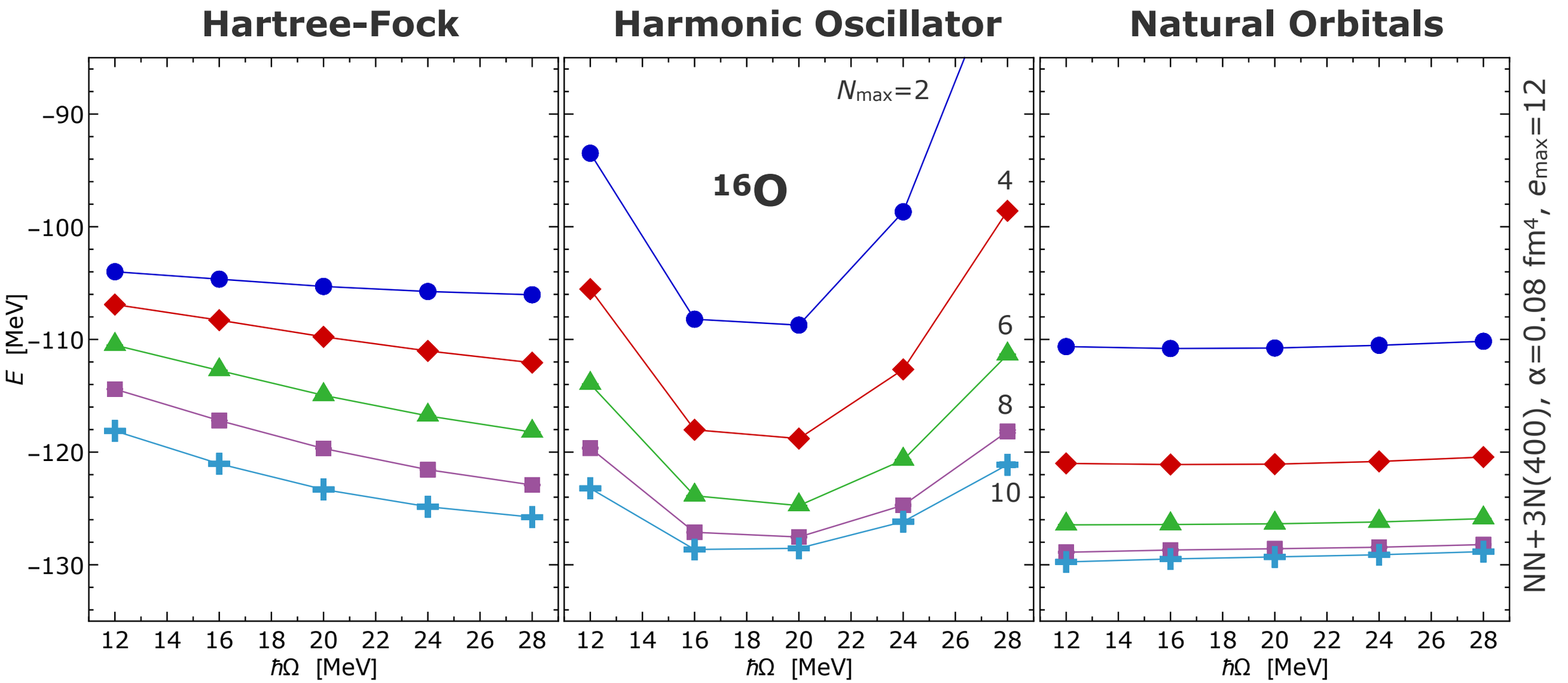
- **Harmonic-Oscillator Basis**
  - essential for computation of matrix elements, always first step
  - separation of center of mass and intrinsic states, translational invariance
  - wrong asymptotic behavior, slow convergence of long-range observables

- **Hartree-Fock Basis**
  - spherical Hartree-Fock calculation to optimize single-particle basis
  - adapt basis to typical size of nuclear ground state
  - only for soft interactions, pathological asymptotics for unbound states

- **Natural-Orbital Basis**
  - one-body density matrix obtained from second-order MBPT calculation
  - natural orbital basis adapted to size of correlated ground state
  - correct asymptotic behavior, independence of underlying basis

NCSM Convergence: Energies

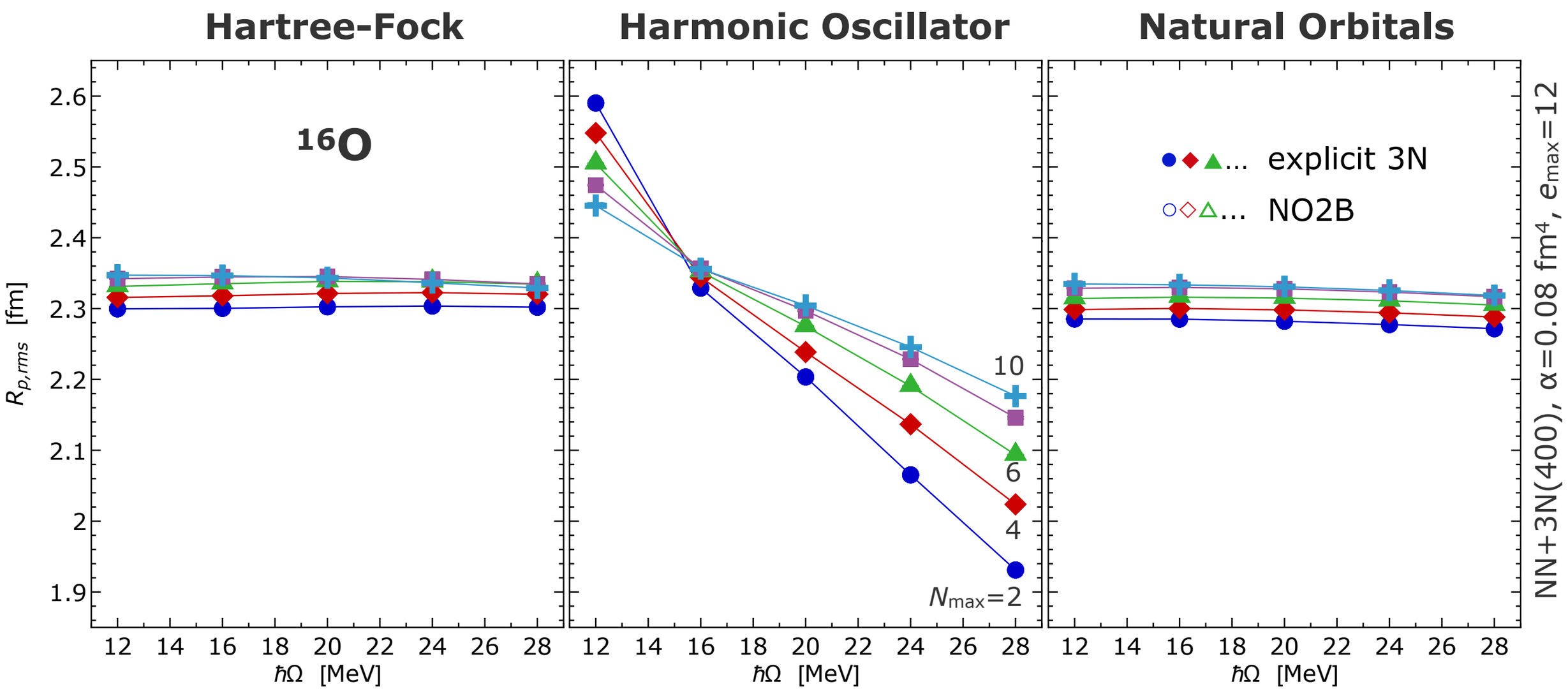
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



- MBPT natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

NCSM Convergence: Radii

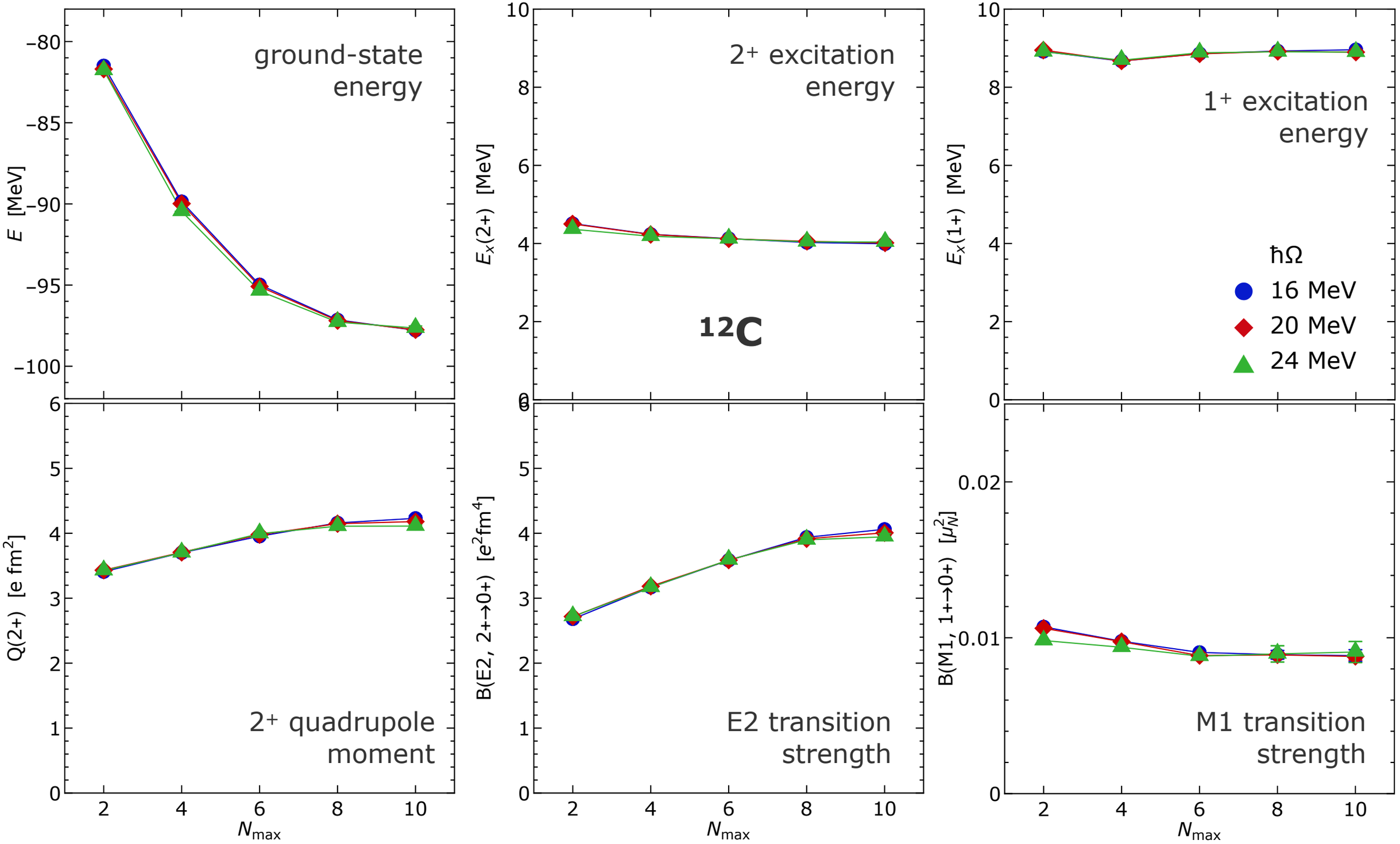
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



- MBPT natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

NCSM Convergence: Spectroscopy

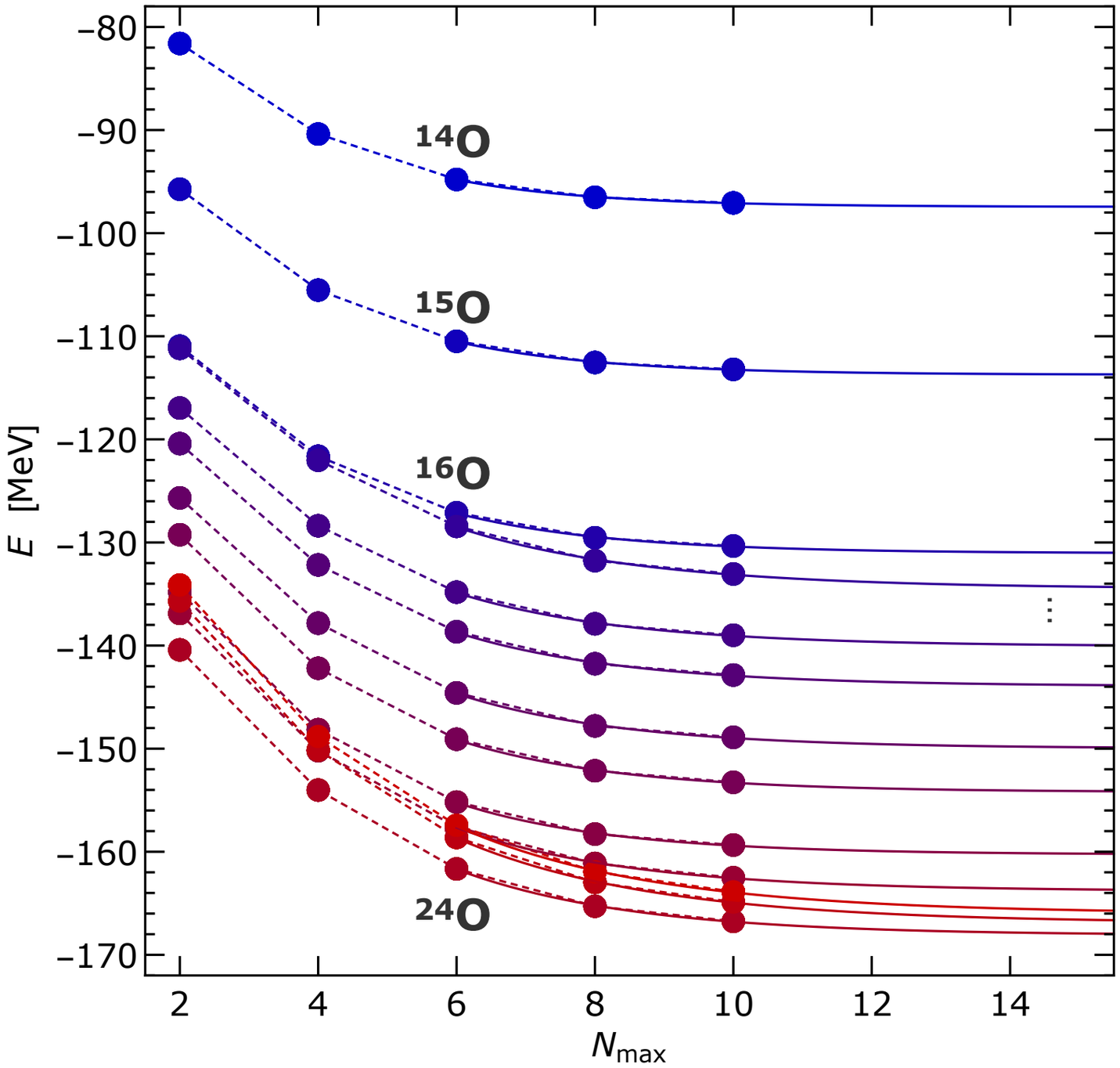
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



NN+3N(500), α=0.08 fm⁴, e_{max}=12

Oxygen Isotopes

Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)

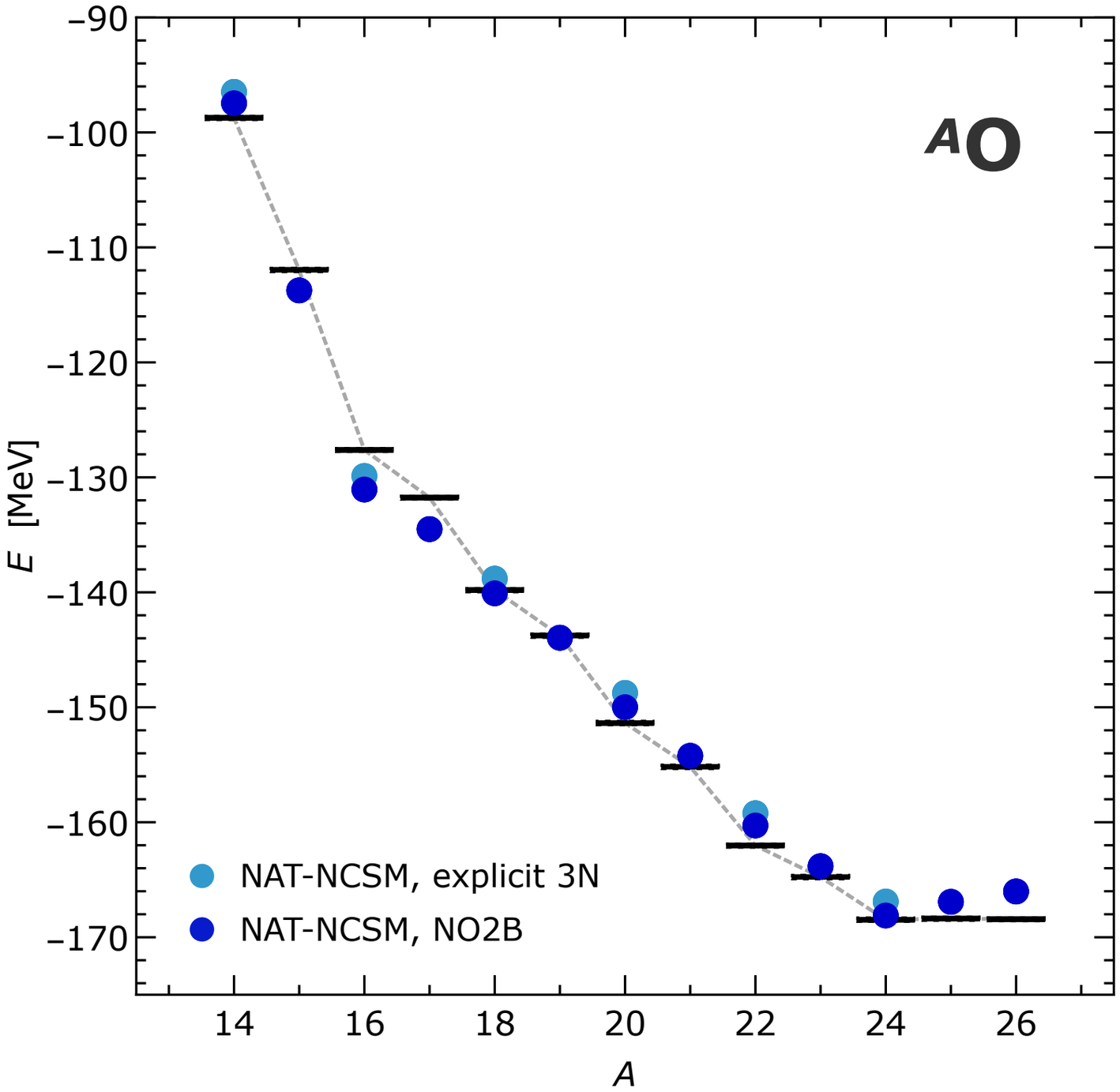


- excellent convergence with natural-orbital basis for all oxygen isotopes

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

Oxygen Isotopes

Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



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

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

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

- **Natural-Orbital NCSM**
  use optimized single-particle basis to accelerate convergence

- **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

Overview

- **Lecture 1: Hamiltonian**

  Prelude • Many-Body Quantum Mechanics • 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 • Basis Optimization

- **Lecture 3: Medium-Mass Nuclei**

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

- **Project: Do-It-Yourself NCSM**

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

- **Lecture 4: Precision, Uncertainties, and Applications**

  Chiral Interactions for Precision Calculations • Uncertainty Quantification • Applications to Nuclei and Hypernuclei