Ab Initio Nuclear Structure Theory

Lecture 2: Correlations

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Overview

- **Lecture 1: Hamiltonian**

  Prelude ● Many-Body Quantum Mechanics ● Nuclear Hamiltonian ● Matrix Elements

- **Lecture 2: Correlations**

  Two-Body Problem ● Correlations & Unitary Transformations ● Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Many-Body Problem ● Configuration Interaction ● No-Core Shell Model ● Applications

- **Lecture 4: Beyond Light Nuclei**

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

Two-Body Problem

Solving the Two-Body Problem

- **simplest ab initio problem**: the only two-nucleon bound state, the deuteron

- start from **Hamiltonian in two-body space**, change to center of mass and intrinsic coordinates

$$\begin{aligned} \mathrm{H} &= \mathrm{H}_{\mathrm{cm}} + \mathrm{H}_{\mathrm{int}} = \mathrm{T}_{\mathrm{cm}} + \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{\mathrm{NN}} \\ &= \frac{1}{2M}\vec{\mathrm{P}}^2_{\mathrm{cm}} + \frac{1}{2\mu}\vec{\mathrm{q}}^2 + \mathrm{V}_{\mathrm{NN}} \end{aligned}$$

- **separate** two-body state into center of mass and intrinsic part

$$|\psi\rangle = |\Phi_{\mathrm{cm}}\rangle \otimes |\phi_{\mathrm{int}}\rangle$$

- solve **eigenvalue problem for intrinsic part** (effective one-body problem)

$$\mathrm{H}_{\mathrm{int}}\,|\phi_{\mathrm{int}}\rangle = E\,|\phi_{\mathrm{int}}\rangle$$

Solving the Two-Body Problem

- expand eigenstates in a **relative partial-wave HO basis**

$$|\phi_{\text{int}}\rangle = \sum_{NLSJMTM_T} C_{NLSJMTM_T} \, |N(LS)JM; TM_T\rangle$$

$$|N(LS)JM; TM_T\rangle = \sum_{M_L M_S} c\left(\begin{smallmatrix} L & S \\ M_L & M_S \end{smallmatrix} \middle| \begin{smallmatrix} J \\ M \end{smallmatrix}\right) \, |NLM_L\rangle \otimes |SM_S\rangle \otimes |TM_T\rangle$$

- **symmetries** simplify the problem dramatically:
  - H_{int} does not connect/mix different J, M, S, T, M_T and parity π
  - angular mom. coupling only allows $J=L+1$, L, L-1 for S=1 or $J=L$ for S=0
  - total antisymmetry requires $L+S+T$=odd

- for given J^π at most two sets of angular-spin-isospin quantum numbers contribute to the expansion

Deuteron Problem

- assume $J^\pi = 1^+$ for the **deuteron ground state**, then the basis expansion reduces to

$$|\phi_{\text{int}}, J^\pi = 1^+\rangle = \sum_N C_N^{(0)} \, |N(01)\,1M;00\rangle + \sum_N C_N^{(2)} \, |N(21)\,1M;00\rangle$$

- inserting into Schrödinger equation and multiplying with basis bra leads to **matrix eigenvalue problem**

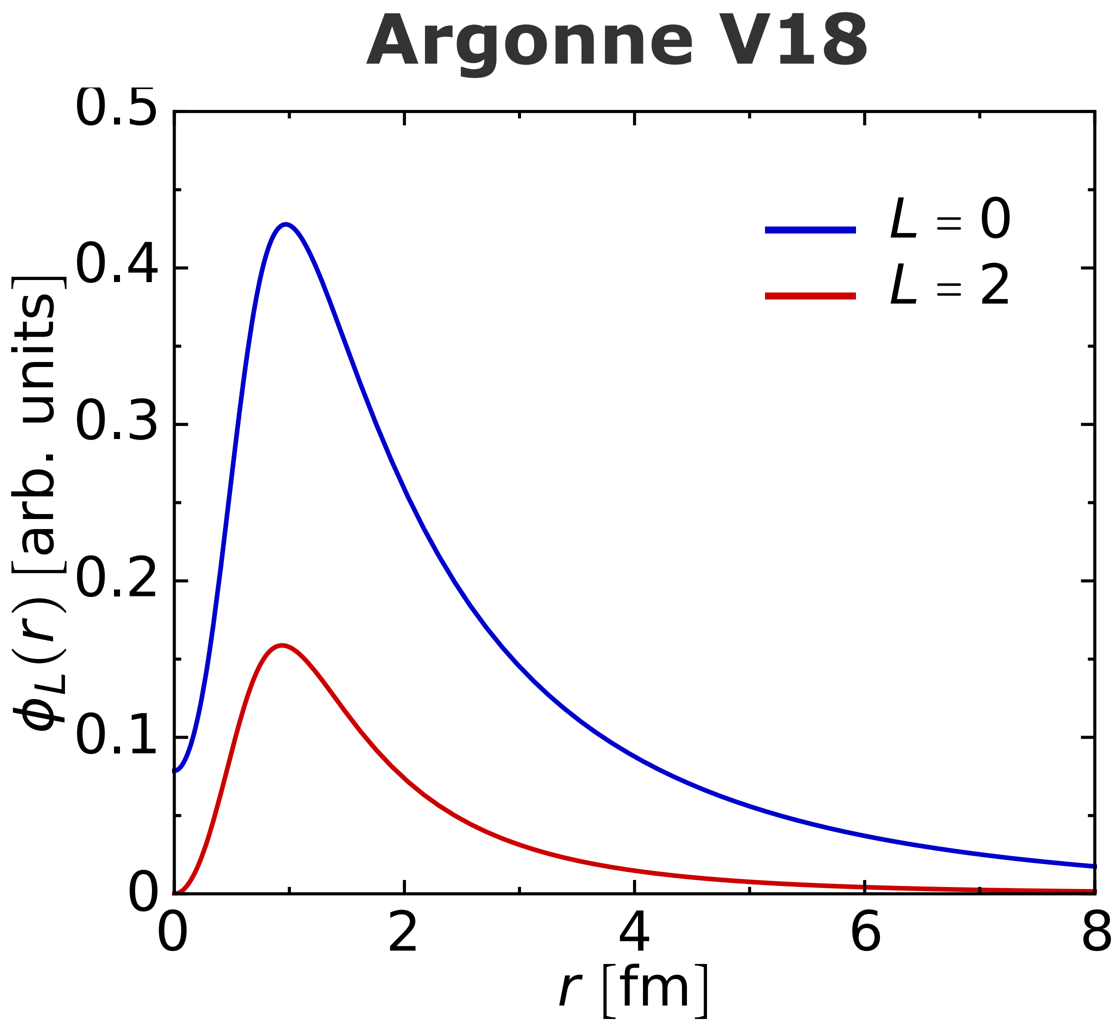
$$\left(\begin{array}{c|c} \langle N'(01)\ldots|\,\mathrm{H}_{\text{int}}\,|N(01)\ldots\rangle & \langle N'(01)\ldots|\,\mathrm{H}_{\text{int}}\,|N(21)\ldots\rangle \\ \hline \langle N'(21)\ldots|\,\mathrm{H}_{\text{int}}\,|N(01)\ldots\rangle & \langle N'(21) \ldots \end{array}\right) \begin{pmatrix} C_N^{(0)} \\ \hline C_N^{(2)} \end{pmatrix} \quad \begin{pmatrix} C_{N'}^{(0)} \\ \hline C_{N'}^{(2)} \end{pmatrix}$$

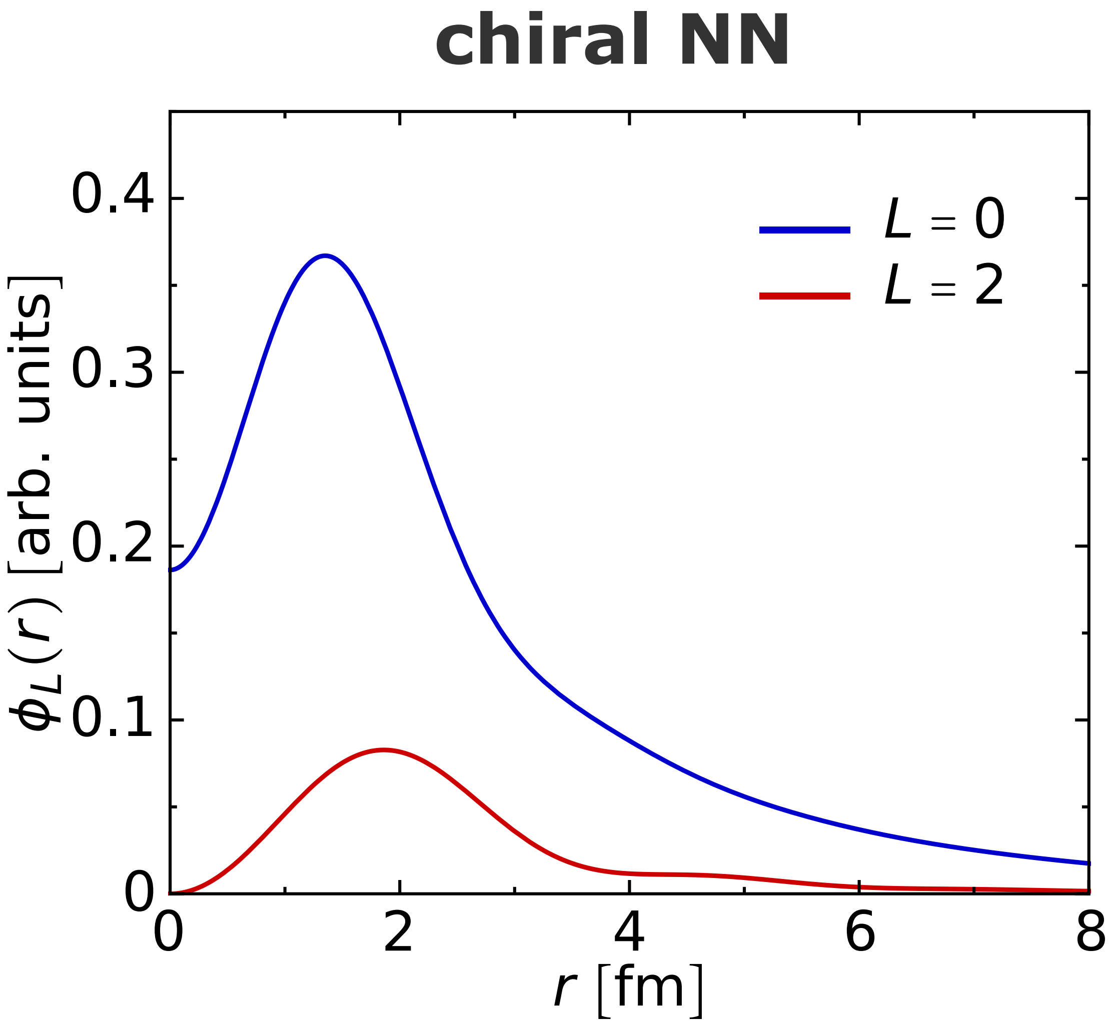
simplest possible Jacobi-NCSM calculation

- eigenvectors ... ...cients and eigenvalues the energies

- **truncate** ... **...ces to $N \leq N_{\text{max}}$** and choose N_{max} large enough so that observables are converged, i.e., do not depend on N_{max} anymore

Deuteron Solution





- deuteron wave function show two characteristics that are **signatures of correlations** in the two-body system:
  - suppression at small distances due to short-range repulsion
  - L=2 admixture generated by tensor part of the NN interaction

Correlations &
Unitary Transformations

Correlations

correlations:
everything beyond the independent particle picture

- many-body eigenstates of independent-particle models described by one-body Hamiltonians are **Slater determinants**
- thus, a single Slater determinant **does not describe correlations**
- but Slater determinants are a basis of the antisym. A-body Hilbert space, so any state can be expanded in Slater determinants
- to describe **short-range correlations**, a superposition of many Slater determinants is necessary

Why Unitary Transformations ?

realistic nuclear interactions generate strong short-range correlations in many-body states

Unitary Transformations

- adapt Hamiltonian to truncated low-energy model space
- improve convergence of many-body calculations
- preserve the physics of the initial Hamiltonian and all observables

many-body methods rely on truncated Hilbert spaces not capable of describing these correlations

Unitary Transformations

- unitary transformations **conserve the spectrum** of the Hamiltonian, with a unitary operator U we get

$$\begin{aligned} \mathrm{H}\,|\psi\rangle &= E\,|\psi\rangle \\ \mathrm{U}^\dagger\mathrm{H}\mathrm{U}\,\mathrm{U}^\dagger\,|\psi\rangle &= E\,\mathrm{U}^\dagger\,|\psi\rangle \\ \tilde{\mathrm{H}}\,|\tilde{\psi}\rangle &= E\,|\tilde{\psi}\rangle \end{aligned} \qquad \text{with} \qquad \begin{aligned} 1 &= \mathrm{U}^\dagger\mathrm{U} = \mathrm{U}\mathrm{U}^\dagger \\ \tilde{\mathrm{H}} &= \mathrm{U}^\dagger\mathrm{H}\mathrm{U} \\ |\tilde{\psi}\rangle &= \mathrm{U}^\dagger\,|\psi\rangle \end{aligned}$$

- for **other observables** defined via matrix elements of an operator A with the eigenstates we obtain

$$\langle\psi|\,\mathrm{A}\,|\psi'\rangle = \langle\psi|\,\mathrm{U}\,\mathrm{U}^\dagger\mathrm{A}\mathrm{U}\,\mathrm{U}^\dagger\,|\psi'\rangle = \langle\tilde{\psi}|\,\tilde{\mathrm{A}}\,|\tilde{\psi}'\rangle$$

unitary transformations conserve all observables as long as the Hamiltonian and all other operators are transformed consistently

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

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

- **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 fixed 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 $|q\,(LS)\,JT\rangle$

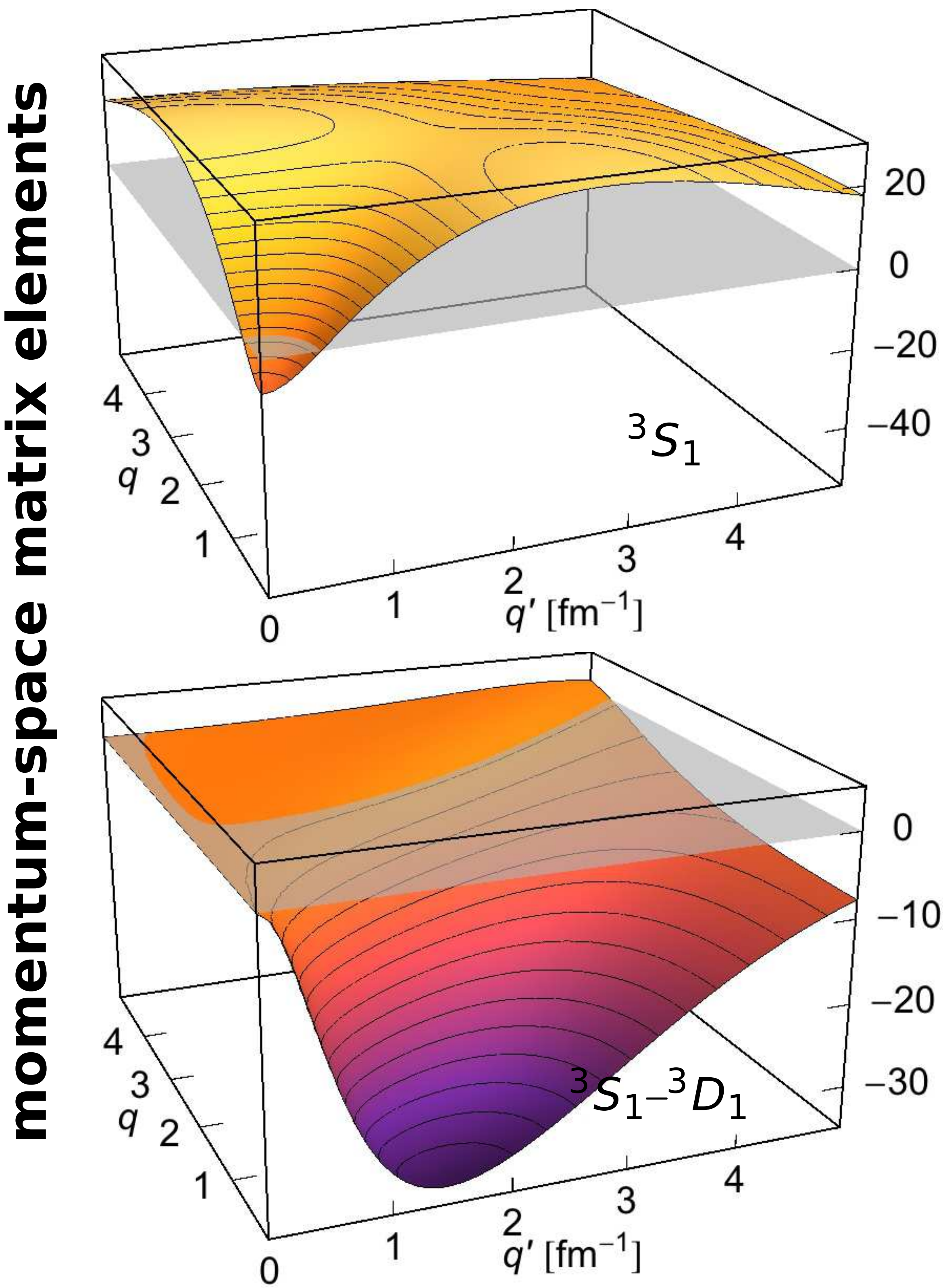
n=3: antisym. three-body Jacobi HO $|Ei J^\pi T\rangle$

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

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

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

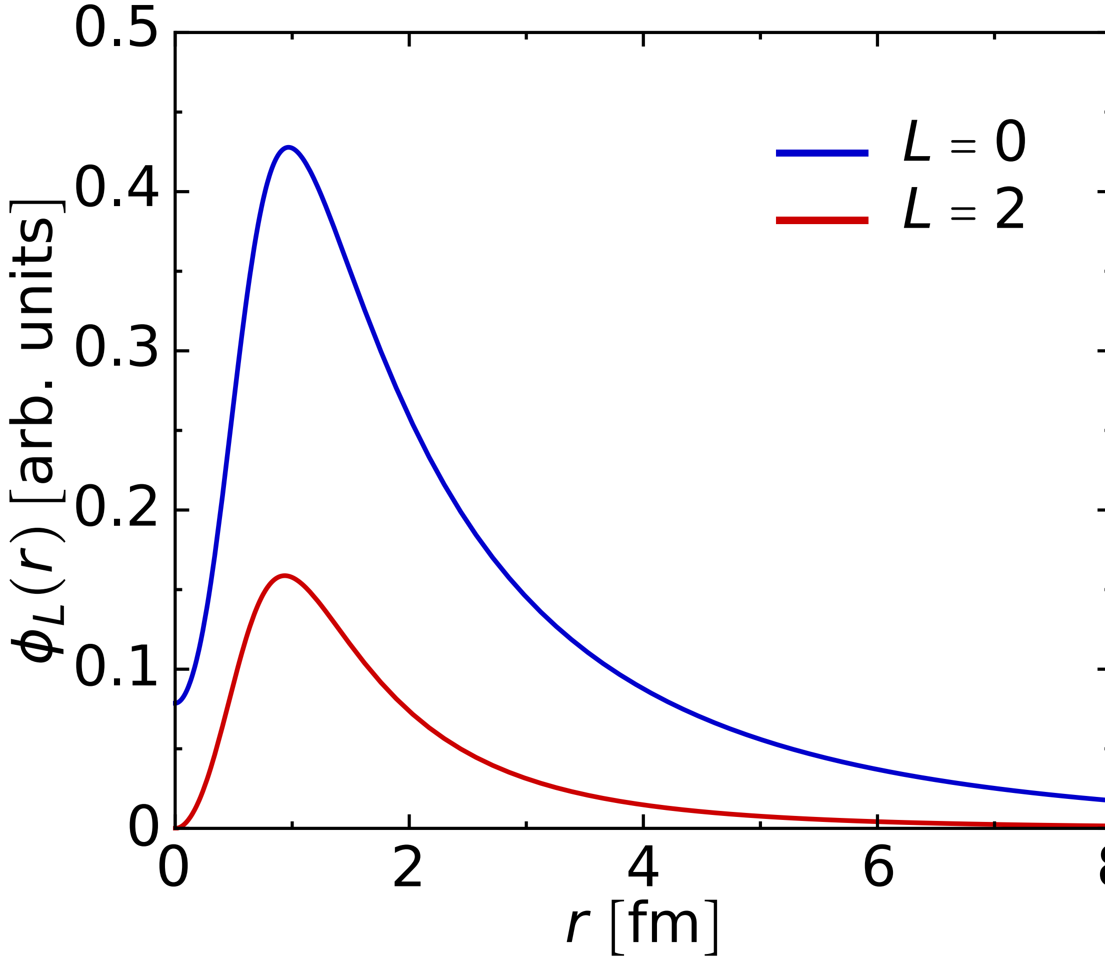
SRG Evolution in Two-Body Space



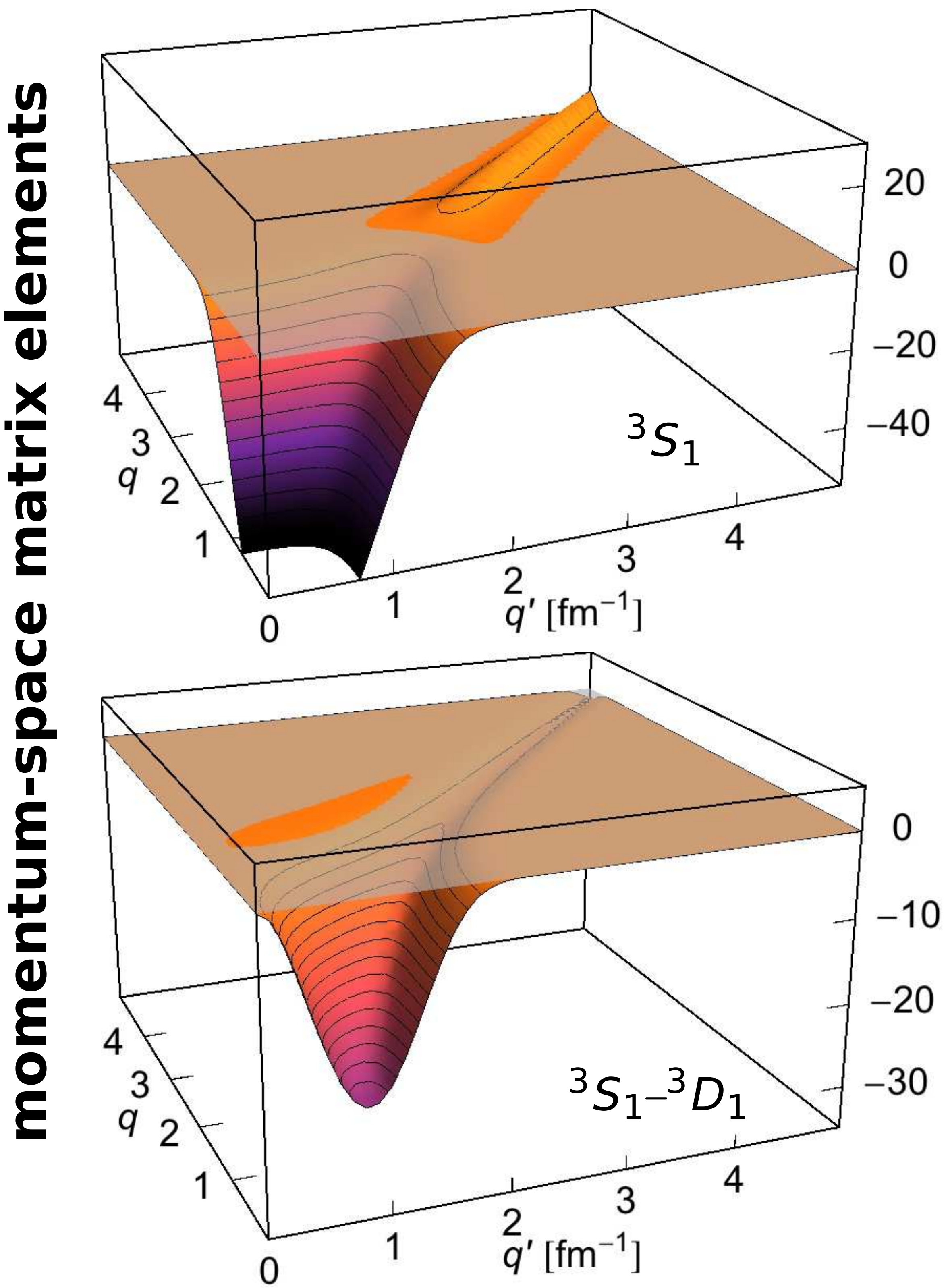
Argonne V18

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

deuteron wave-function



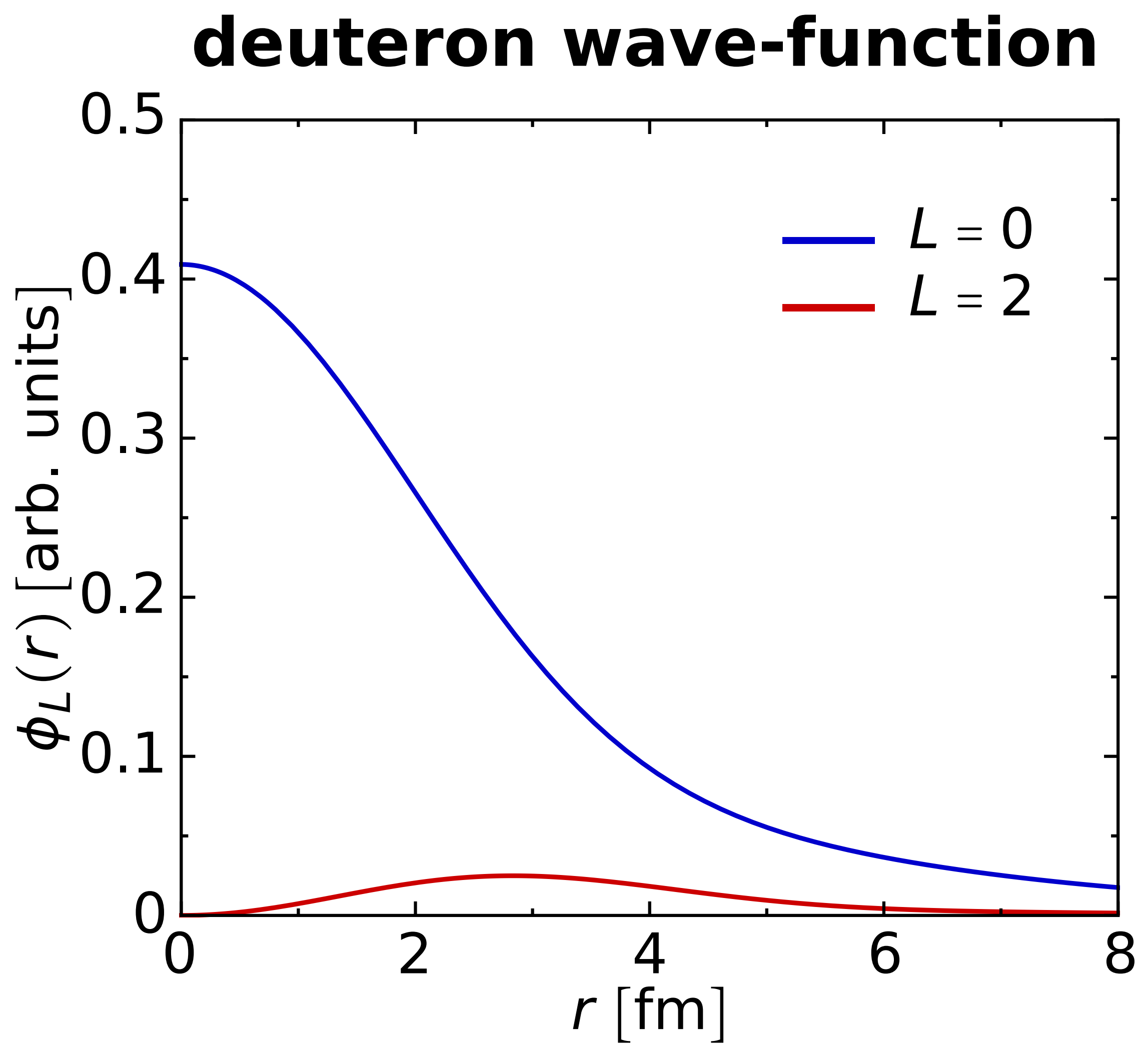
SRG Evolution in Two-Body Space



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

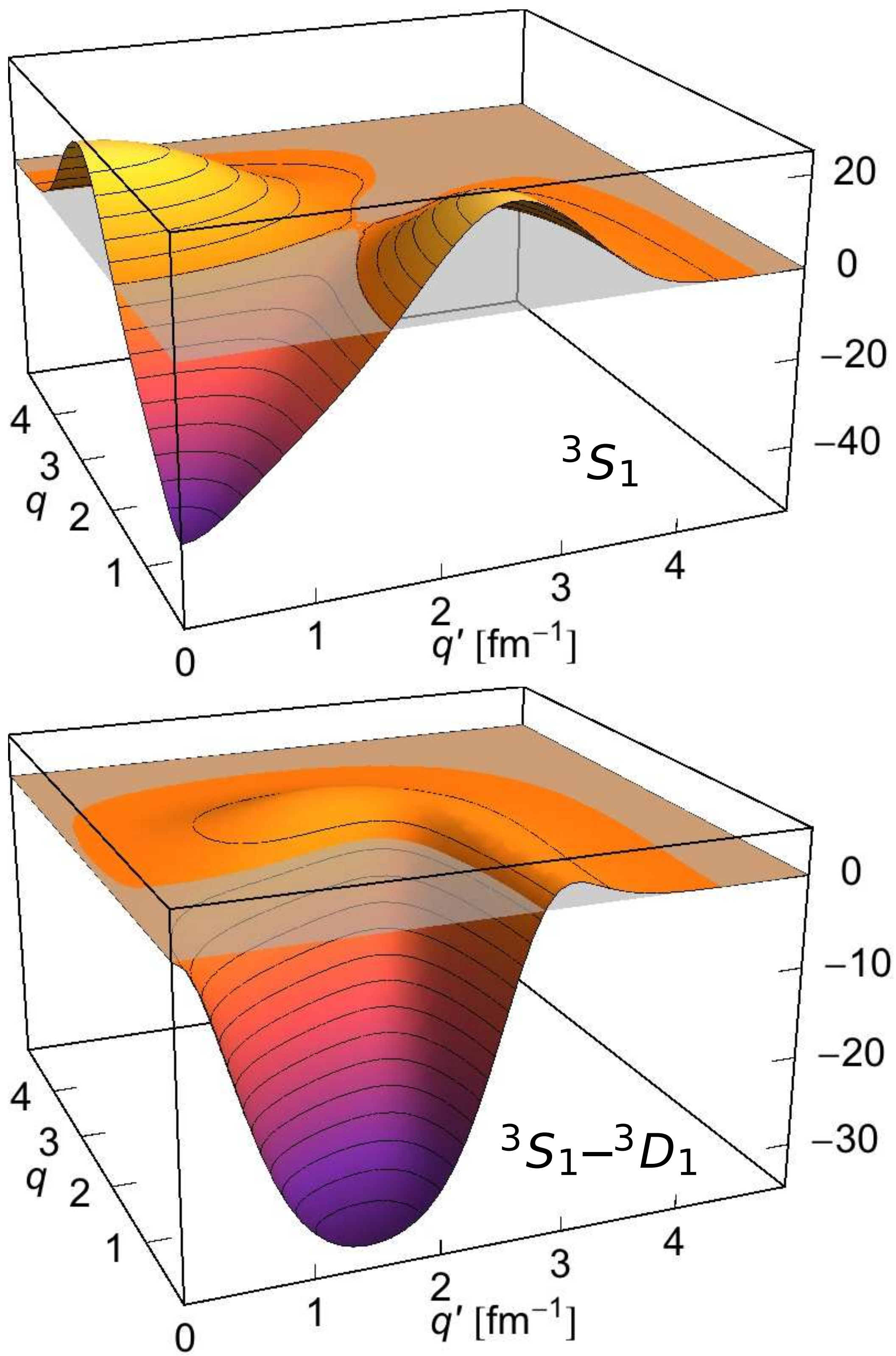
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

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



SRG Evolution in Two-Body Space

momentum-space matrix elements

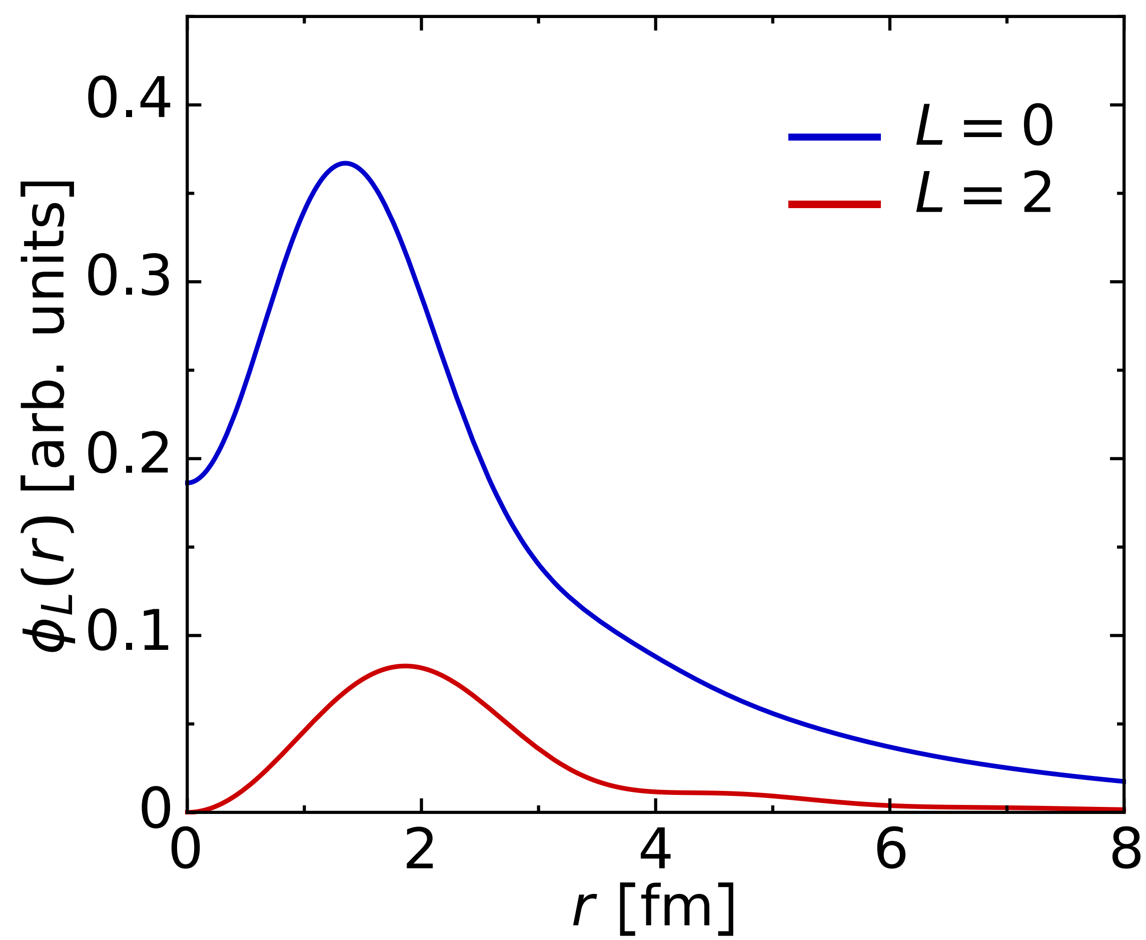


chiral NN

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

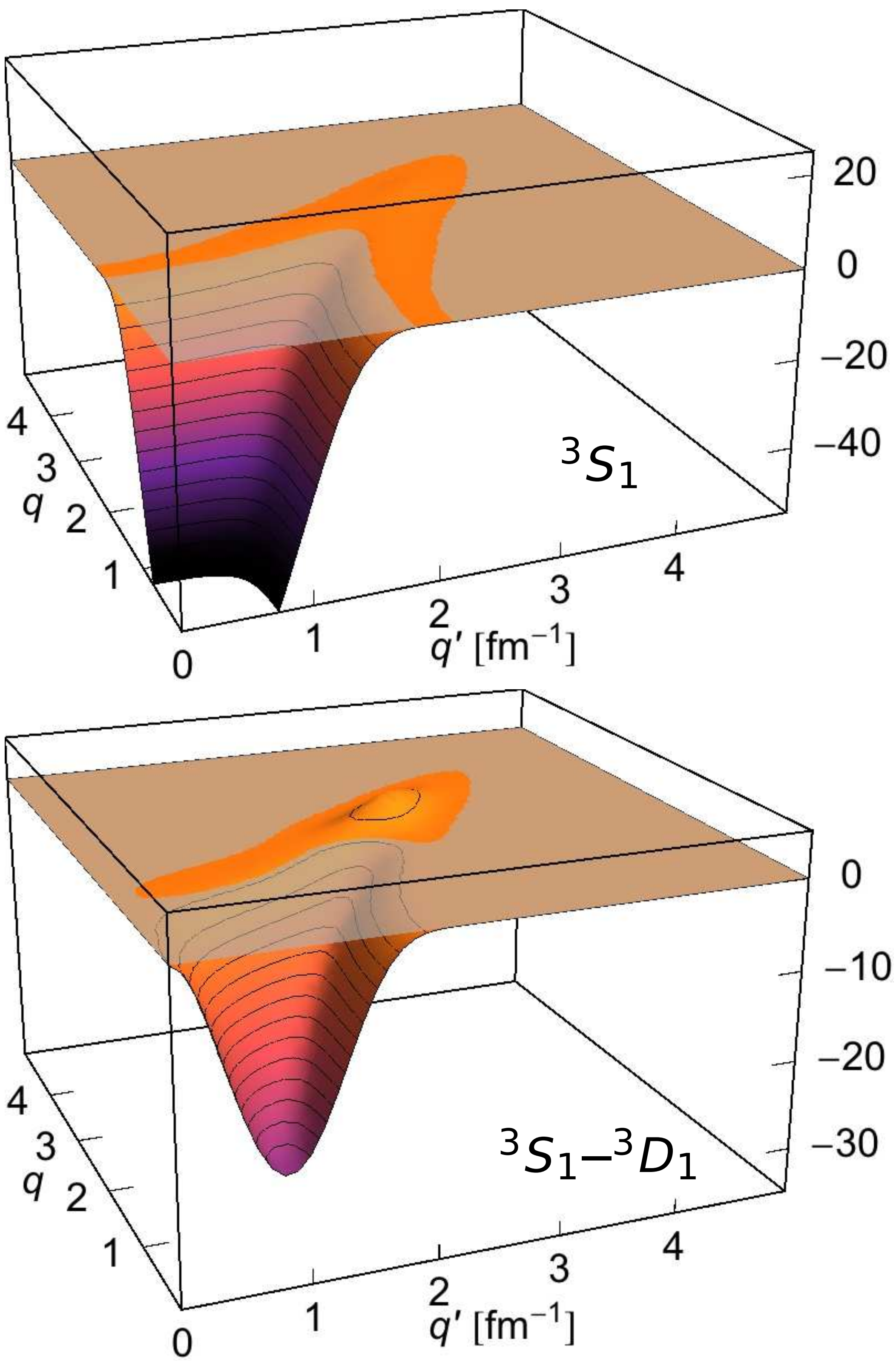
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements



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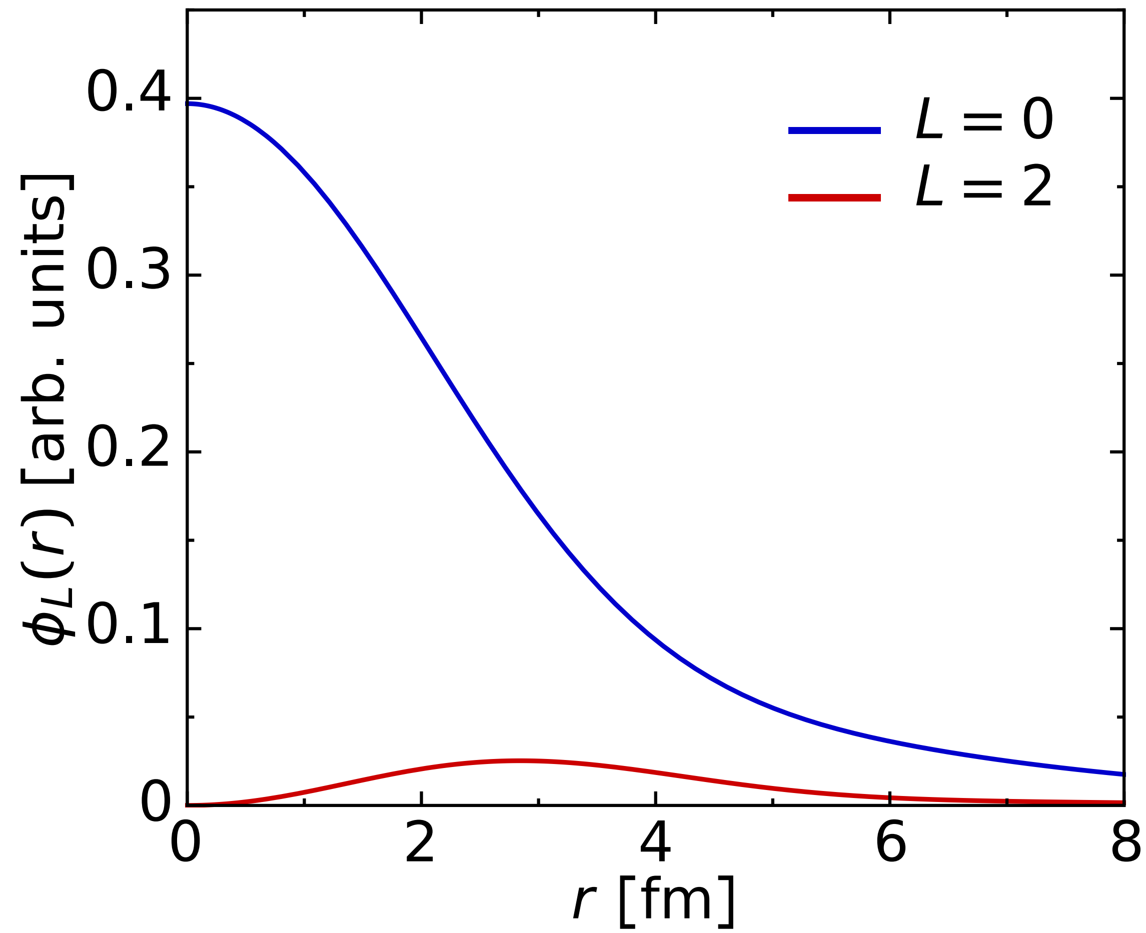
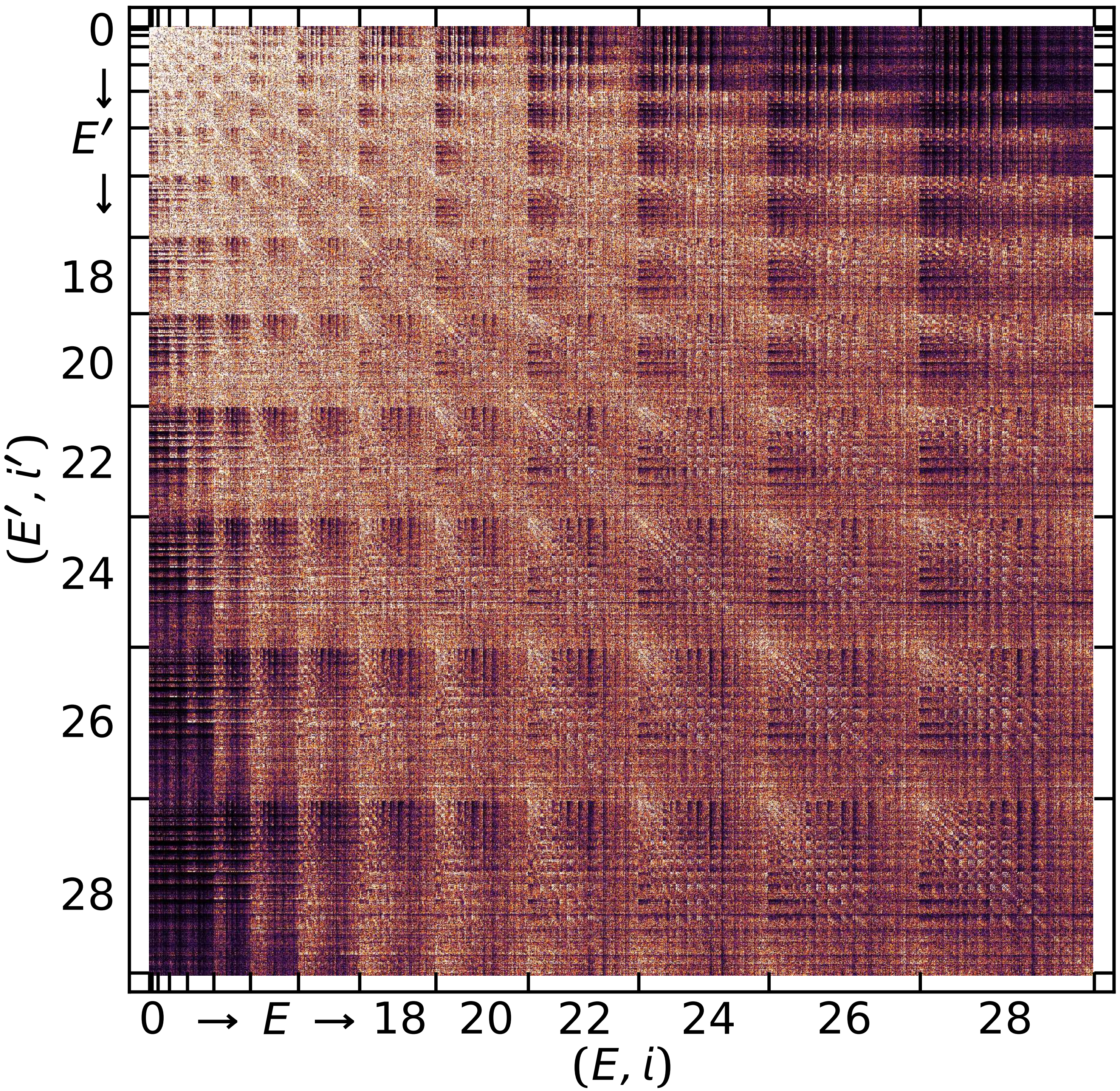
deuteron wave-function



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

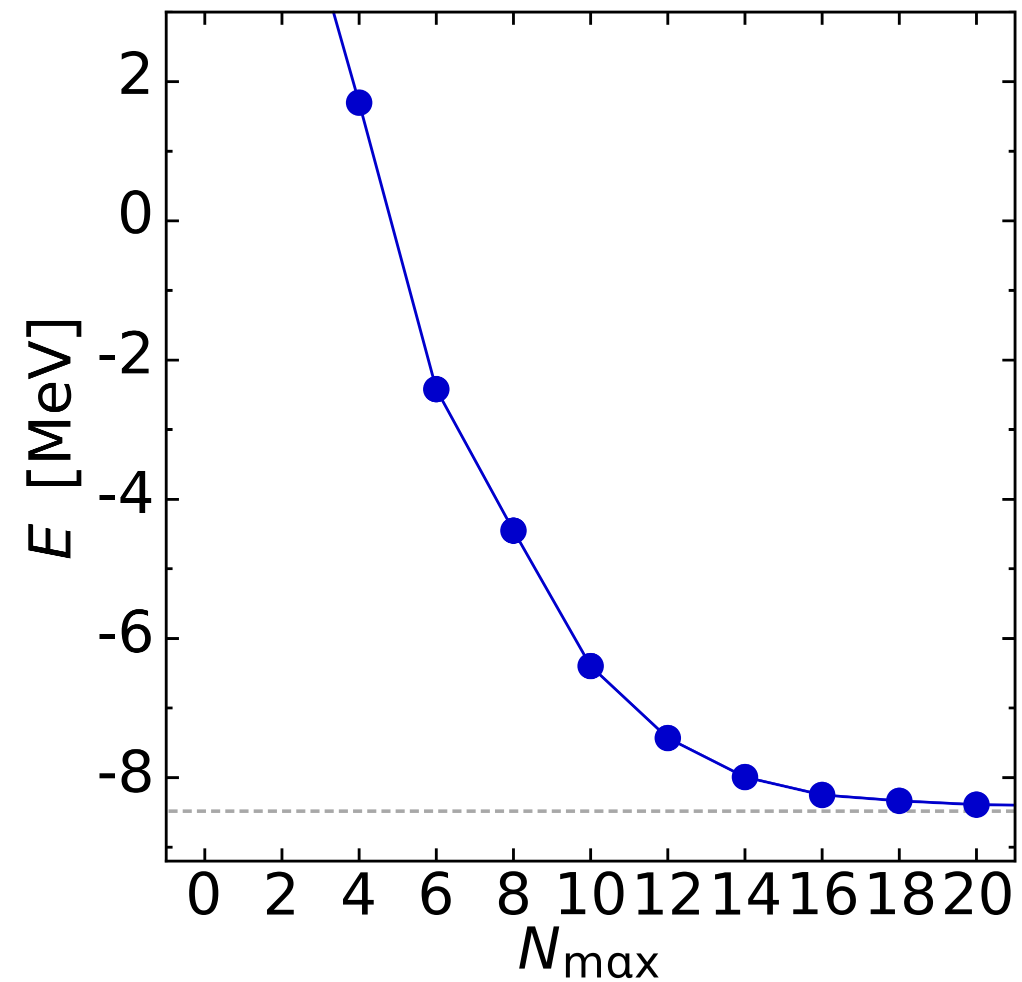


chiral NN+3N

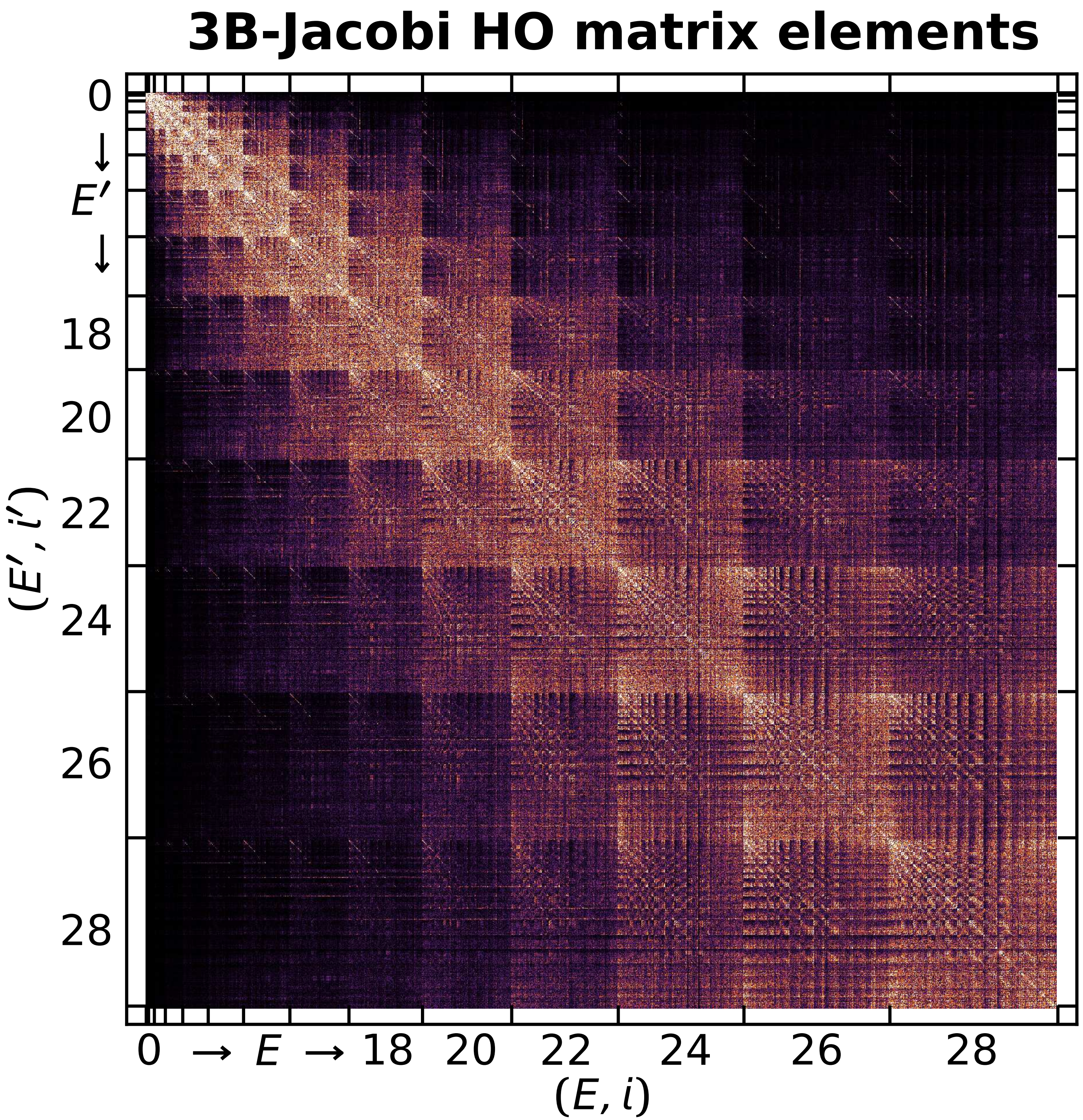
$N^3LO + N^2LO$, triton-fit, 500 MeV

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

NCSM ground state ^{3}H



SRG Evolution in Three-Body Space



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

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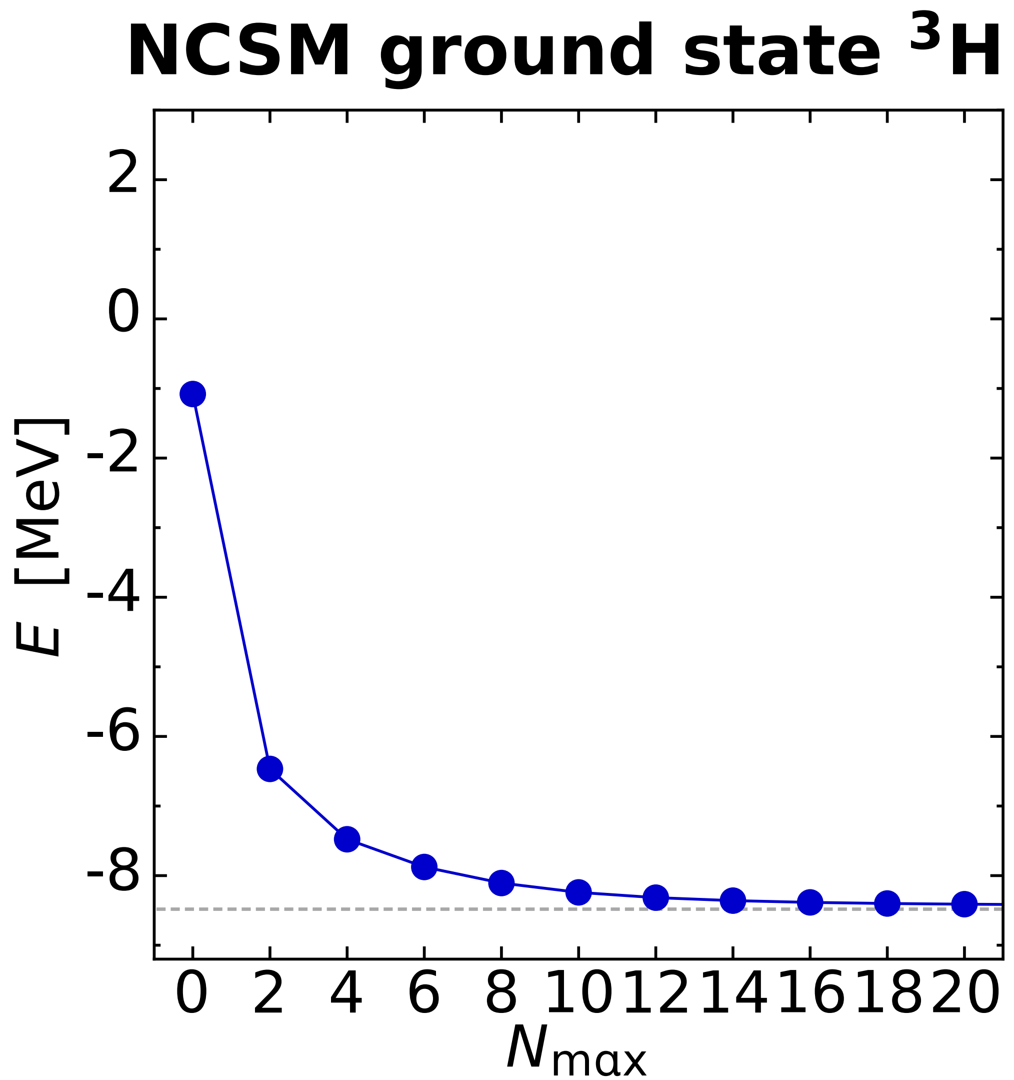
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\text{MeV}$



SRG Evolution in A-Body Space

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

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

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

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

- 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

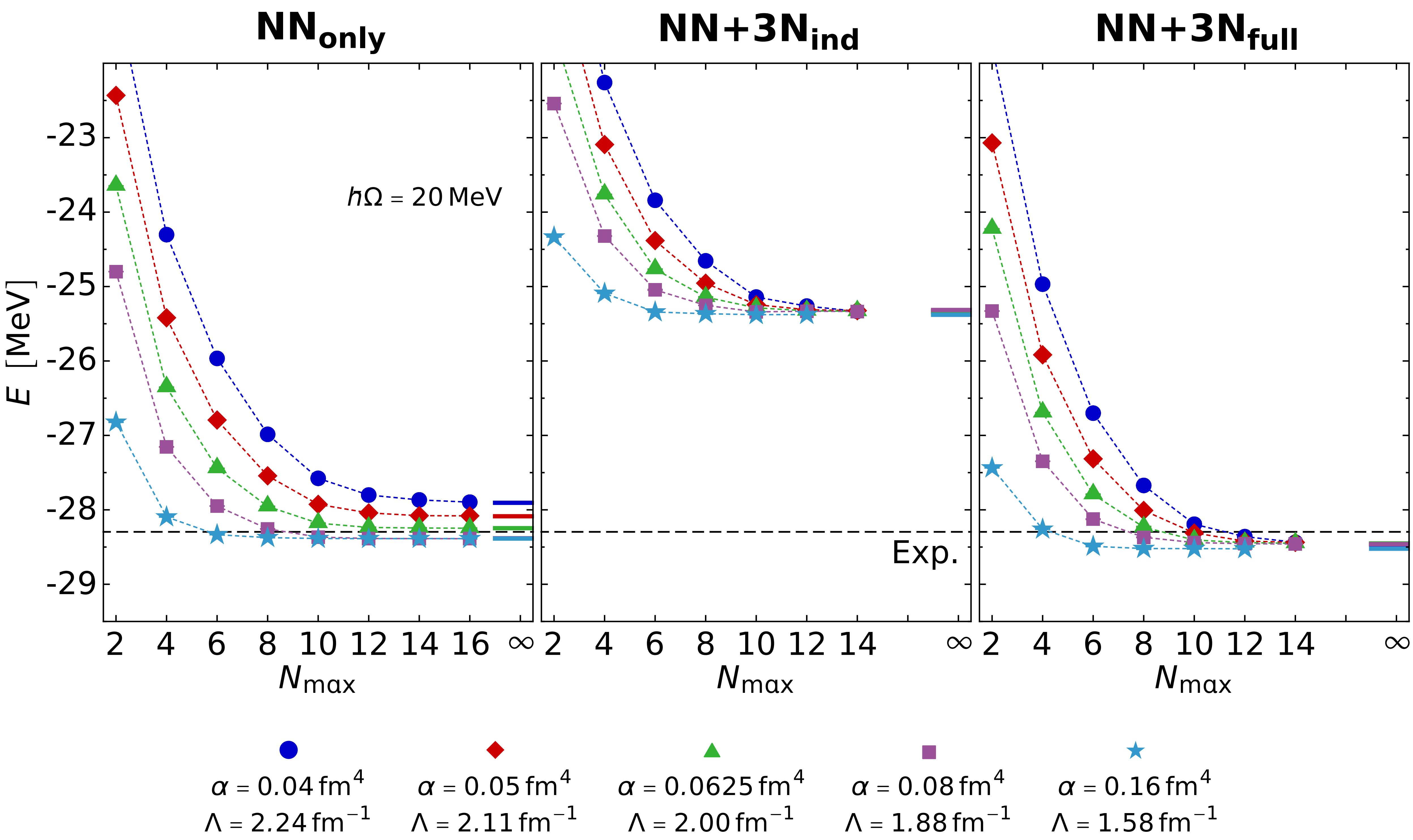
$NN+3N_{ind}$: use initial NN, keep evolved NN+3N

$NN+3N_{full}$: 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)