Ab initio calculations of atomic nuclei

Recent progress and future challenges

Lecture 2: Many-body techniques

Part 1: Exact methods

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Many-body Schrödinger equation

⊙ Goal: solve ***A*-body Schrödinger equation** (for any A)

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

- H: many-nucleon Hamiltonian
- $|\Psi_k^A\rangle$: A-body wave function
- E_k^A: A-body energies of ground and excited states

⊙ **Only input**

$$H = H_{\text{int}} = T_{\text{int}} + V_{\text{NN}} + V_{\text{3N}} + \dots$$

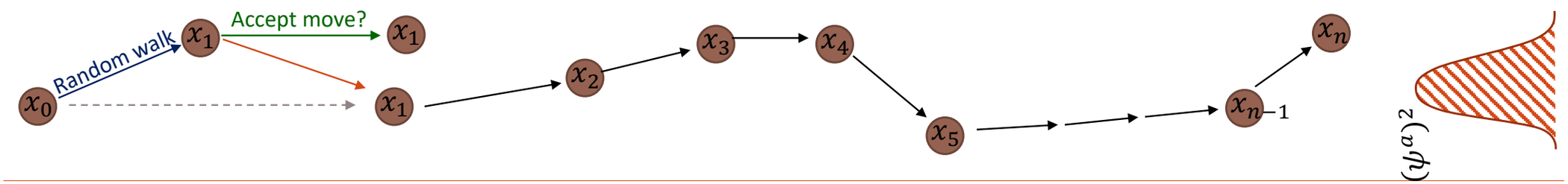
○ Given as a sum of many operators in momentum space (⊗ spin & isospin)

○ Coupling constants in X-body sector (ideally) fitted on X-body observables

○ Increasingly complicated as more nucleons are involved

Coordinate-space vs configuration-space methods

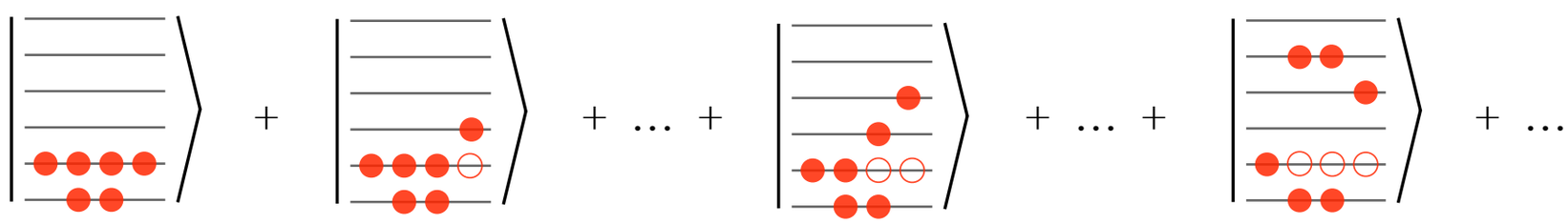
- **Coordinate-space methods**
  - Directly work with many-body wave function (e.g. Monte Carlo sampling)



✓ Flexible (any spatial configuration is accessible) + no intensive memory requirement

✗ Sign problem → constrained choice of operators + expensive in processor time

- **Configuration-space methods**
  - Expand eigenstates on a basis of known many-body states



✓ Universally applicable to any operator + amenable to controlled approximations

✗ Expensive in memory usage + constrained by the properties of basis states

One-body (= single-particle) basis

- Basic constituents: nucleons characterised by **position, spin and isospin**
  - Single-nucleon states expressed as

$$|\varphi_k\rangle = \Big[|\varphi_k^{\rm space}\rangle \otimes |\varphi_k^{\rm spin}\rangle\Big] \otimes |\varphi_k^{\rm isospin}\rangle$$

- Standard choice for nuclear structure approaches

$|\varphi_k^{\rm space}\rangle = |n\,\ell\,m_\ell\rangle$ e.g., solutions of **one-body harmonic oscillator**

$|\varphi_k^{\rm spin}\rangle = |s\,m_s\rangle = |\frac{1}{2}\,m_s\rangle$ eigenstates of s^2 and s_z with s=1/2

$|\varphi_k^{\rm isospin}\rangle = |t\,m_t\rangle = |\frac{1}{2}\,m_t\rangle$ eigenstates of t^2 and t_z with t=1/2

- **Orbital angular momentum and spin are typically coupled**

$$|\varphi_k\rangle = |n\,(\ell\,\frac{1}{2})\,j\,m;\frac{1}{2}\,m_t\rangle = \sum_{m_l,m_s} c\left(\begin{array}{cc|c}\ell & \frac{1}{2} & j\\ m_l & m_s & m\end{array}\right)|n\,\ell\,m_\ell\rangle \otimes |\frac{1}{2}\,m_s\rangle \otimes |\frac{1}{2}\,m_t\rangle$$

Many-body basis

⊙ When dealing with fermions, **many-body states have to be explicitly antisymmetrised**

Antisymmetrisation operator $\mathcal{A} = \frac{1}{A!} \sum_{\pi} \mathrm{sgn}(\pi)\, P_\pi$

Direct product of A 1-body states

$$
\begin{aligned}
|\Phi^A\rangle &= \mathcal{A}\left\{|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle \otimes \cdots \otimes |\varphi_{k_A}\rangle\right\} \\
&= \frac{1}{\sqrt{A!}} \sum_{\pi} \mathrm{sgn}(\pi)\, P_\pi \left(|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle \otimes \cdots \otimes |\varphi_{k_A}\rangle\right) \\
&\equiv |k_1\, k_2\, \cdots\, k_A\rangle
\end{aligned}
$$

Slater determinants

- ○ Antisymmetric under **exchange** $P_{ij}\,|\cdots k_i \cdots k_j \cdots\rangle = |\cdots k_j \cdots k_i \cdots\rangle = -|\cdots k_i \cdots k_j \cdots\rangle$
- ○ Encodes **Pauli principle** $|\cdots k_i \cdots k_i \cdots\rangle = 0$ → minimal intrinsic correlations

⊙ Any antisymmetric state can be expanded in the **Slater determinant basis**

$$
|\Psi^A\rangle = \sum_{k_1 > k_2 \cdots > k_A} c_{k_1\, k_2\, \ldots\, k_A} |k_1\, k_2\, \cdots\, k_A\rangle \equiv \sum_i c_i\, |\Phi_i\rangle
$$

Configuration interaction

⊙ The strategy is the following

1. Select a one-body basis

$$|\alpha\rangle \equiv |n\,\ell\,j\,m\,m_t\rangle$$

2. Construct *A*-body basis of Slater determinants

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

3. Convert Schrödinger equation into a matrix eigenvalue problem

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle \qquad \rightarrow \text{ expand} \qquad |\Psi_k\rangle = \sum_i C_i^{(k)}|\Phi_i\rangle$$

$$\langle\Phi_j| \times \left[H\sum_i C_i^{(k)}|\Phi_i\rangle = E_k\sum_i C_i^{(k)}|\Phi_i\rangle\right]$$

$$\sum_i \underbrace{\langle\Phi_j|H|\Phi_i\rangle}_{\equiv H_{ji}} C_i^{(k)} = E_k\sum_i C_i^{(k)}\underbrace{\langle\Phi_j\,|\,\Phi_i\rangle}_{=\delta_{ij}} \rightarrow$$

$$\begin{bmatrix} \vdots & \\ \cdots & H_{ji} \quad \cdots \\ \vdots & \end{bmatrix} \begin{bmatrix} \vdots \\ C_i^{(k)} \\ \vdots \end{bmatrix} = E_k \begin{bmatrix} \vdots \\ C_j^{(k)} \\ \vdots \end{bmatrix}$$

Model space truncations

⊙ Expansion on Slater determinants involves an **infinite number of basis states**

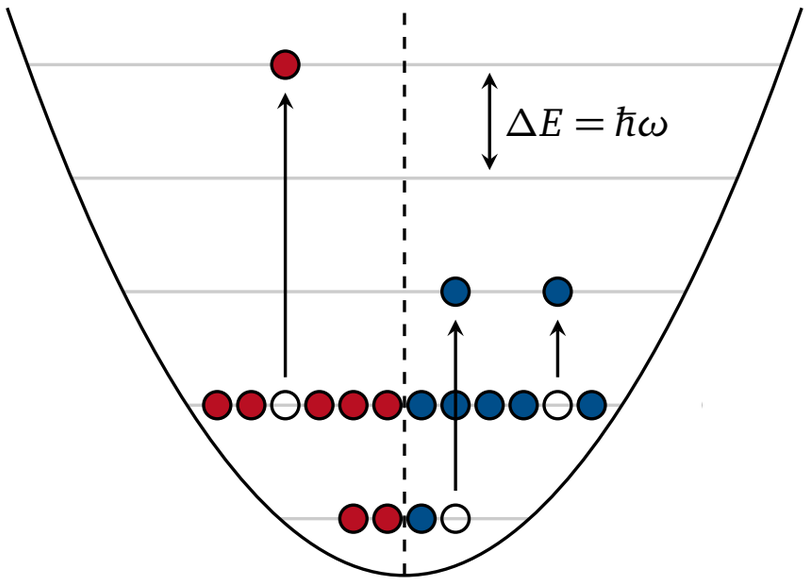
$$|\Psi_k\rangle = \sum_{i=1}^{\infty} C_i^{(k)} |\Phi_i\rangle \qquad \Rightarrow \qquad |\Psi_k(D)\rangle = \sum_{i=1}^{D} C_i^{(k)} |\Phi_i\rangle$$

obviously cannot store an infinite vector… ➪ truncations have to be necessarily introduced

⊙ **Two main ways** of truncating the basis

○ **Full CI**: truncate the **one-body** basis (at some maximum single-particle energy $\mathbf{e_{max}}$)

○ **No-core shell model**: cut the **many-body** basis (total number of HO excitation quanta $N_{\mathbf{max}}$)

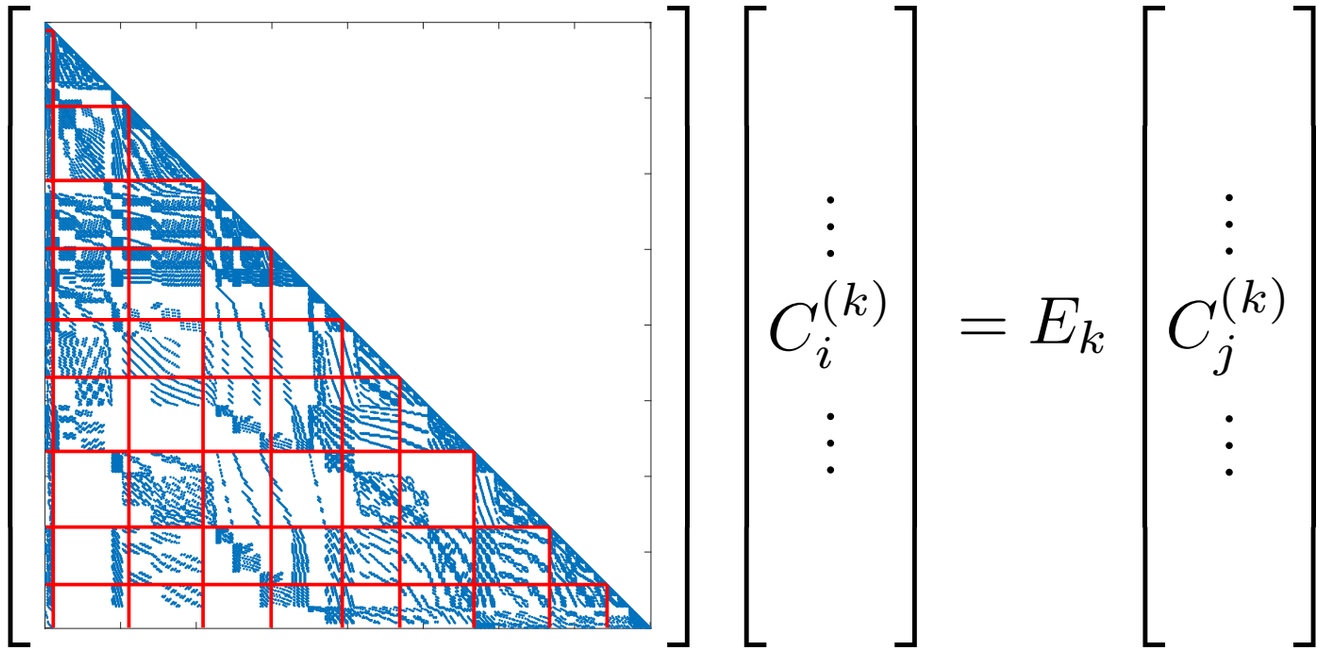


Example: $N_{\mathbf{max}} = 6$

[*Figure*: R.Roth]

Computational strategy

- **Involved computational problem as A increases**
- Key features
  - One is only interested in a **few low-lying eigenstates**
  - Hamiltonian matrix is **sparse** ($< 0.01\%$ of non-zeros at working values of $N_{\max}$)



- **Computational solutions & limitations**
  - **Lanczos-type algorithms** employed to extract first few eigenstates and associated eigenvalues
  - Fast storage of non-zero matrix elements sets the **limits of matrix dimensions**
  - Extensive use of parallelisation, matrix transformations, optimisation techniques, …

CI dimensionality

- "Back-of-the-envelope" estimate of matrix dimensions
  - **Case of Full CI** (recall: truncation acts on the single-particle basis)

- How many Slater determinants can be built from a given number of single-particle states?
  - Take ***A* nucleons** and ***n* single-particle states**
    - ➪ Number of different possible Slater determinants $\left(\begin{array}{c} n \\ A \end{array} \right) = \dfrac{n!}{(n-A)!\,A!}$

- **Example: ^{16}O** ($Z = 8$, $N = 8$) in 40 single-particle states

$$\left(\begin{array}{c} 40 \\ 8 \end{array} \right) = \frac{40!}{(40-8)!\,8!} \approx 8 \cdot 10^7 \quad \text{for protons} \quad \text{x} \quad \left(\begin{array}{c} 40 \\ 8 \end{array} \right) = \frac{40!}{(40-8)!\,8!} \approx 8 \cdot 10^7 \quad \text{for neutrons}$$

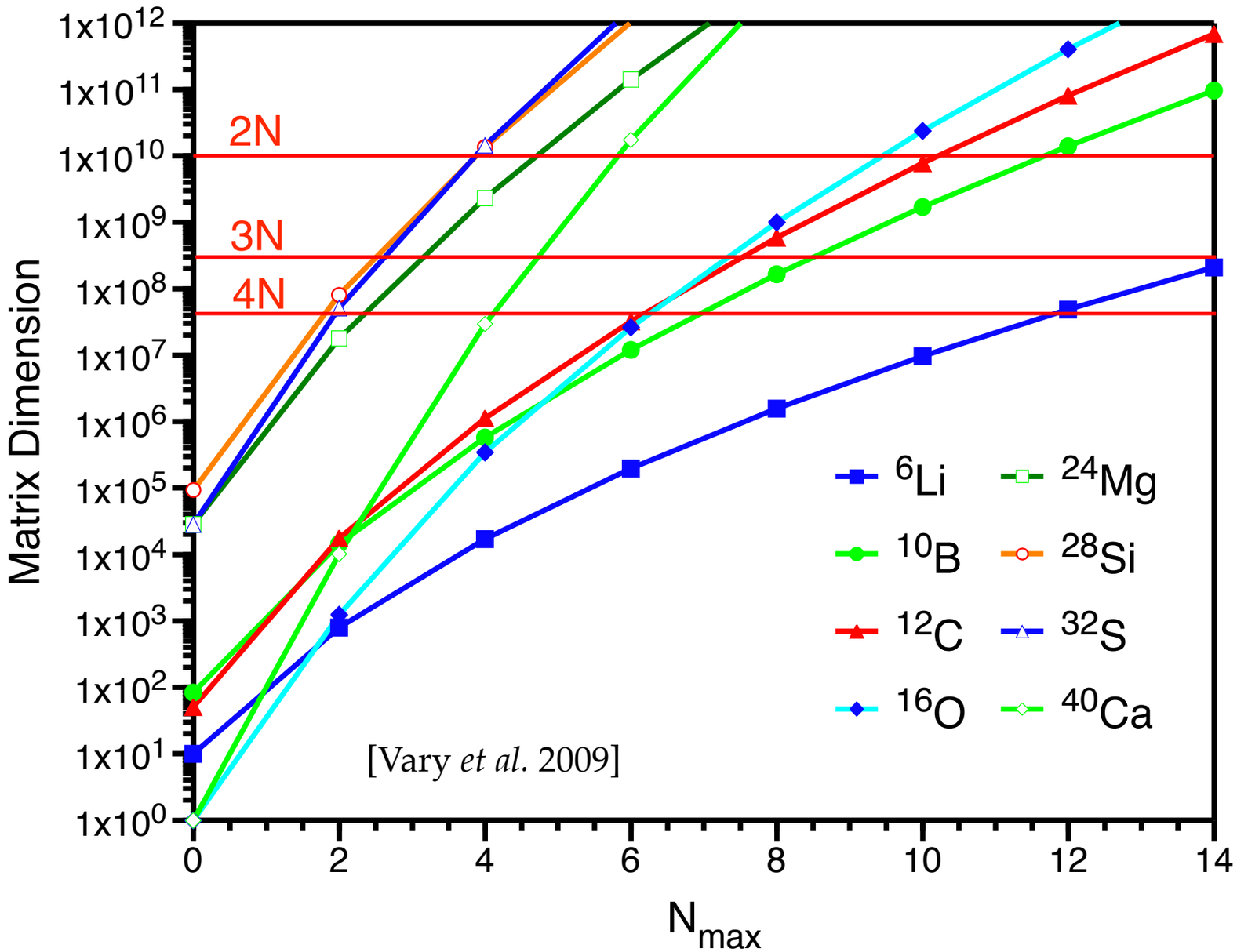
  - ➪ Total of D = $6 \cdot 10^{15}$ Slater determinants
  - ➪ Number of non-zero matrix elements (*NN* only!) scales as $D^{1.2}$ → ~ 10^{18} non-zero entries
  - ➪ Size in memory beyond EB → well beyond current capabilities

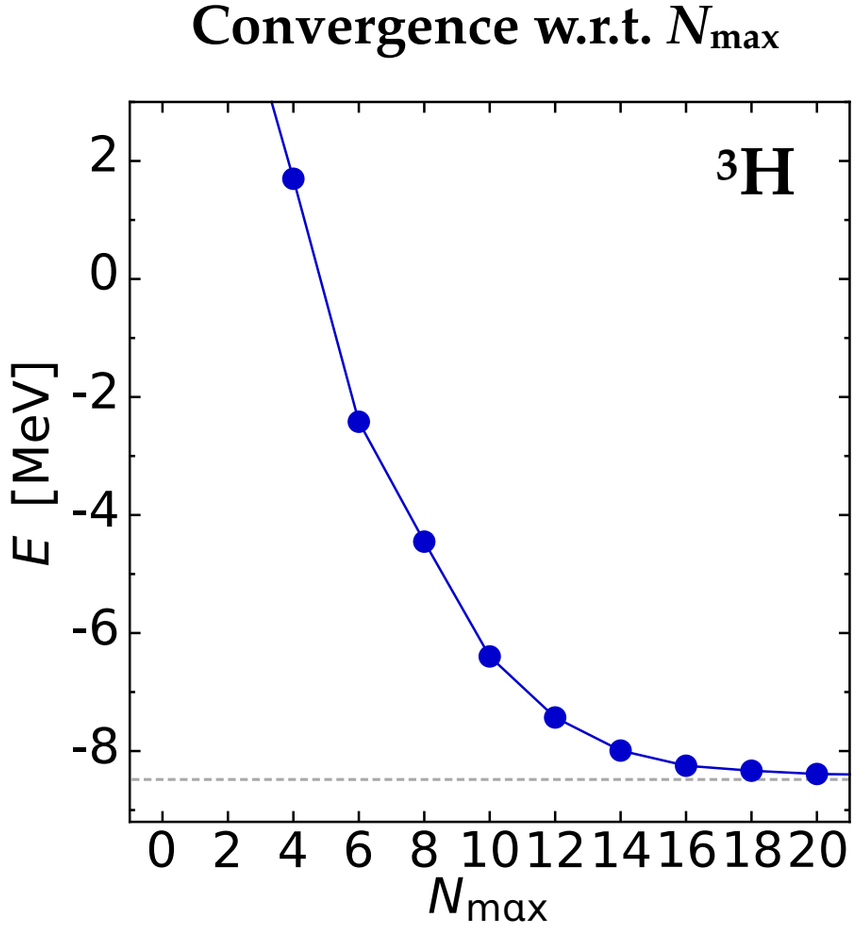
- **Current computational limits** for the storage and diagonalisation of a large matrix
  - Petascale machines: **D ~ 10^{10}** // Exascale machines: **D ~ 10^{12}**

NCSM dimensionality

⊙ **No-core shell model**

○ More gentle scaling (recall: truncation $N_{\max}$ acts on the many-body basis)



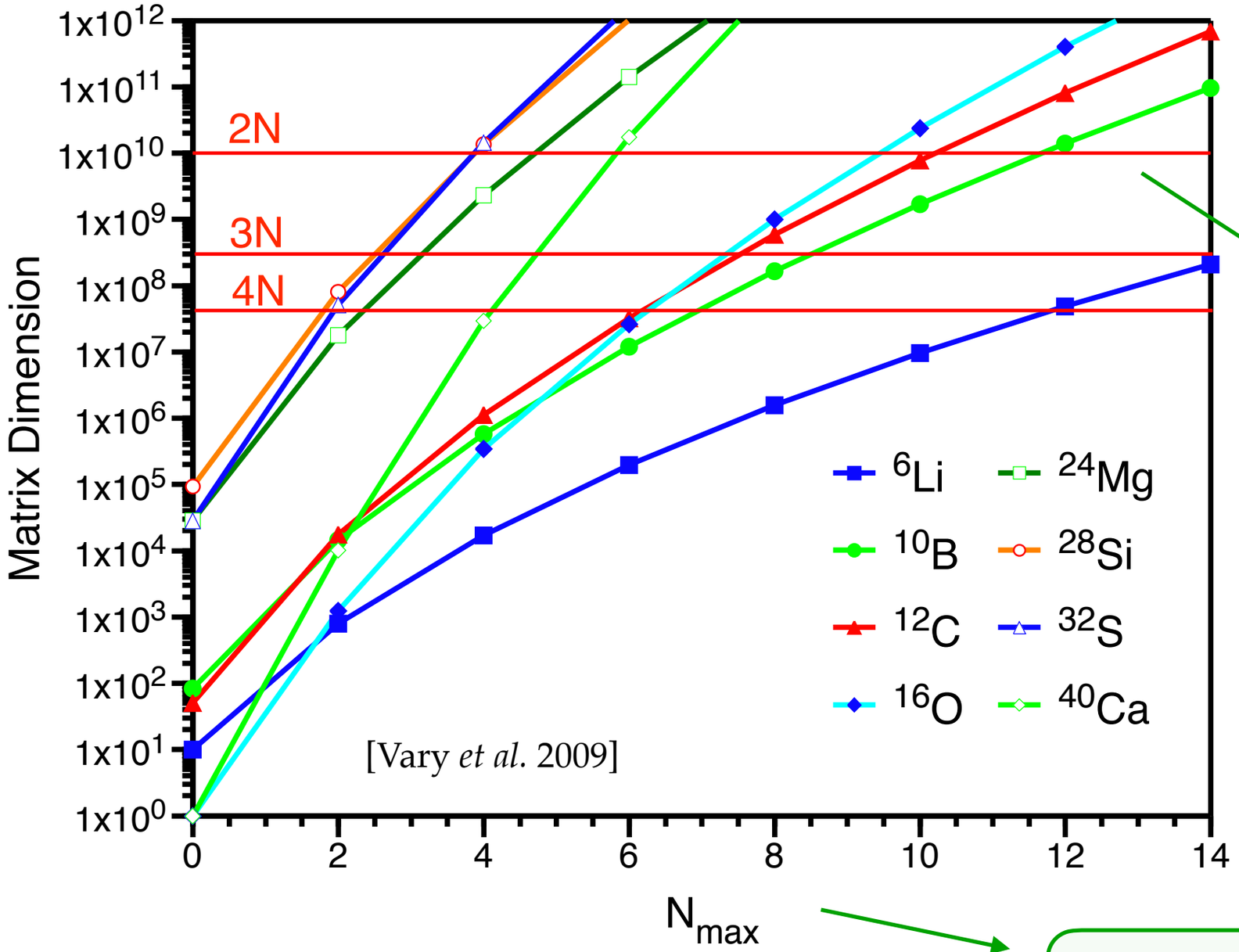


➪ Very quickly one reaches the computational limits

NCSM dimensionality

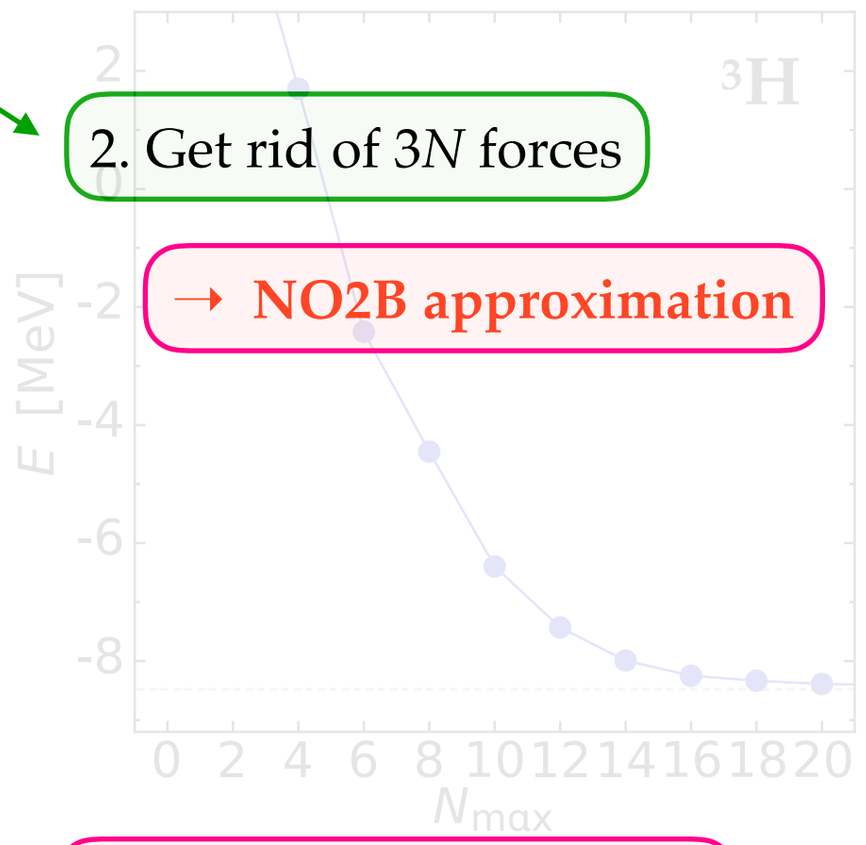
3. Get rid of some matrix elements

→ **Importance truncation**



2. Get rid of 3*N* forces

→ **NO2B approximation**



→ **SRG transformations**

1. Improve $N_{\max}$ convergence

Contents

Short-range correlations & “low-momentum” interactions

⊙ **Why do we need to include such high values of $N_{\max}$ / large matrix dimensions?**

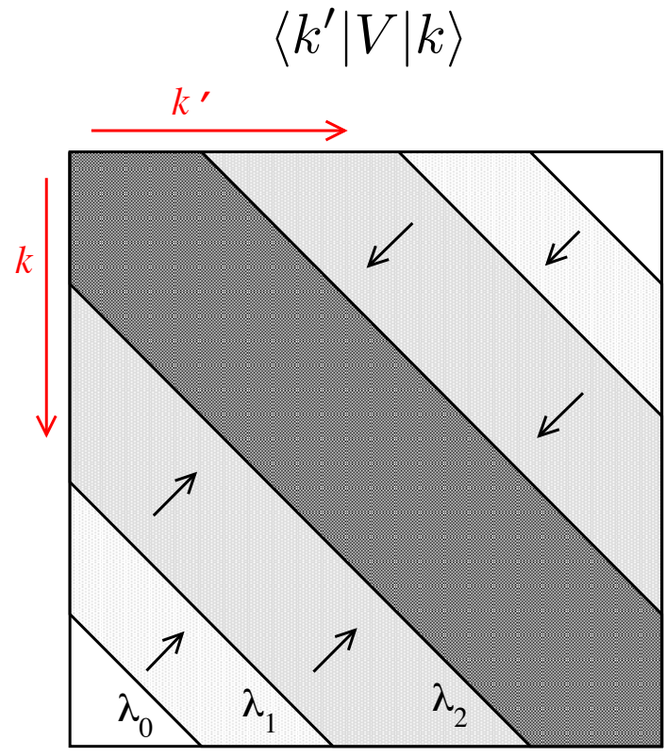
⊙ Nuclear interactions generate **short-range correlations** in many-body states

- ○ Traditionally linked to “**hard core**” of one-boson exchange potentials
- ○ **Weaker but present** in modern chiral interactions
- ○ Short distance / high momenta / high energy → **large Hilbert space needed**

⊙ **Idea: use unitary transformations on H to suppress these correlations**

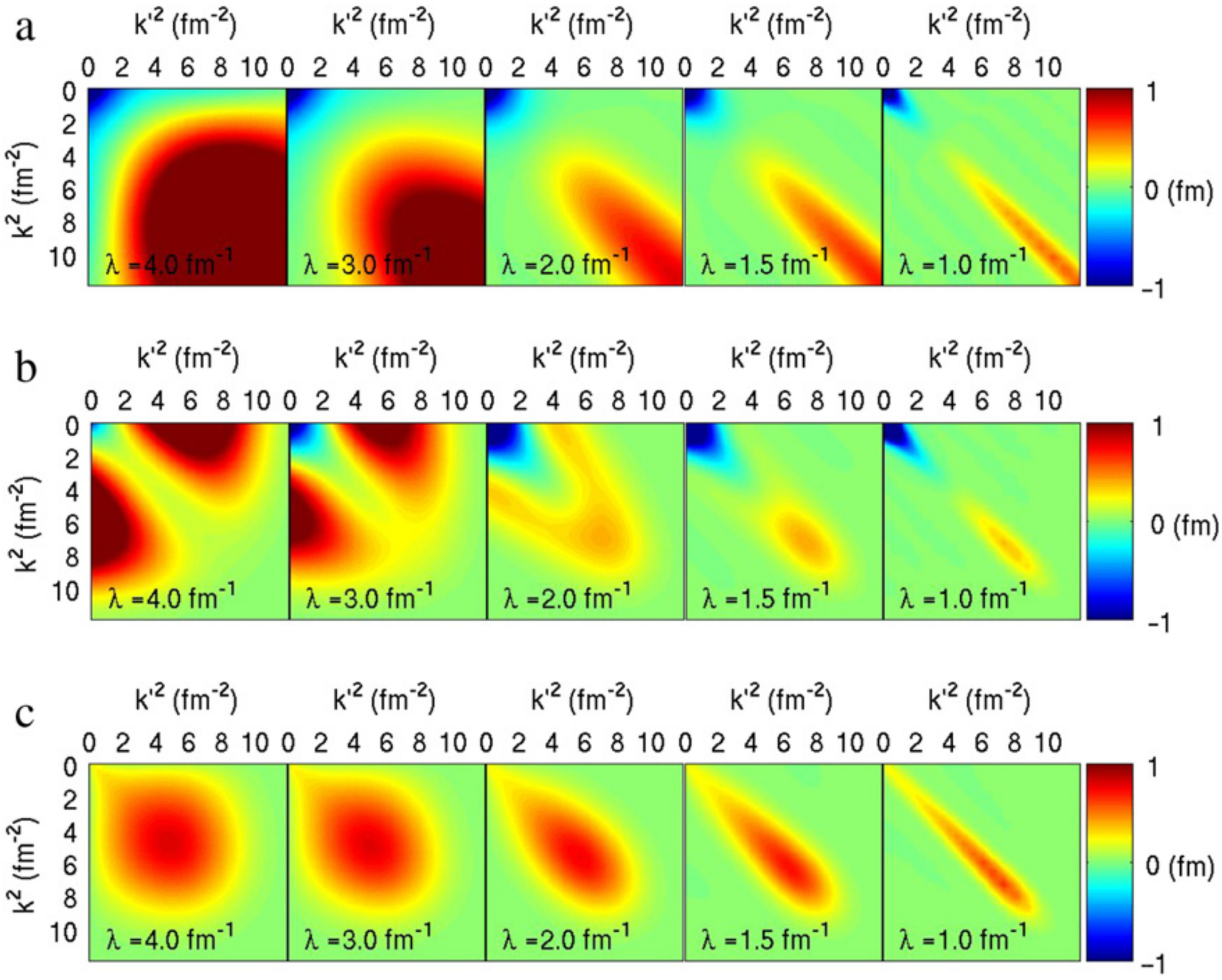
- ○ Goal: achieve decoupling between low- and high-momenta
- ○ Builds on EFT ideas (further change in “resolution”)
- ○ Low-energy observables unchanged
- ○ Corresponding wave functions are less correlated
- ○ Drawback: **additional many-body forces generated**

➪ **Similarity renormalisation group (SRG) transformation**



SRG transformation

$\lambda \equiv \alpha^{-1/4}$ $[\mathrm{fm}^{-1}]$



$^1S_0$

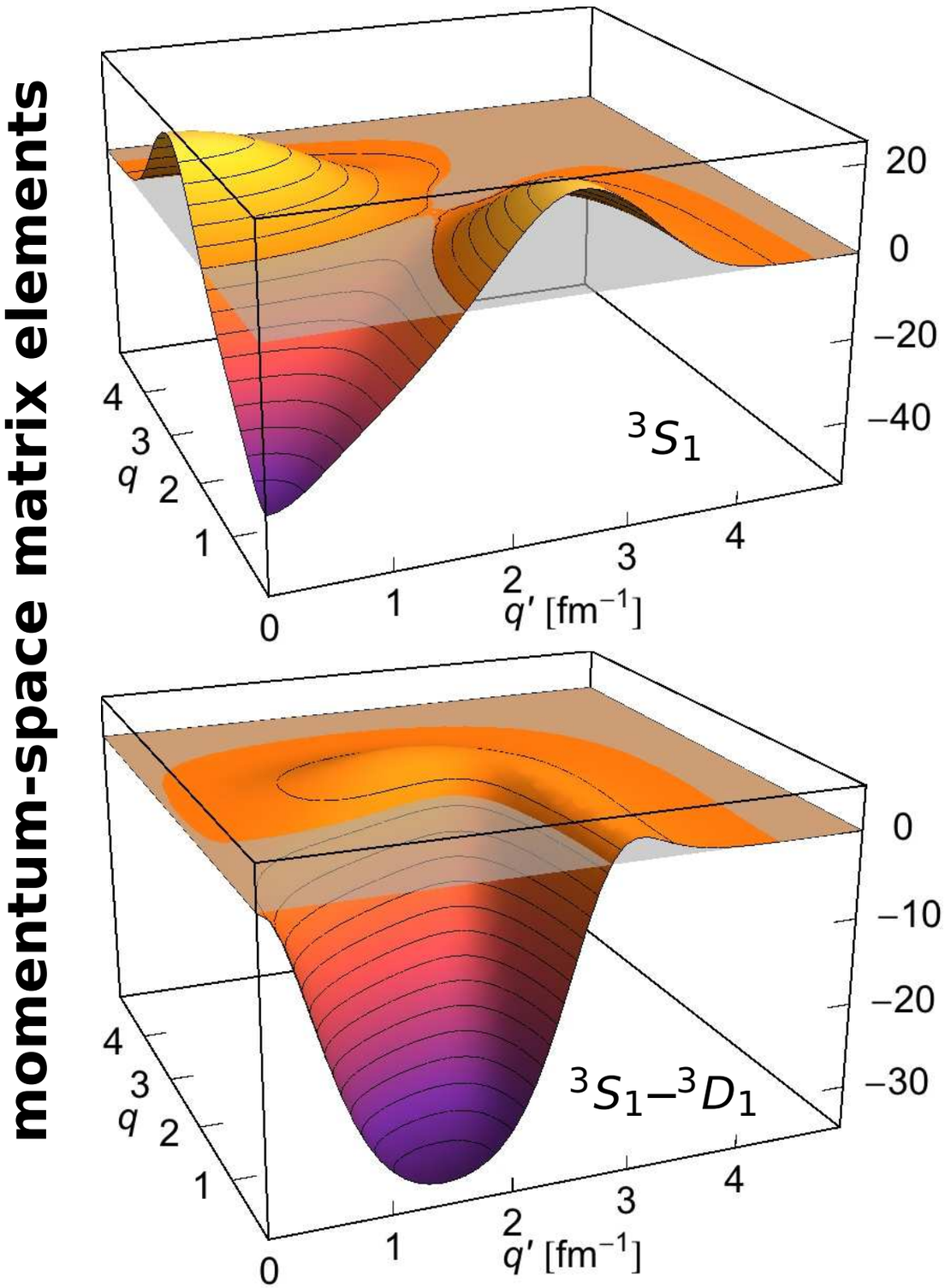
$^3S_1$

$^1P_1$

[Bogner *et al.* 2010]

SRG transformation

[*Figures*: R. Roth]

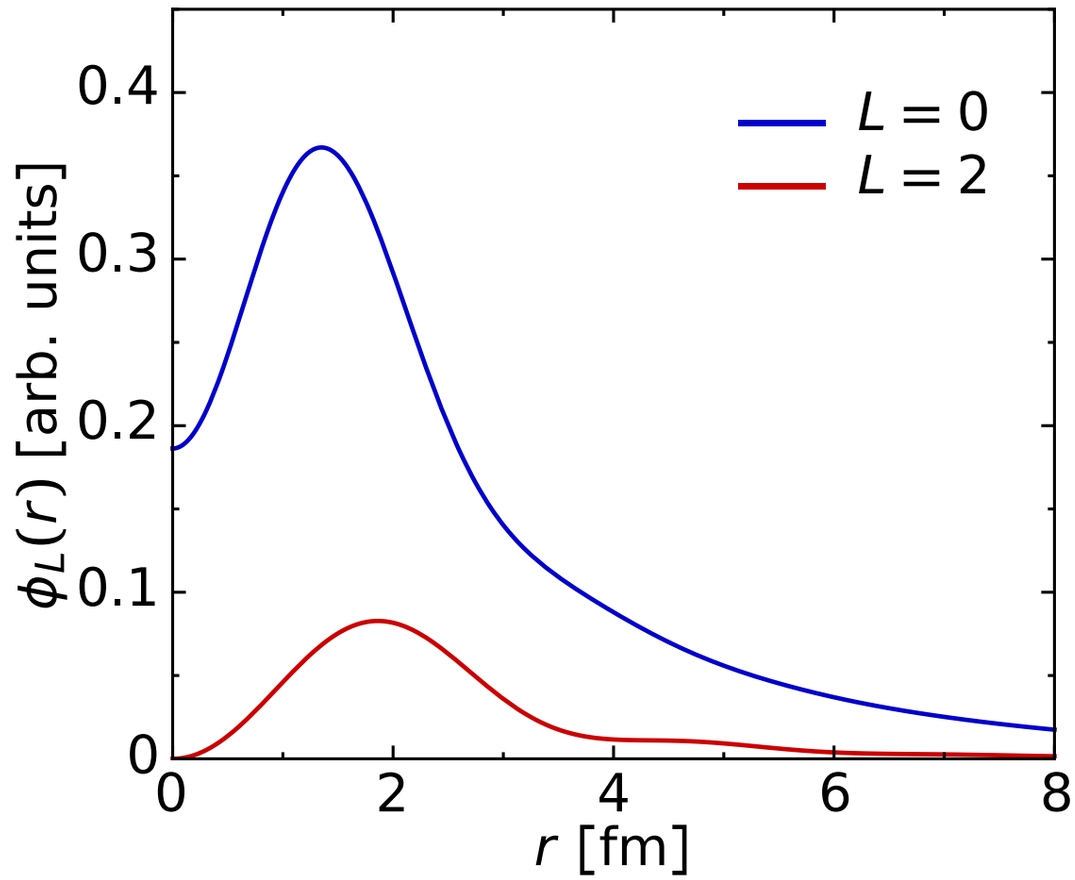


chiral NN

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

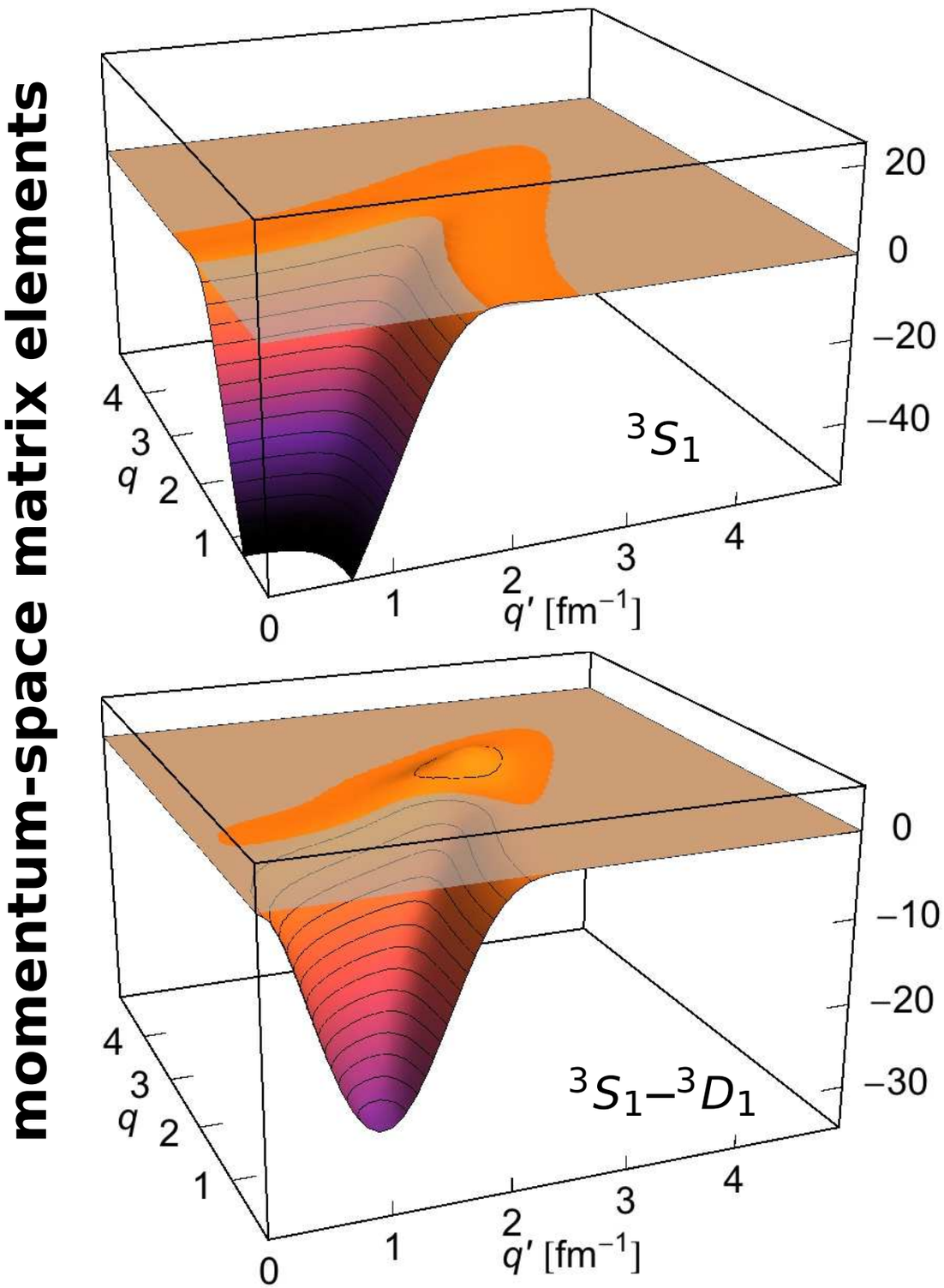
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG transformation

[*Figures*: R. Roth]

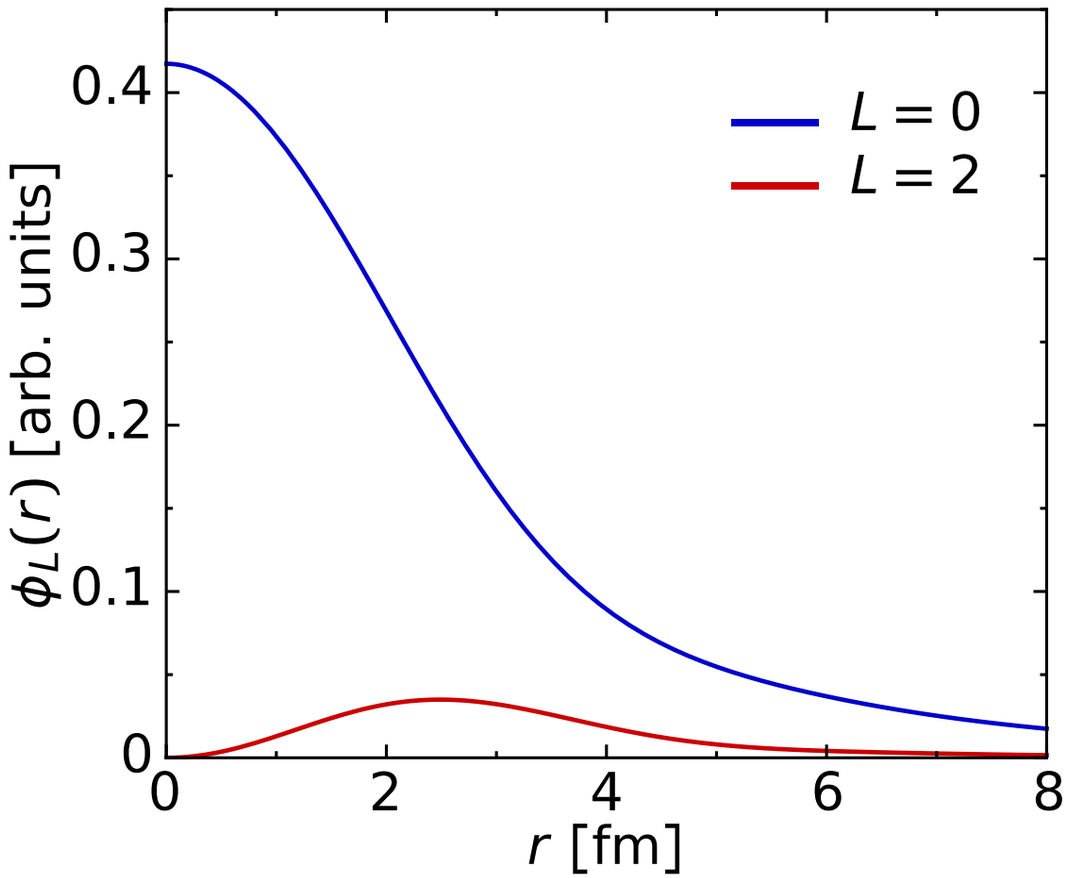


$$\alpha = 0.160\,\mathrm{fm}^4$$

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

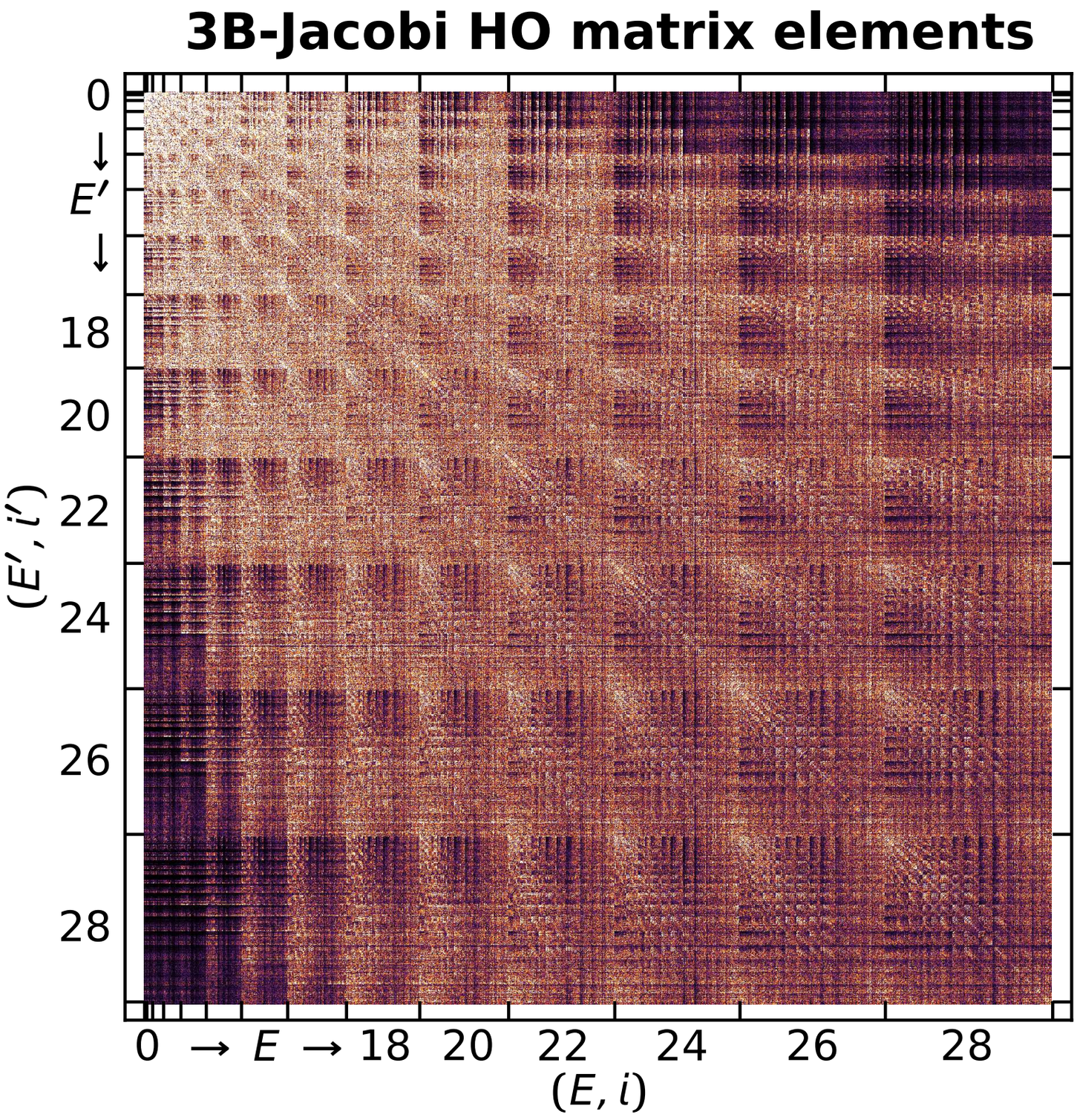
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG transformation

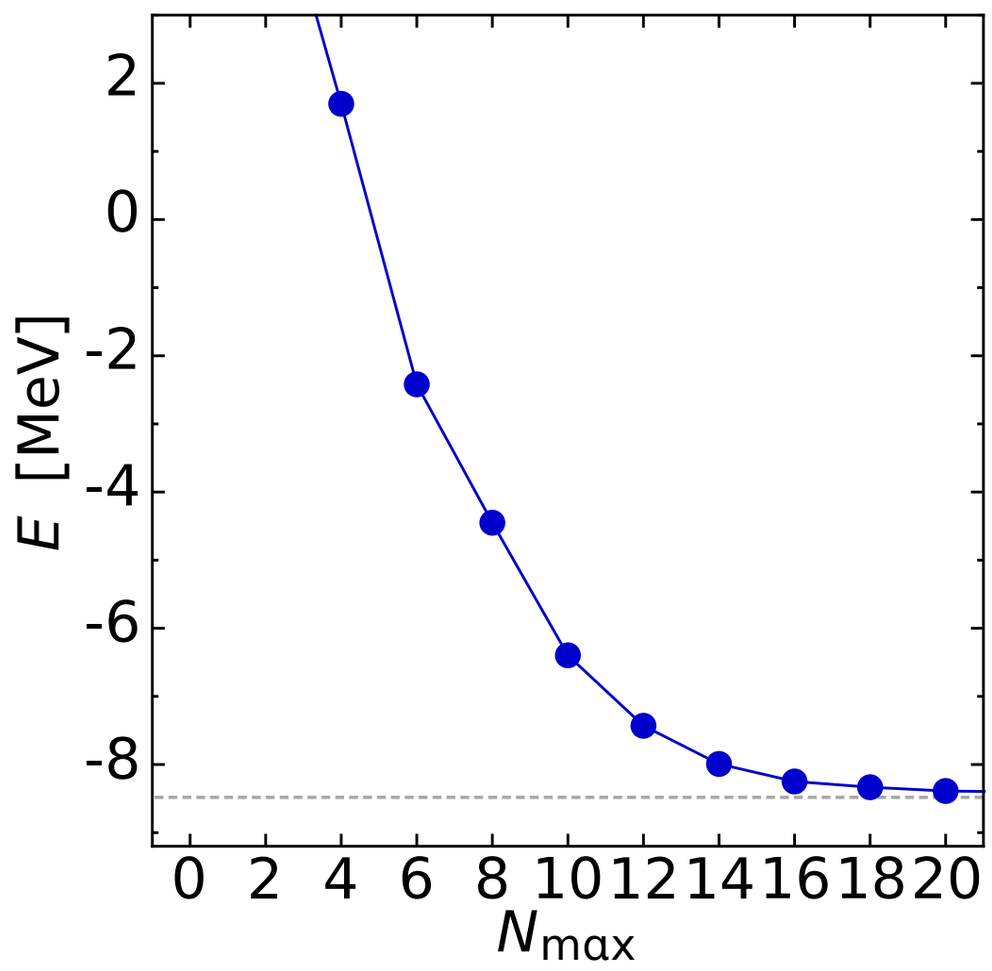
[*Figures*: R. Roth]



chiral NN+3N

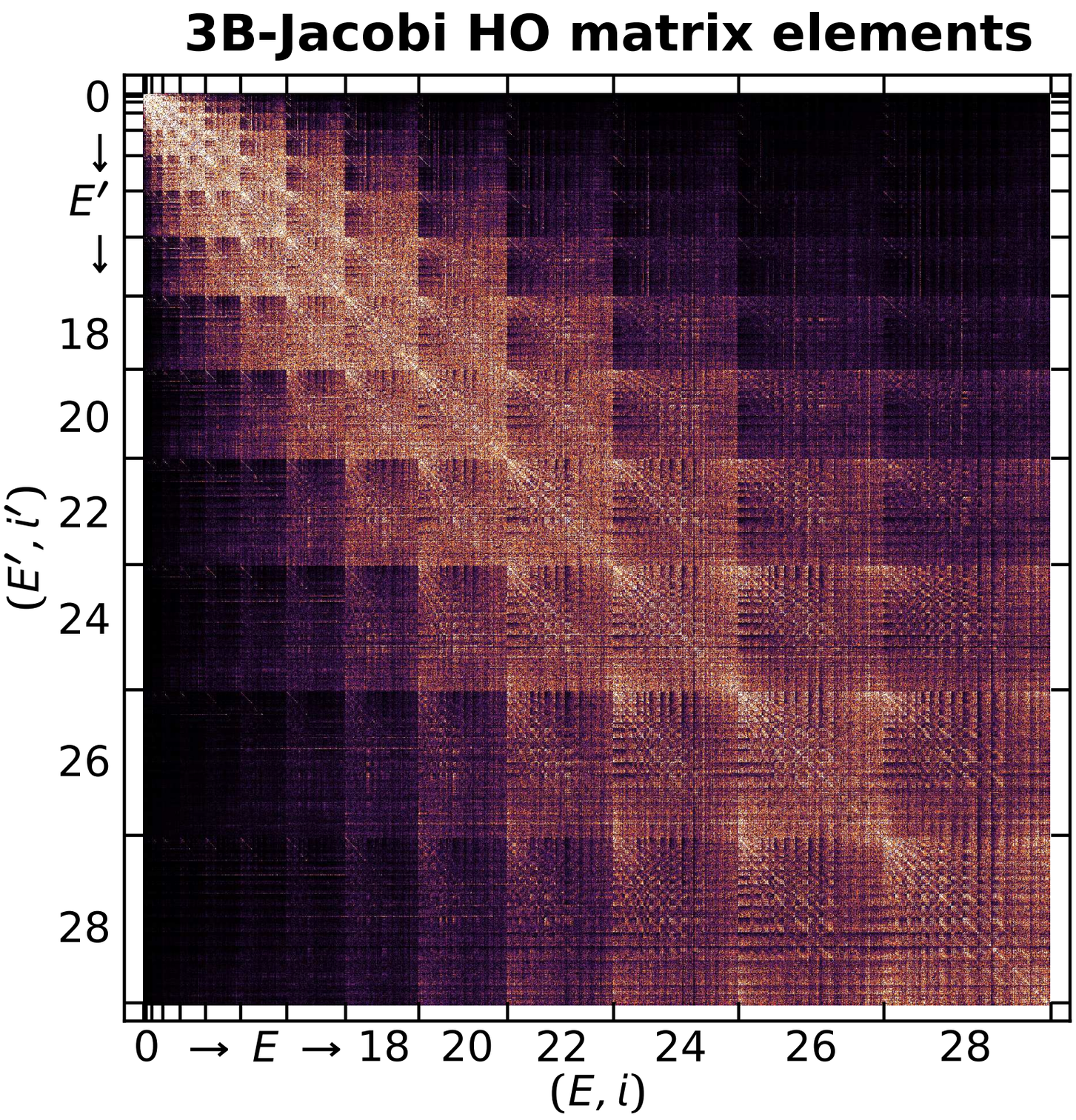
$N^3LO + N^2LO$, triton-fit, 500 MeV

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



SRG transformation

[*Figures*: R. Roth]



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

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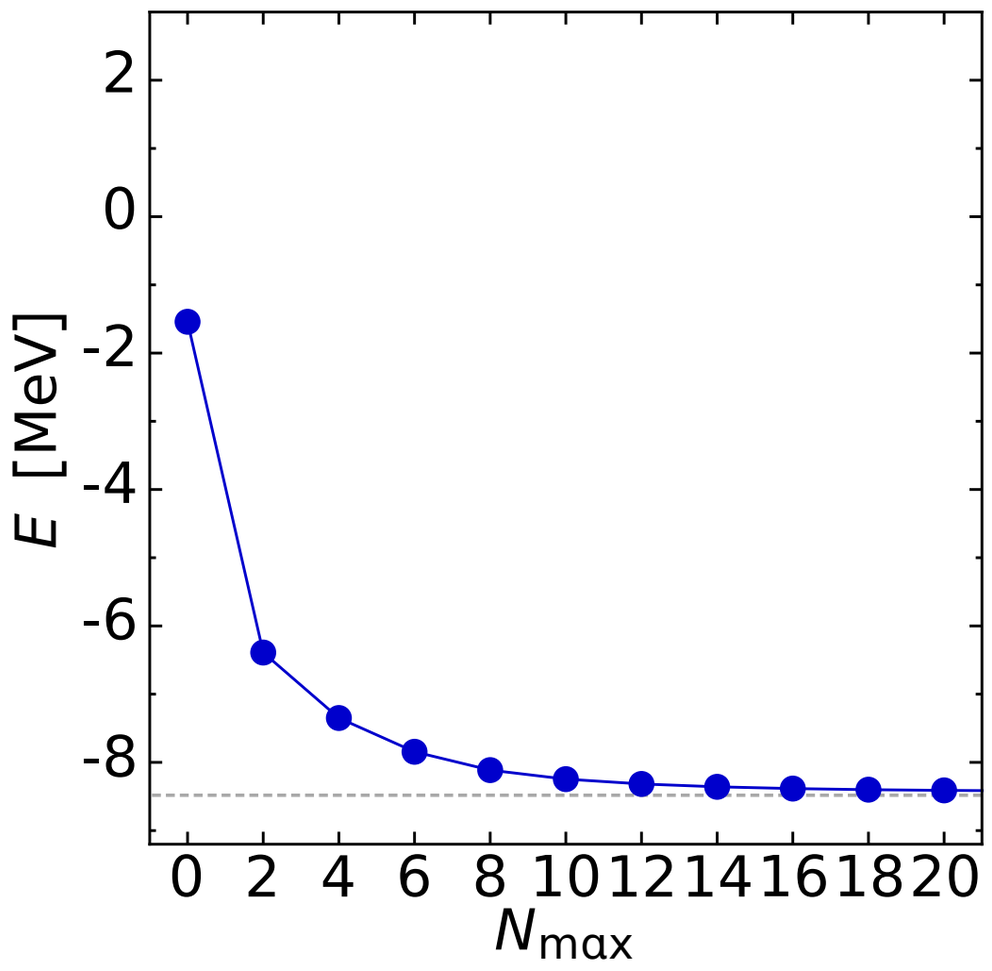
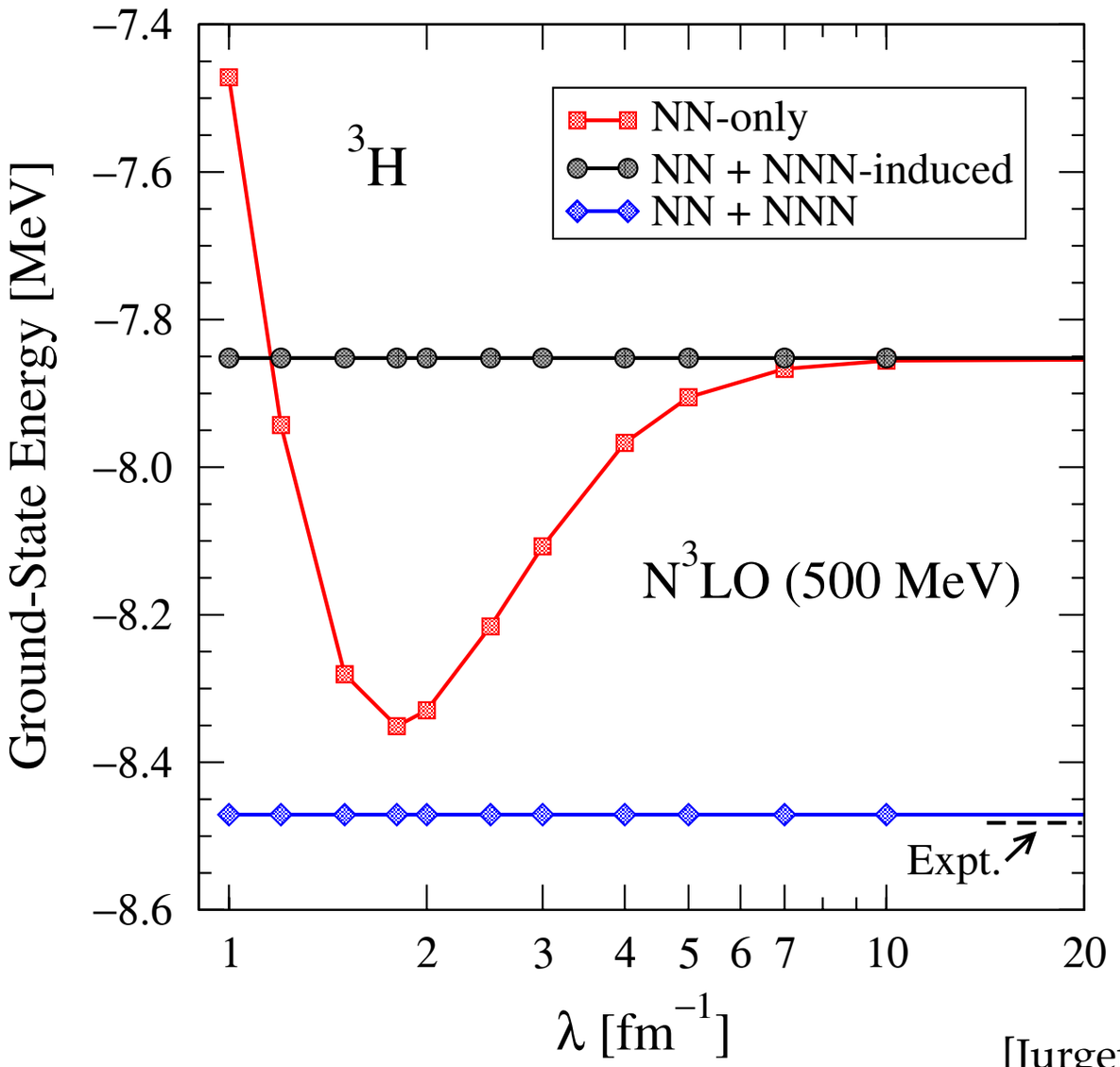
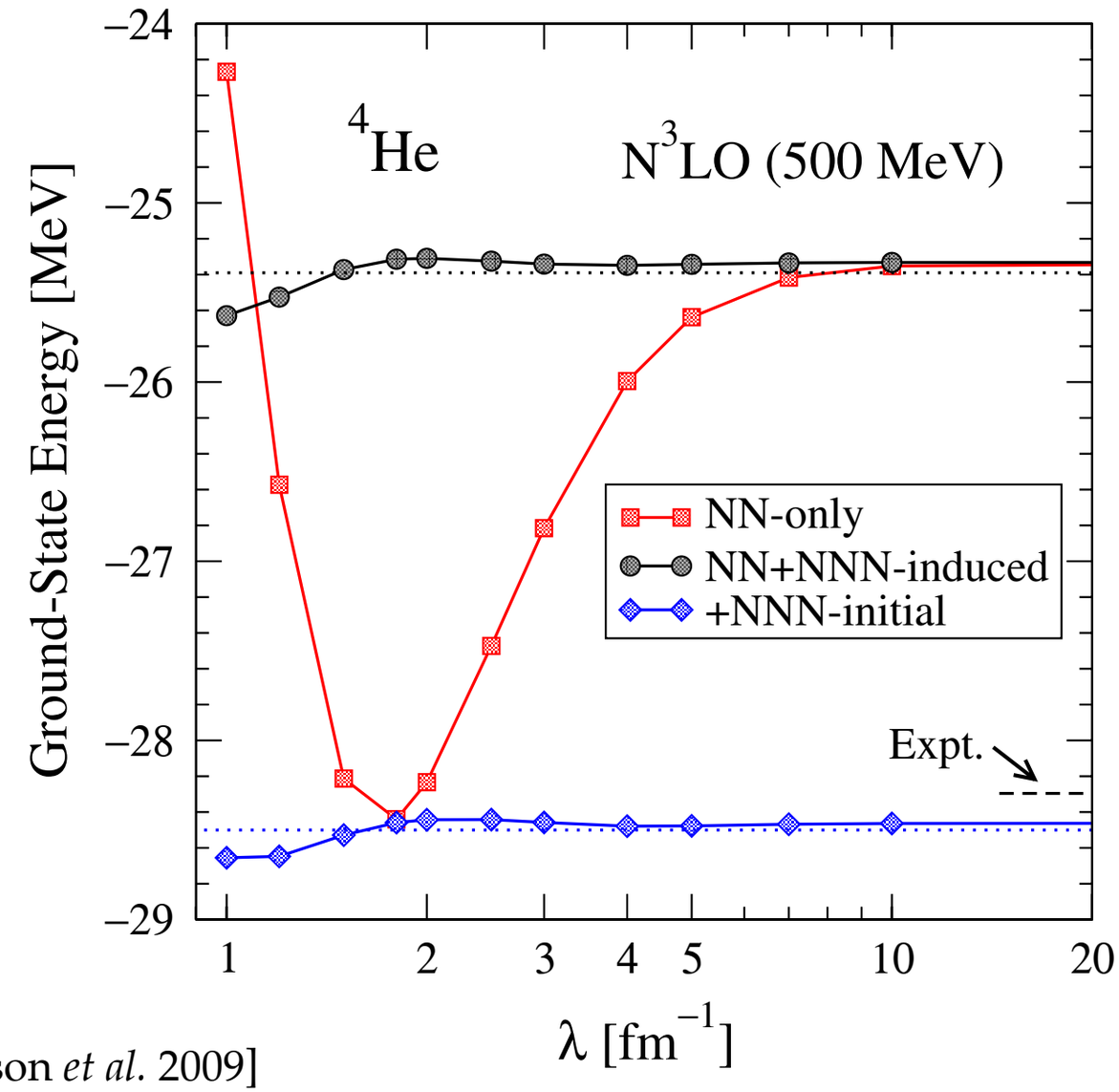
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



SRG in *A*-body systems

⊙ **Effect of induced many-body forces is non-negligible already in small systems**





[Jurgenson *et al.* 2009]

○ **Initial** ("genuine") **4-body** forces assumed to be very small

○ λ-dependence provides estimate of neglected **induced 4-body** contributions in ^{4}He

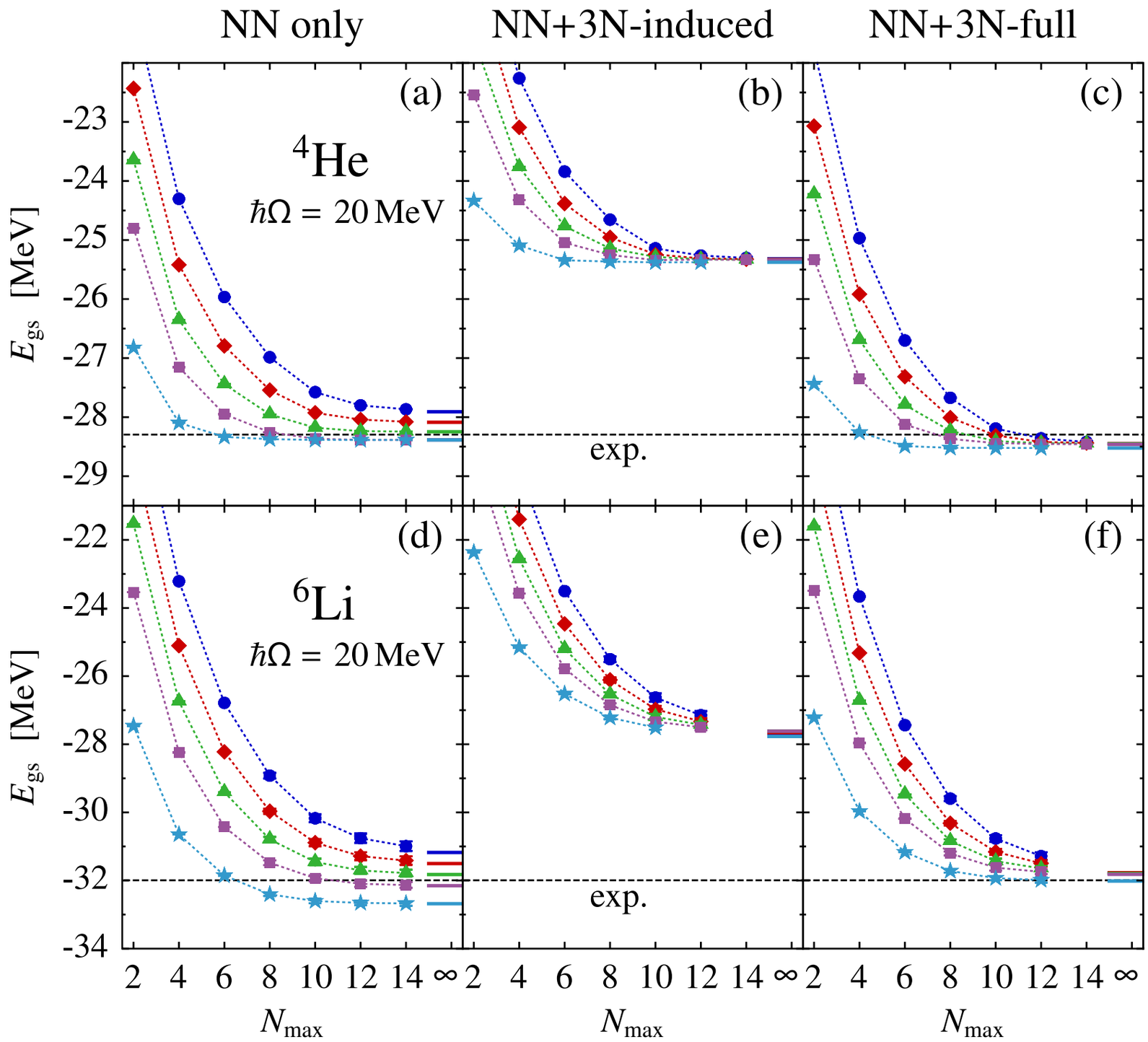
SRG in *A*-body systems

⊙ **Example: no-core shell model calculations of ^{4}He and ^{6}Li ground-state energies**

Flow parameters [fm^{-1}]

- 2.24
- 2.11
- 2.00
- 1.88
- 1.58

SRG evolution



[Roth *et al.* 2011]

Normal-ordered two-body approximation

⊙ From original Hamiltonian (normal-ordered w.r.t. the **particle vacuum**)…

$$H = \sum_{pq} t_{pq}\, c_p^\dagger c_q + \frac{1}{(2!)^2} \sum_{pqrs} v_{pqrs}\, c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2} \sum_{pqrstu} w_{pqrstu}\, c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

⬇ introduce Slater determinant $|\phi_0\rangle = \prod_{i=1}^{A} a_i^\dagger |0\rangle$

… to a Hamiltonian normal-ordered w.r.t. to a **reference Slater determinant**

$$H = h^{(0)} + \sum_{pq} h_{pq}^{(1)}\ :a_p^\dagger a_q: + \frac{1}{2!} \sum_{pqrs} h_{pqrs}^{(2)}\ :a_p^\dagger a_q^\dagger a_s a_r: + \frac{1}{6!} \sum_{pqrstu} h_{pqrstu}^{(3)}\ :a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s:$$

⊙ Define density matrix & occupation numbers

$$\rho_{pq} \equiv \langle \phi_0 | a_p^\dagger a_q | \phi_0 \rangle = n_p\, \delta_{pq} \quad \rightarrow \quad \begin{cases} n_i = 1 & \text{holes} \\ n_a = 0 & \text{particles} \end{cases}$$

Normal-ordered two-body approximation

⊙ **Normal-ordered matrix elements**

$$h^{(0)} = \sum_i t_{ii}\, n_i + \frac{1}{2}\sum_{ij} v_{ijij}\, n_i n_j + \frac{1}{6}\sum_{ijk} w_{ijkijk}\, n_i n_j n_k$$

$$h^{(1)}_{pq} = t_{pq} + \sum_i v_{piqi}\, n_i + \frac{1}{2}\sum_{ij} w_{pijqij}\, n_i n_j$$

$$h^{(2)}_{pqrs} = v_{pqrs} + \sum_i w_{pqirsi}\, n_i$$

$$h^{(3)}_{pqrstu} = \cancel{w_{pqrstu}}$$

Large part of the original 3N transferred into effective lower-rank operators

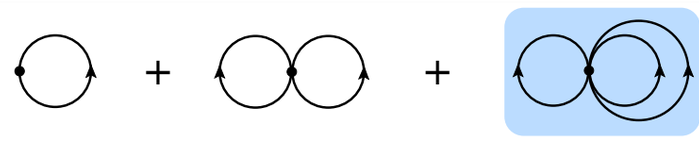
Normal-ordered 2-body approximation (NO2B)

→ Discard residual 3N operator

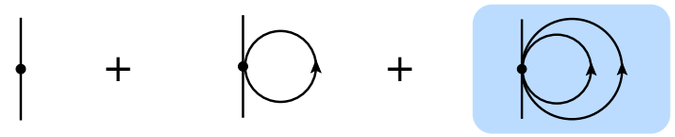
Normal-ordered two-body approximation

⊙ **Normal-ordered matrix elements**

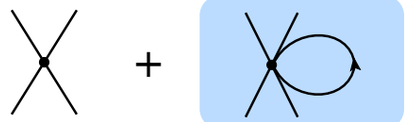
$$h^{(0)} = \sum_i t_{ii}\, n_i + \frac{1}{2}\sum_{ij} v_{ijij}\, n_i n_j + \frac{1}{6}\sum_{ijk} w_{ijkijk}\, n_i n_j n_k =$$



$$h^{(1)}_{pq} = t_{pq} + \sum_i v_{piqi}\, n_i + \frac{1}{2}\sum_{ij} w_{pijqij}\, n_i n_j =$$



$$h^{(2)}_{pqrs} = v_{pqrs} + \sum_i w_{pqirsi}\, n_i =$$



$$h^{(3)}_{pqrstu} = \cancel{w_{pqrstu}}$$

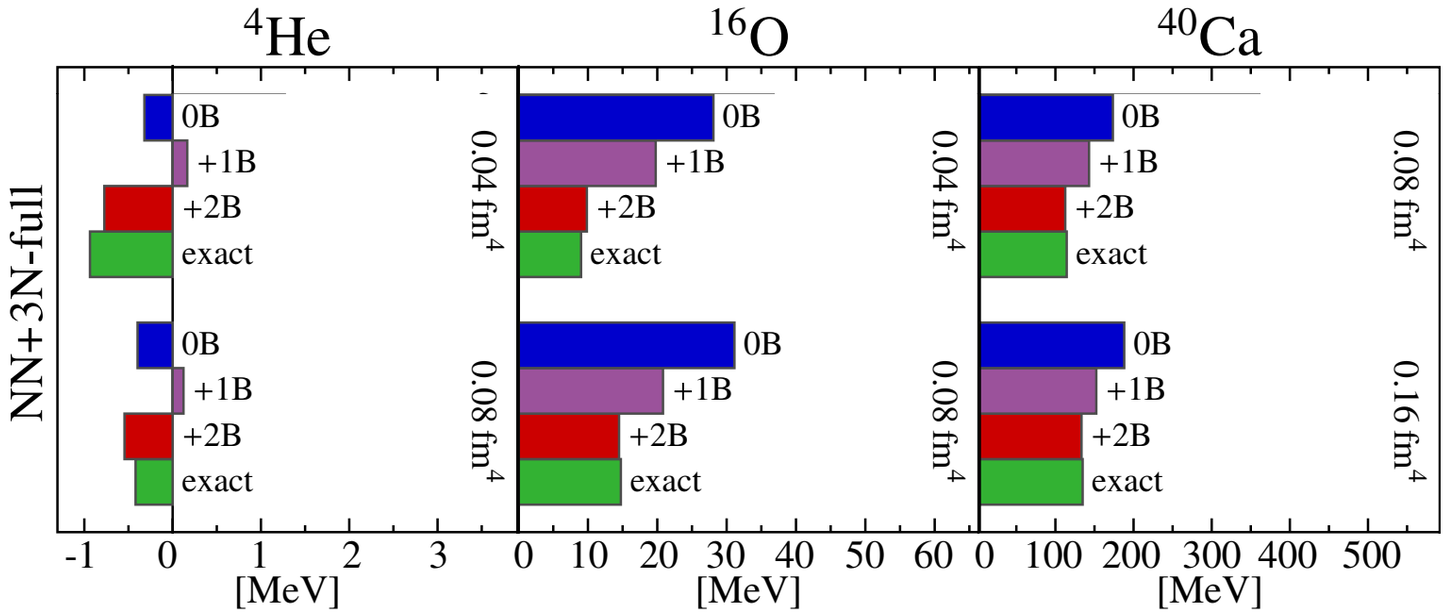
Normal-ordered 2-body approximation (NO2B)

→ Discard residual 3N operator

⊙ **Benchmarked** in light nuclei

- 1-3% error
- Comparable to other errors

[Roth *et al.* 2012]



Importance truncation

- **Not all matrix elements of H are equally relevant**
  - $N_{\max}$ cuts might not be the most efficient way of selecting important entries
  - Is there a way of **discarding *a priori* the most irrelevant entries** for a given $N_{\max}$?

- **Importance truncation**: prior to diagonalisation

  1. Estimate the size of each entry upon a given criterion
  2. Discard irrelevant entries (i.e., make the matrix even more sparse)

     ➪ Construct **importance-truncated space** from all basis states having $|\kappa_\nu| \geq \kappa_{\min}$

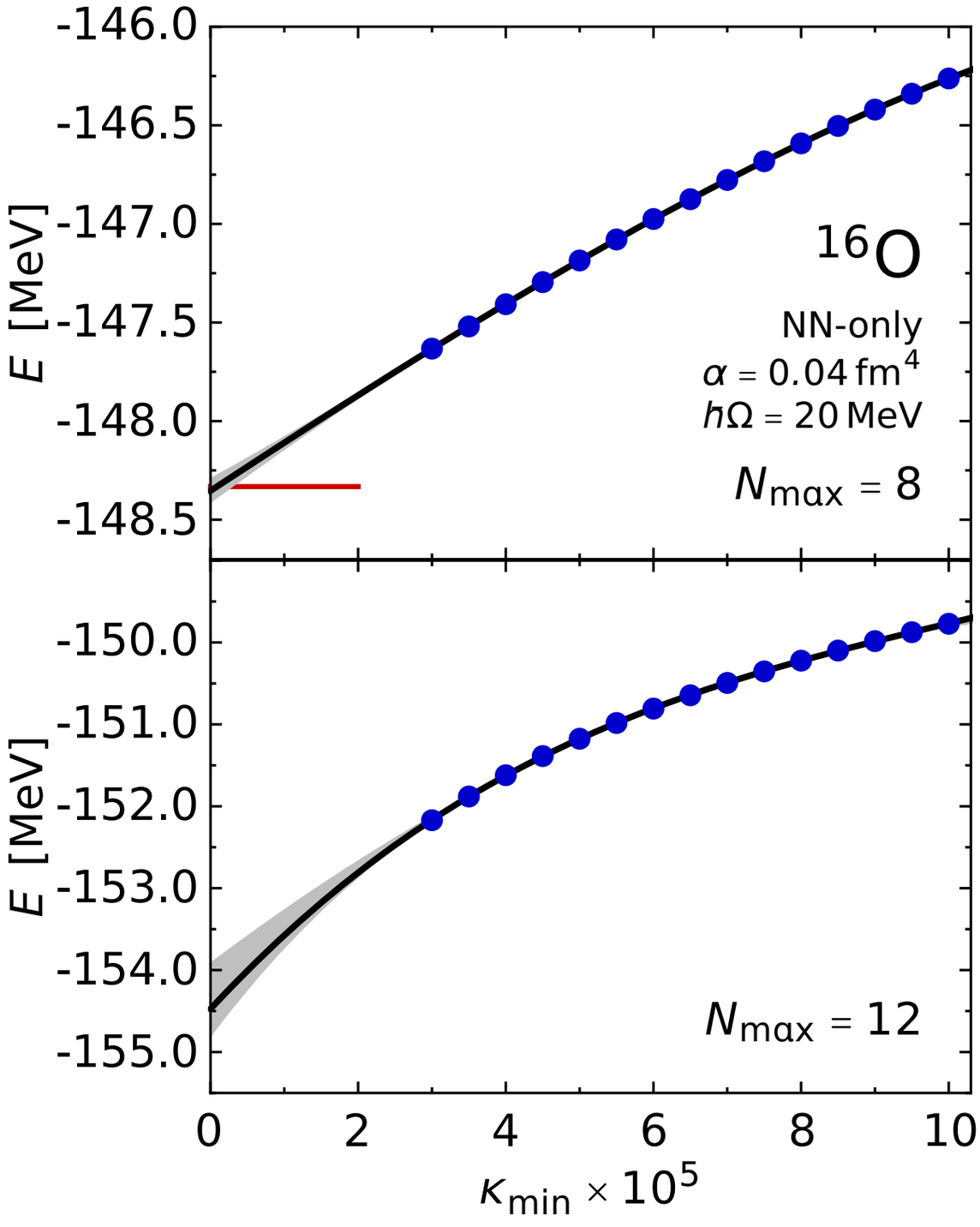
- **Required features**:
  - Estimate has be done with a **cheap** method

    - Typical tool of choice: **many-body perturbation theory**
  - In the limit of null threshold one must recover the original (exact) problem

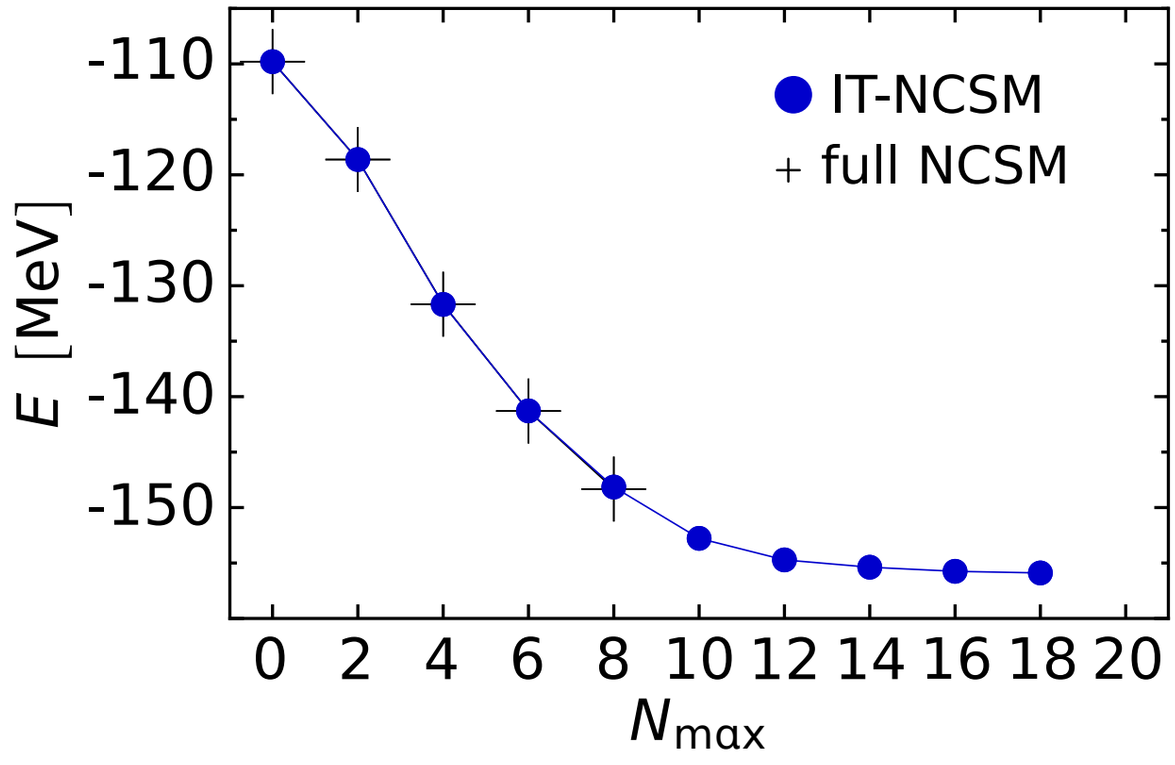
    - Smooth behaviour desirable in order to **perform extrapolations**

Importance truncation

⊙ Example: **no-core shell model calculation of ^{16}O** [Roth 2009]

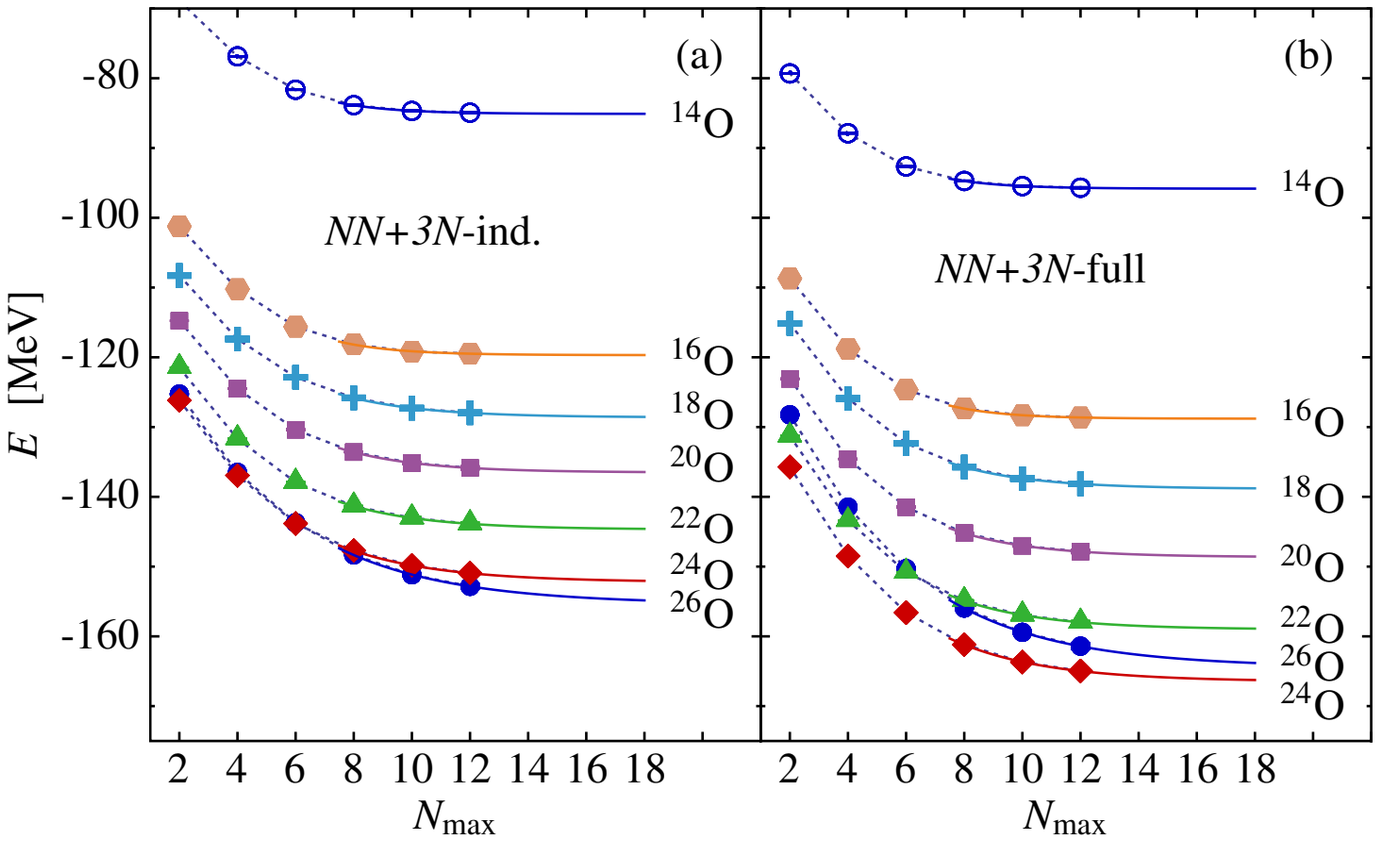


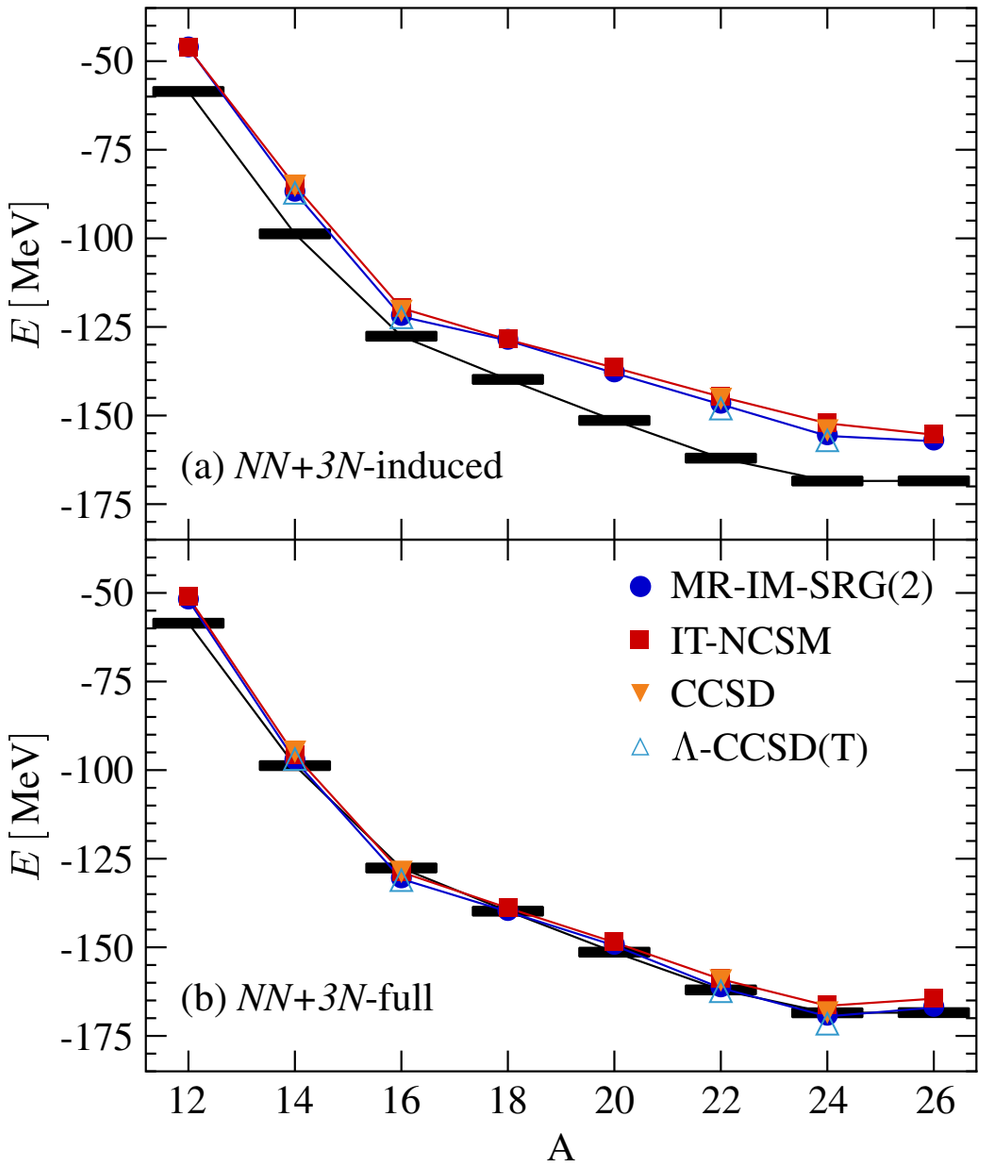
- Smooth threshold dependence
- Extrapolation to un-truncated result
- Uncertainty quantification from fit
- Benchmarks possible for for small $N_{\max}$



Applications: oxygen isotopes

⊙ **First ab initio calculations with NN+3N chiral interactions along the oxygen chain**





○ Converged results achieved **up to ^{24}O**

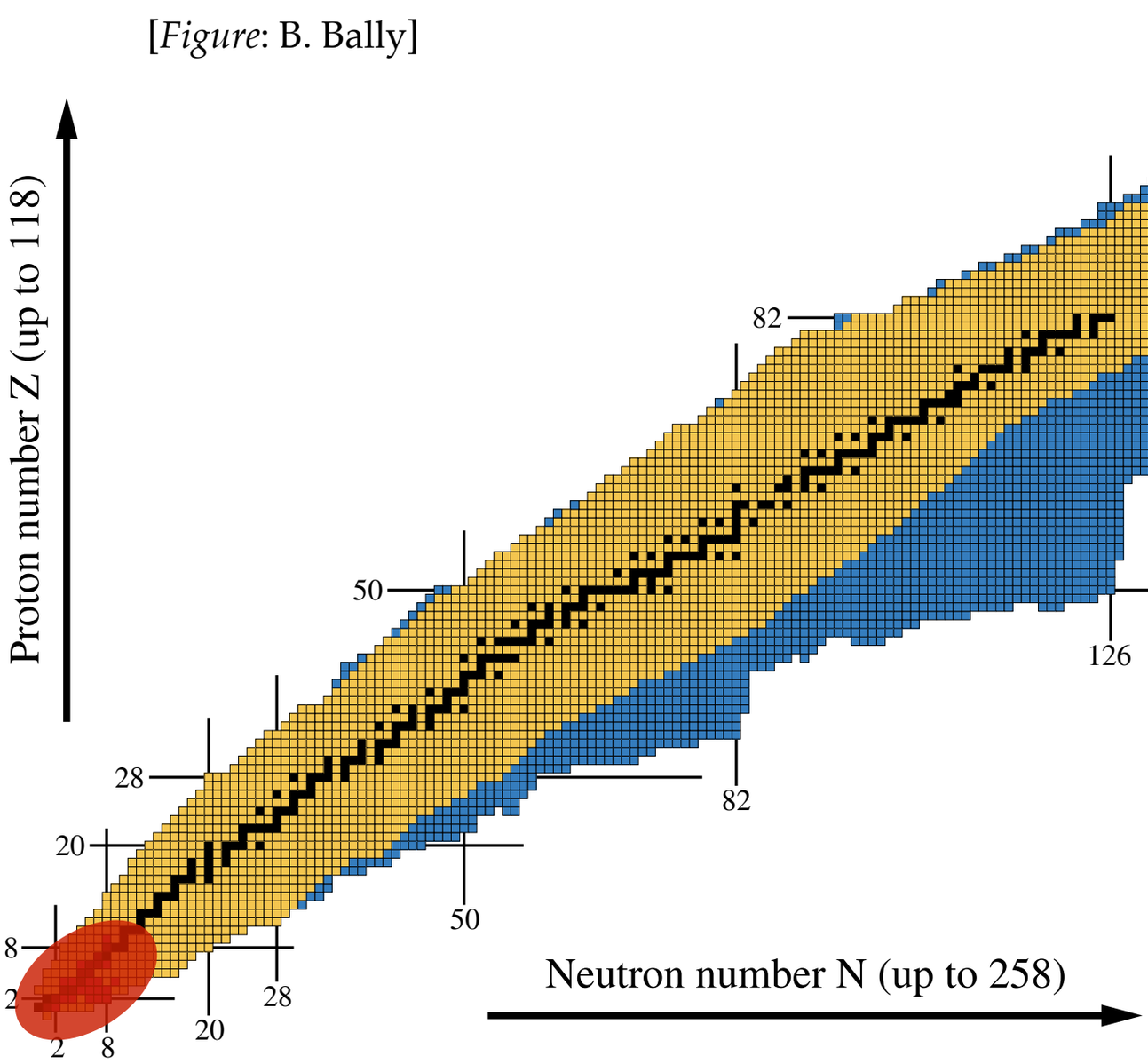
○ **Unbound ^{26}O** harder to compute in HO basis

○ Role of "genuine" 3N forces evident

[Hergert *et al.* 2013]

Applicability of exact ab initio approaches

[*Figure*: B. Bally]



- Stable
- Atomic mass evaluation 2020
- *Ab initio* 2010
- Energy density functional (Gogny D1M)

Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
H. Hergert (private communications)