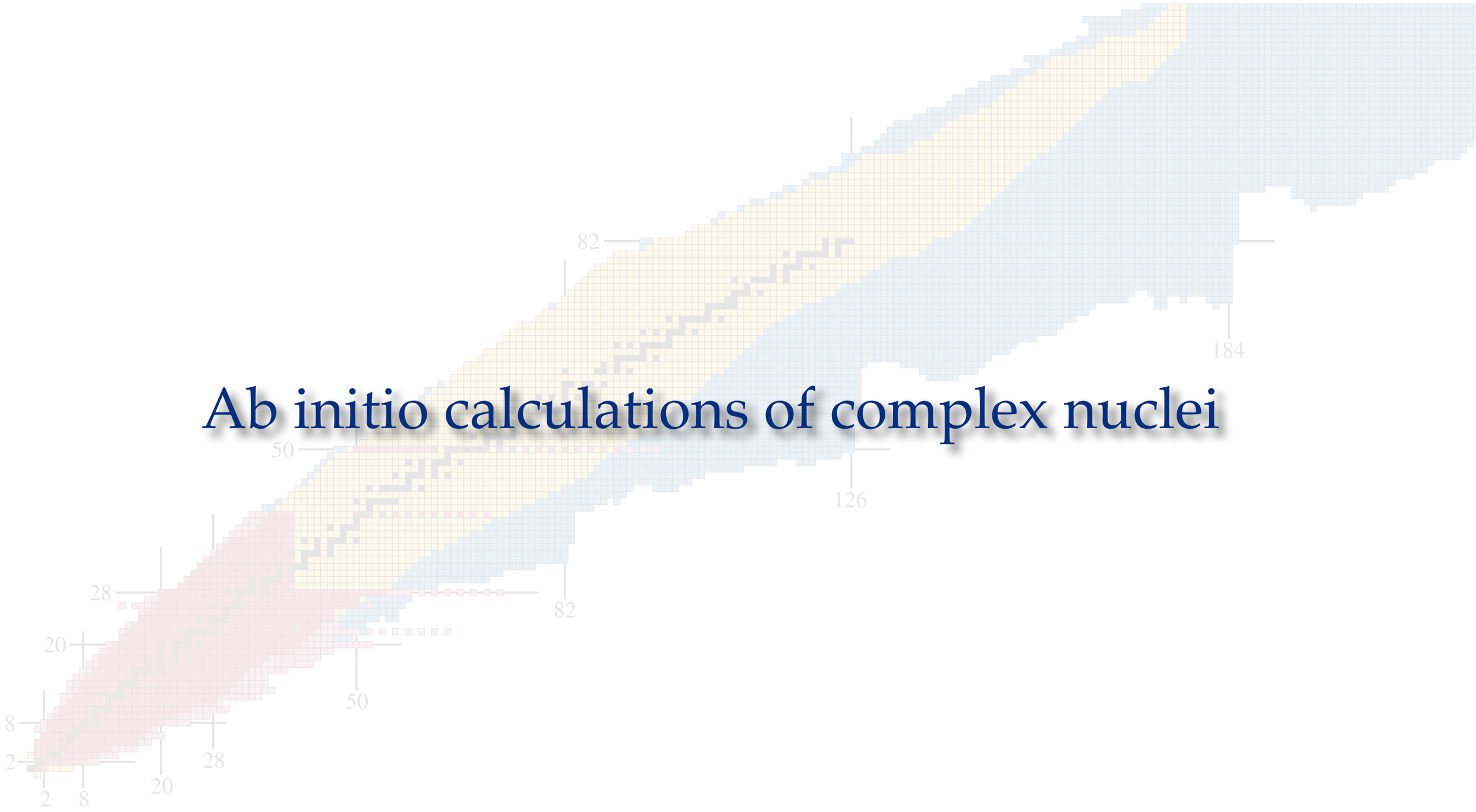


Ab initio calculations of complex nuclei

Fiera di Primiero
26-30 September 2022

Vittorio Somà
CEA Saclay

Programme

1. Ab initio description of nuclei

2. Exact many-body methods

3. Expansion many-body methods for closed-shell nuclei

4. Expansion many-body methods for open-shell nuclei

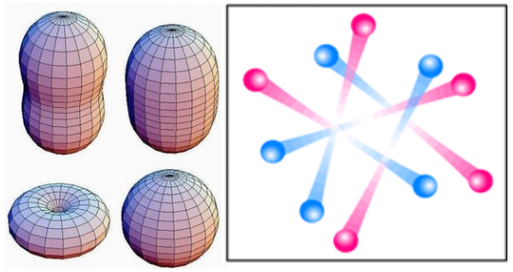
Part 1

Ab initio description of nuclei

Diversity of nuclear phenomena

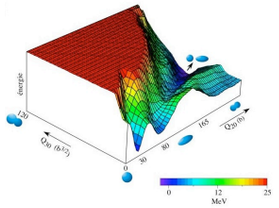
Ground state

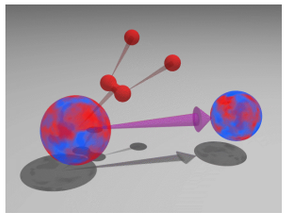
Mass, size, superfluidity, …



Radioactive decays

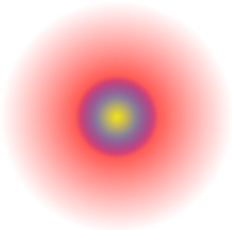
β, 2β, α, p, 2p, fission, …

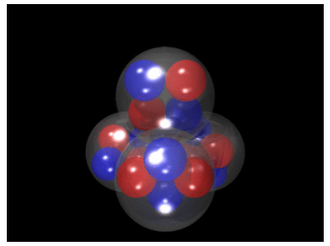


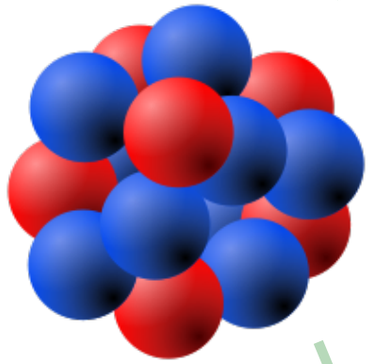


Exotic structures

Clusters, halos, …







Strongly-correlated systems

Angular corr. → Deformation

Pairing corr. → Superfluidity

Quartet corr. → Clustering

Several scales at play

Nucleon momenta ~ **100** MeV

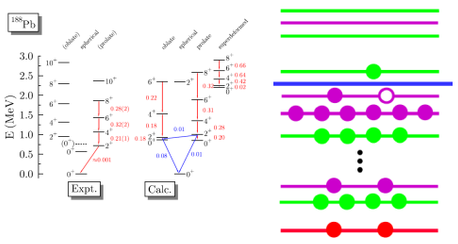
Separation energies ~ **10** MeV

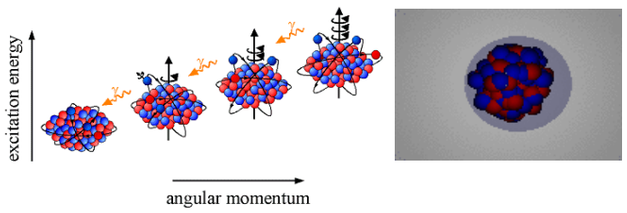
Vibration modes ~ **1** MeV

Rotation modes ~ **0.01-few** MeV

Spectroscopy

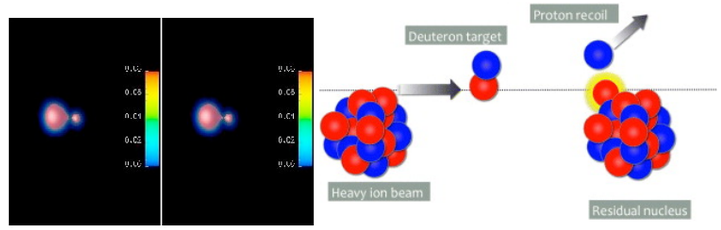
Excitation modes





Reaction processes

Fusion, transfer, knockout, …



Which is the most appropriate theoretical description?

⊙ **Richness of nuclear phenomena propelled the formulation of many models**

Ab initio

Energy density functionals

Shell model

Interacting boson model

Cluster model

Algebraic model

Liquid drop model

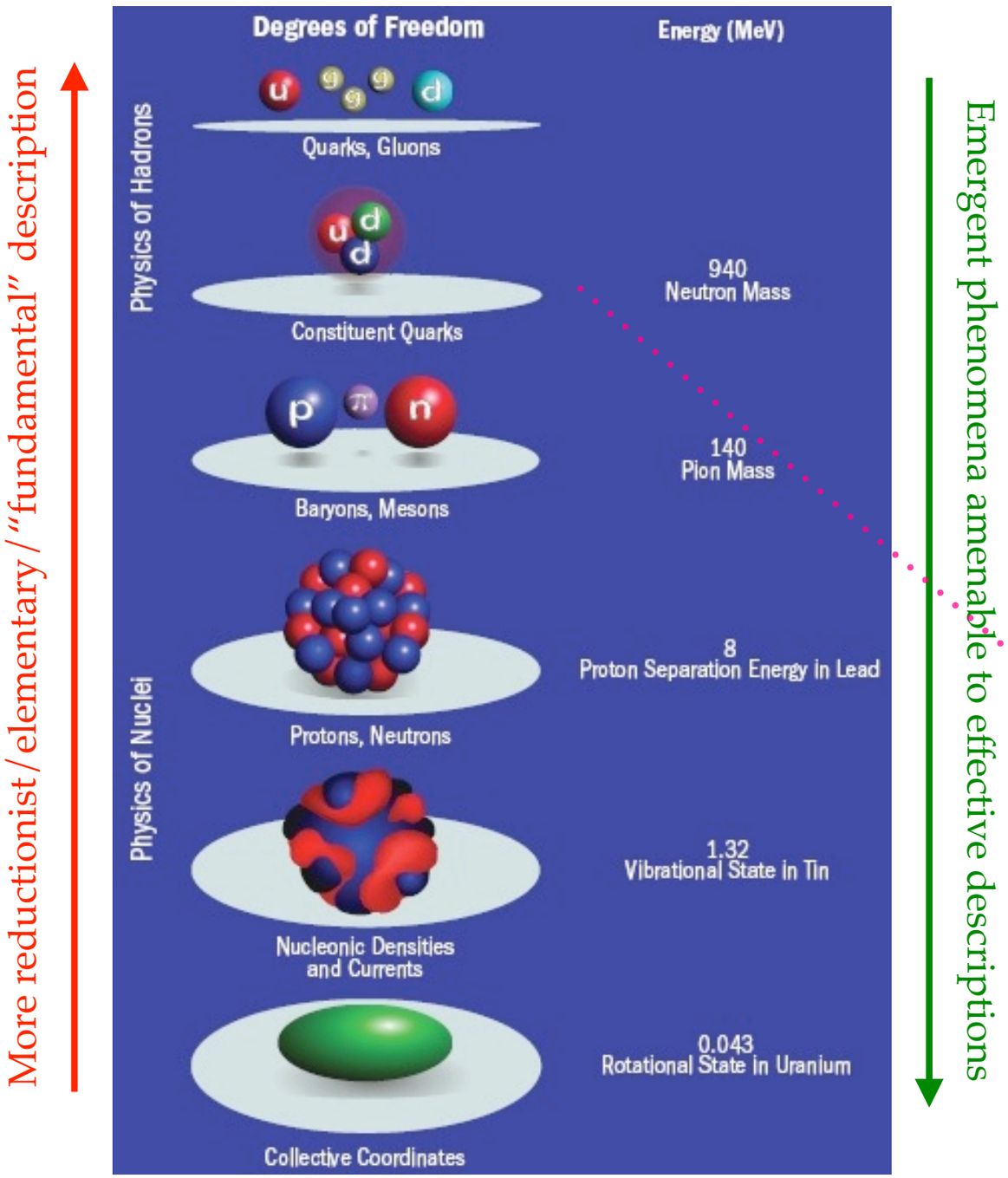
Collective model

- ○ Motivated by regularities observed in data
- ○ Lack of systematic character
- ○ Different models not always consistent

Is a unified / consistent / systematic description possible?

Which is the most appropriate theoretical description?

⊙ **Modern view: effective (field) theories**



1. Separation of scales → Definition of d.o.f.

2. Most general dynamics → All allowed terms

3. Organisation → Power counting

4. Truncation & fit of interaction strengths

➪ **Systematically improvable**

➪ **Internal consistency check**

Possible choices as d.o.f.

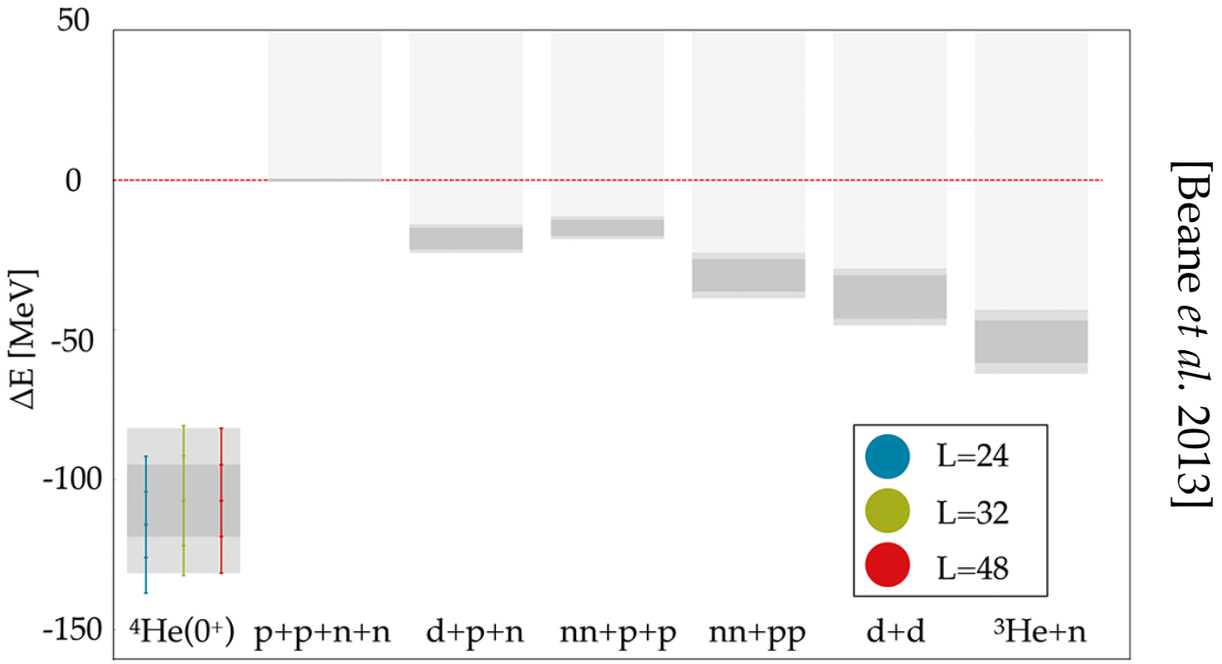
Quarks & gluons

Nuclei from lattice QCD

⊙ **First option: compute directly nuclear observables**

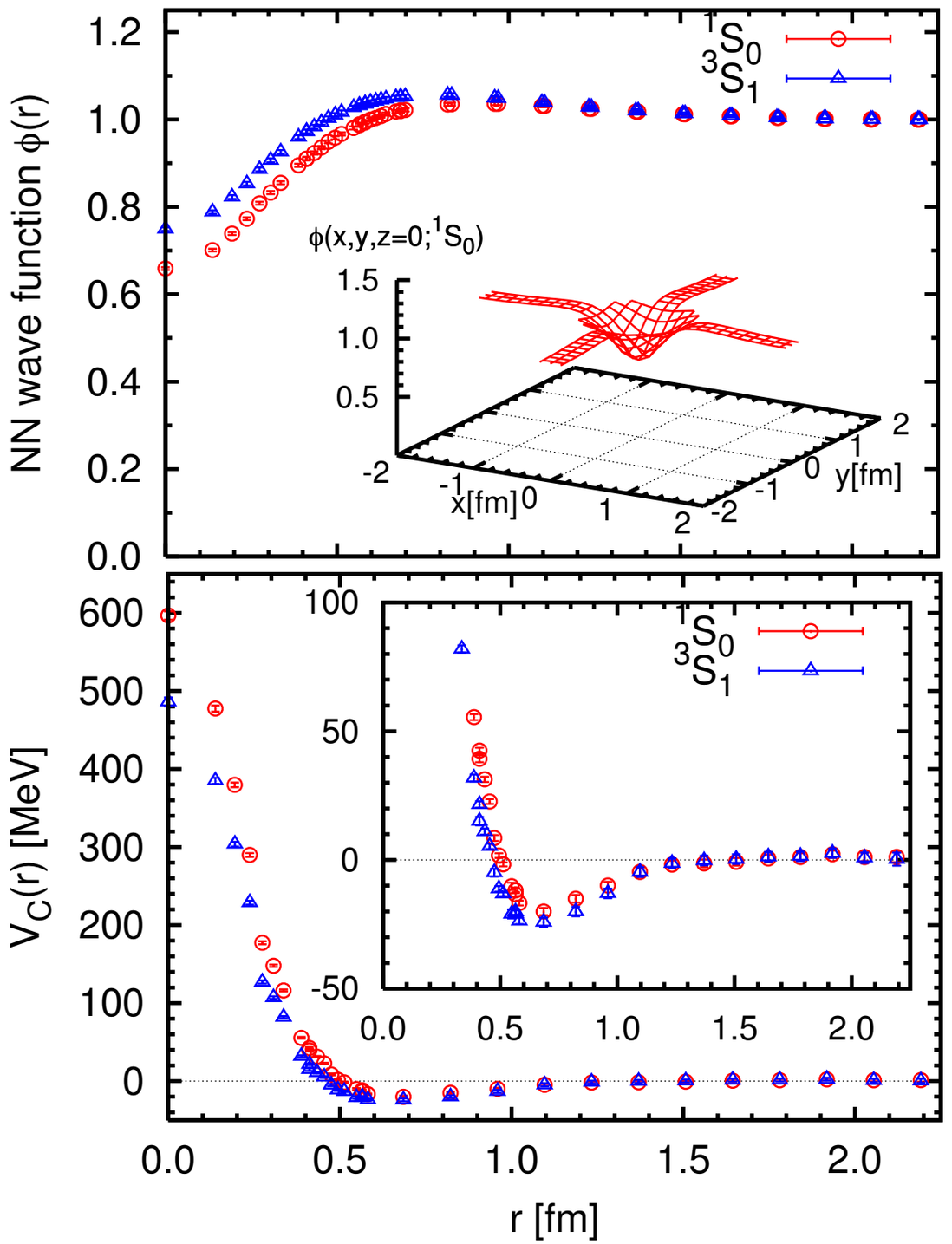
✗ Noise-to-signal ratio of A-nucleon correlation functions scales as $e^{A\left(M_N-\frac{3}{2}m_\pi\right)t}$

✓ Could provide highly useful benchmarks



[Beane *et al.* 2013]

[Ishii *et al.* 2007]



⊙ **Second option: compute NN (& NNN) potential**

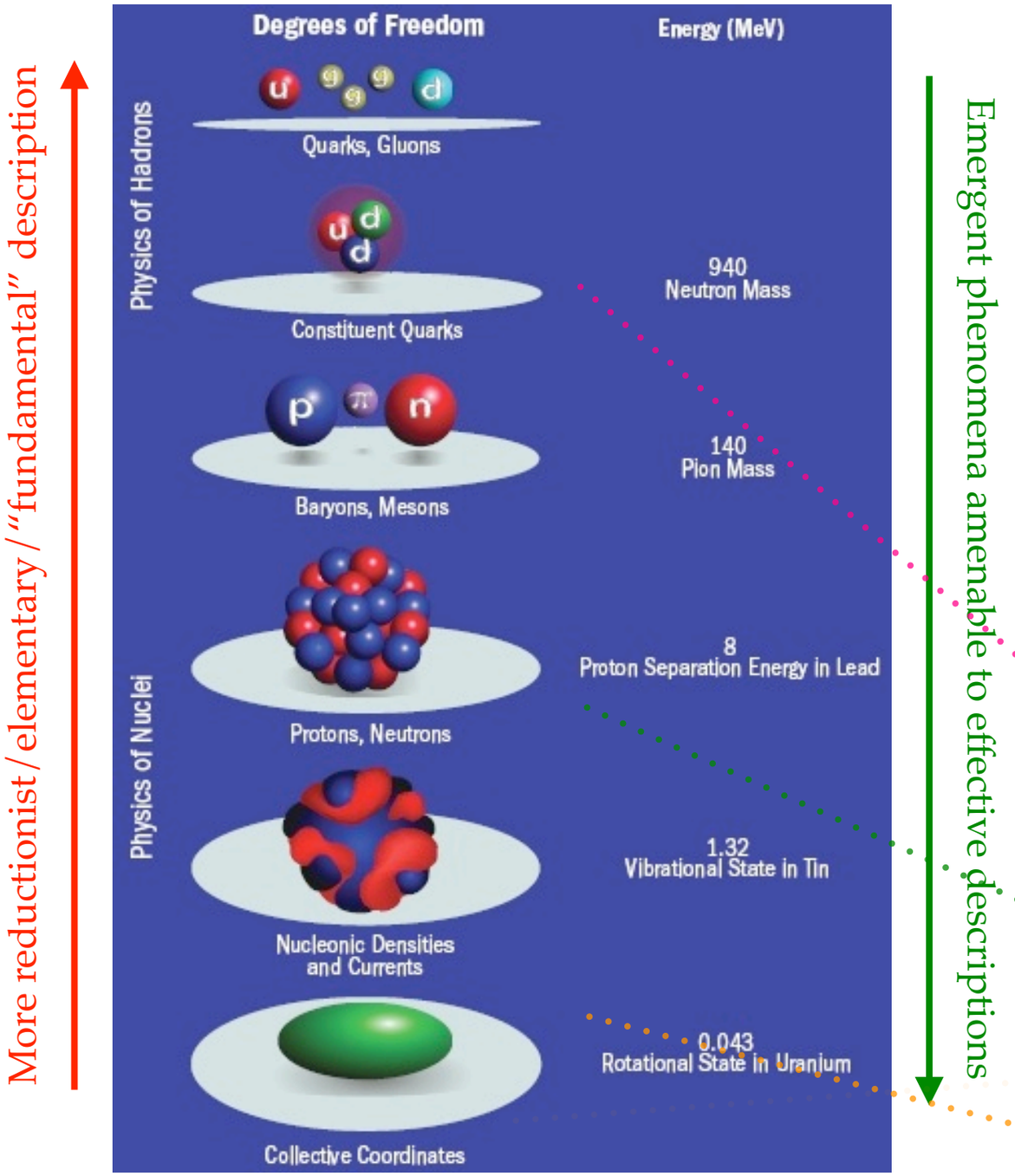
✗ Unphysical pion masses

✗ Difficult to extend to 3-body forces

✓ Extremely useful if extended to hyperons

Which is the most appropriate theoretical description?

⊙ **Modern view: effective (field) theories**



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➪ **Systematically improvable**

➪ **Internal consistency check**

Possible choices as d.o.f.

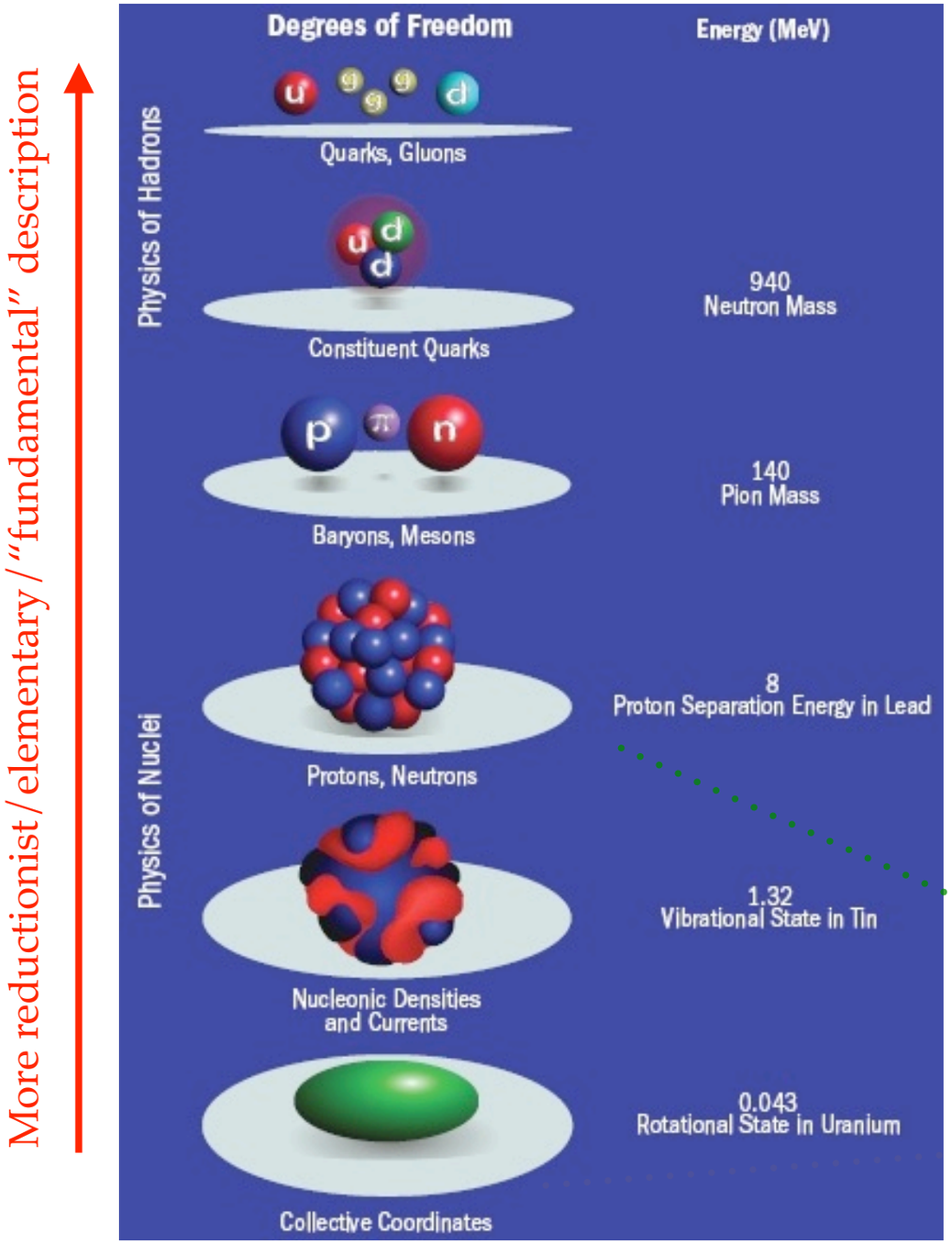
Quarks & gluons

Nucleons

Rotation/vibration modes

Which is the most appropriate theoretical description?

⊙ **Modern view: effective (field) theories**



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➪ **Systematically improvable**

➪ **Internal consistency check**

Possible choices as d.o.f.

Quarks & gluons

Nucleons

Rotation/vibration modes

Ab initio nuclear many-body problem

Goal: solve ***A*-body Schrödinger equation** (for any A=Z+N)

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

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

1. Model interactions between nucleons

a) Model the form of H

b) Fit coupling constants in H

c) Pre-process H

input ⇢

⇠ feedback

2. Solve many-body Schrödinger eq.

a) Formulate many-body approach

b) Implement, benchmark, optimise

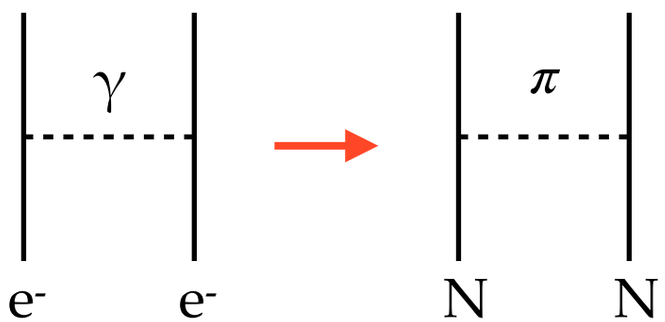
c) Run calculations

➪ **Difficult formal and computational tasks**

- Automatised algebraic derivations
- Techniques from applied maths
- High-performance computing

One-boson exchange potentials

⊙ **Yukawa potential**: nuclear force mediated by massive spin-0 boson (the "mesotron" → later, pion)



Yukawa potential

$$V(r) \propto \frac{e^{-mr}}{r}$$

m ~ 100 MeV ← r ~ 2 fm

Range ~ Compton wavelength of exchanged boson ~ 1/m

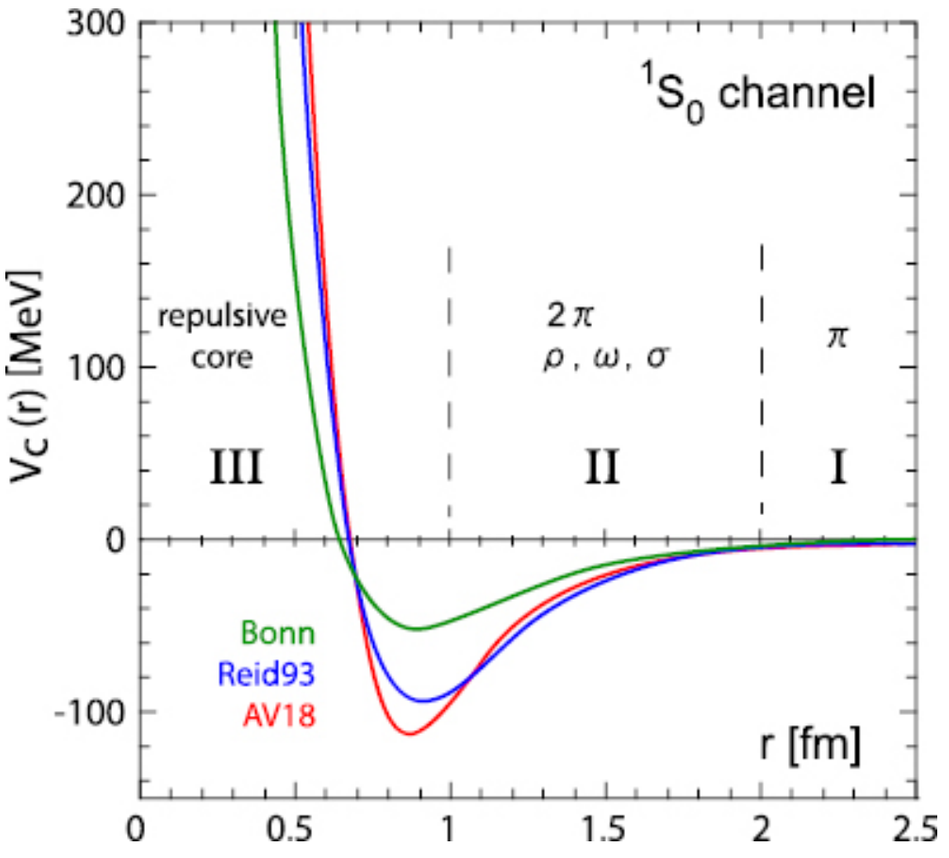
⊙ **OBE potentials**: mesons with larger masses (ρ , ω, σ) can model ranges smaller than $1/m_\pi$

- ○ Different spin/isospin structures generated
- ○ Additional phenomenological terms

✓ High precision → $\chi^2 \approx 2$ in the 1980's, $\chi^2 \approx 1$ in the 1990's

✗ Hard repulsive core → **strong (short-range) correlations**

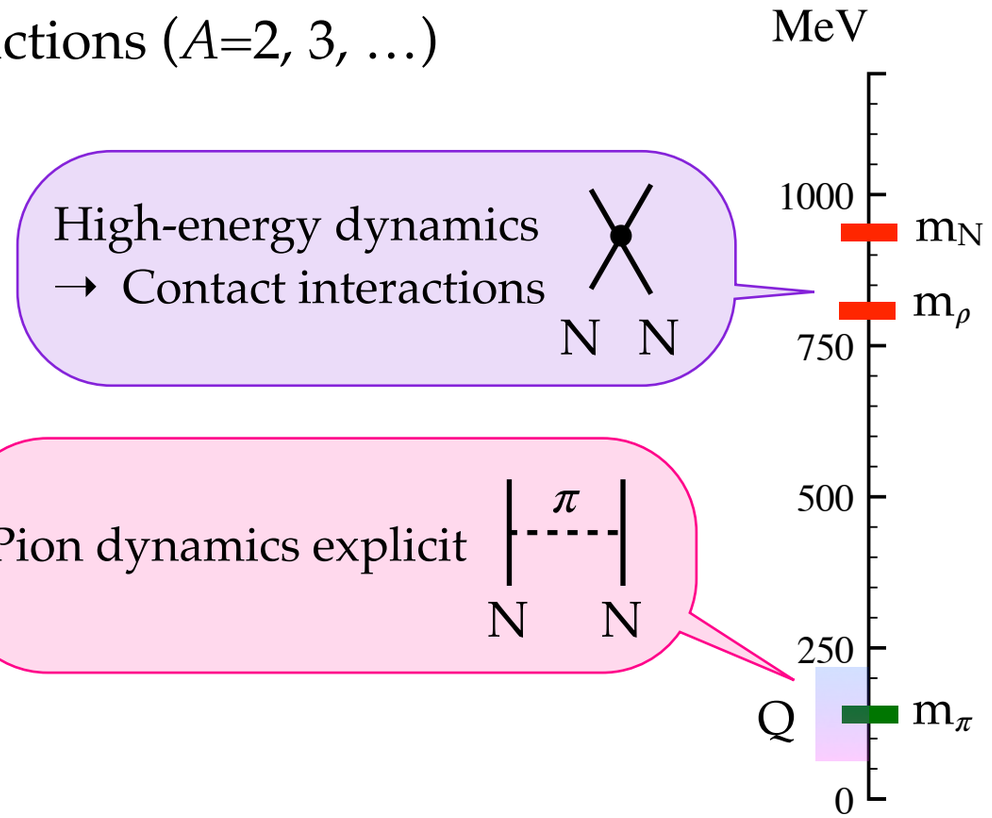
✗ Phenomenological component → **model dependence**



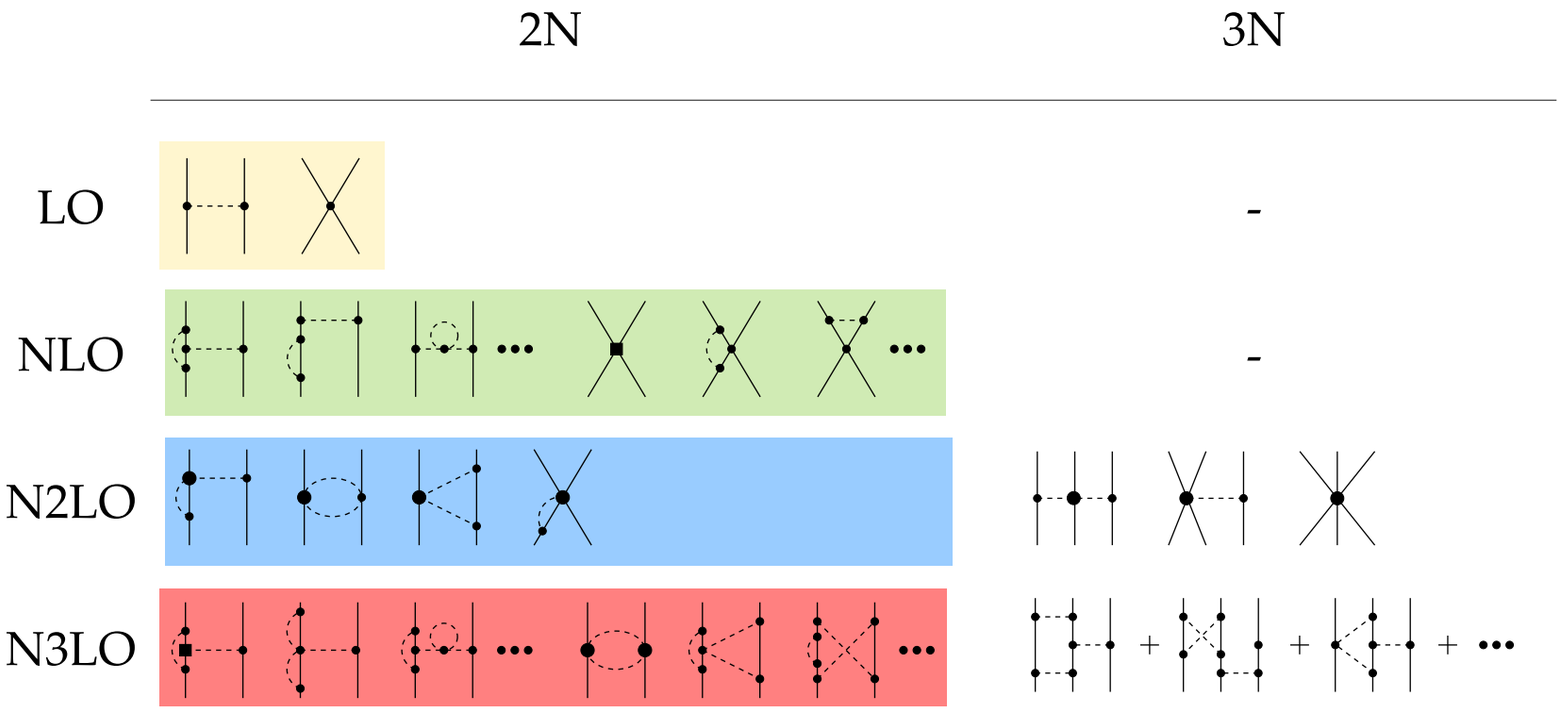
Chiral effective field theory

⊙ Chiral EFT: a **systematic** framework to construct AN interactions (A=2, 3, …)

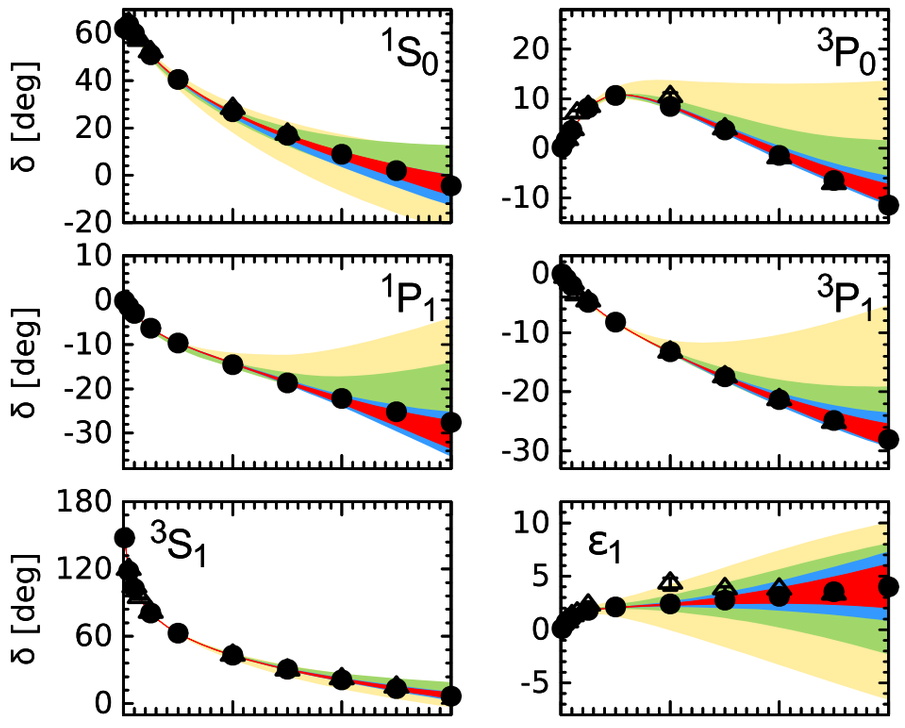
- ○ Expansion around Q ~ m_π → d.o.f.: nucleons and pions
- ○ Interactions organised according to power counting
- ○ Many-body forces/currents consistently derived
- ○ **Theoretical error** assigned to each order



Apply to the many-nucleon system (and propagate the theoretical error)



[Epelbaum *et al.* 2015, 2020]

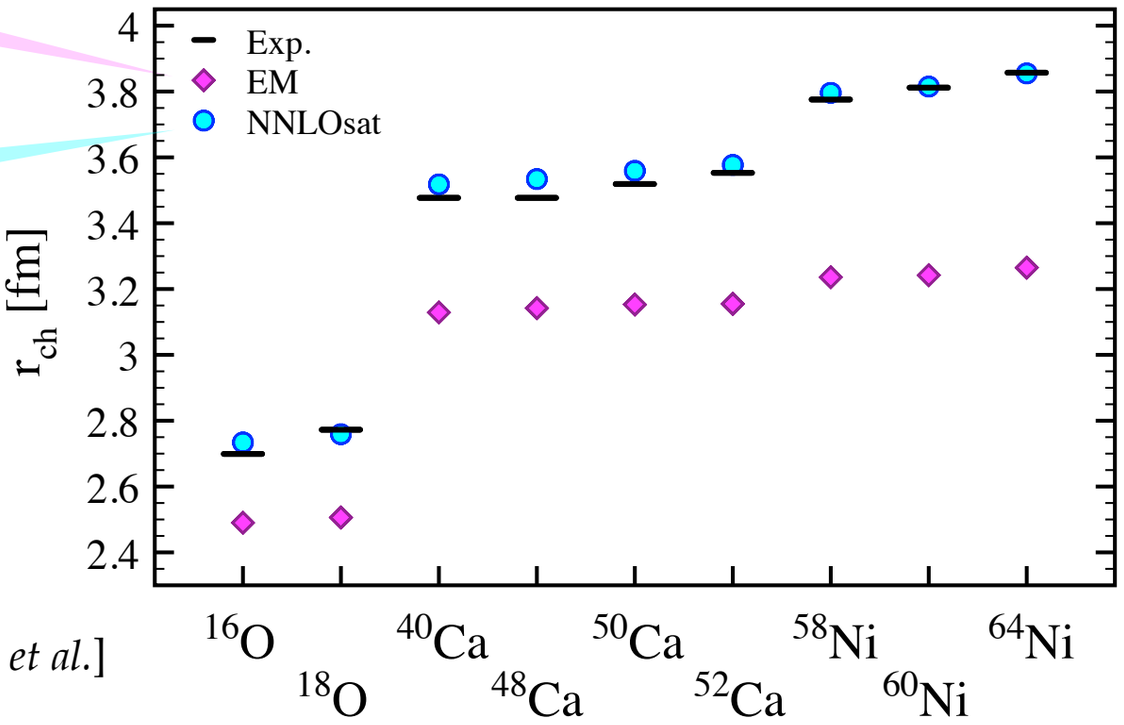


Accuracy of chiral potentials

⊙ **Accuracy of chiral potentials steadily improving**

2010

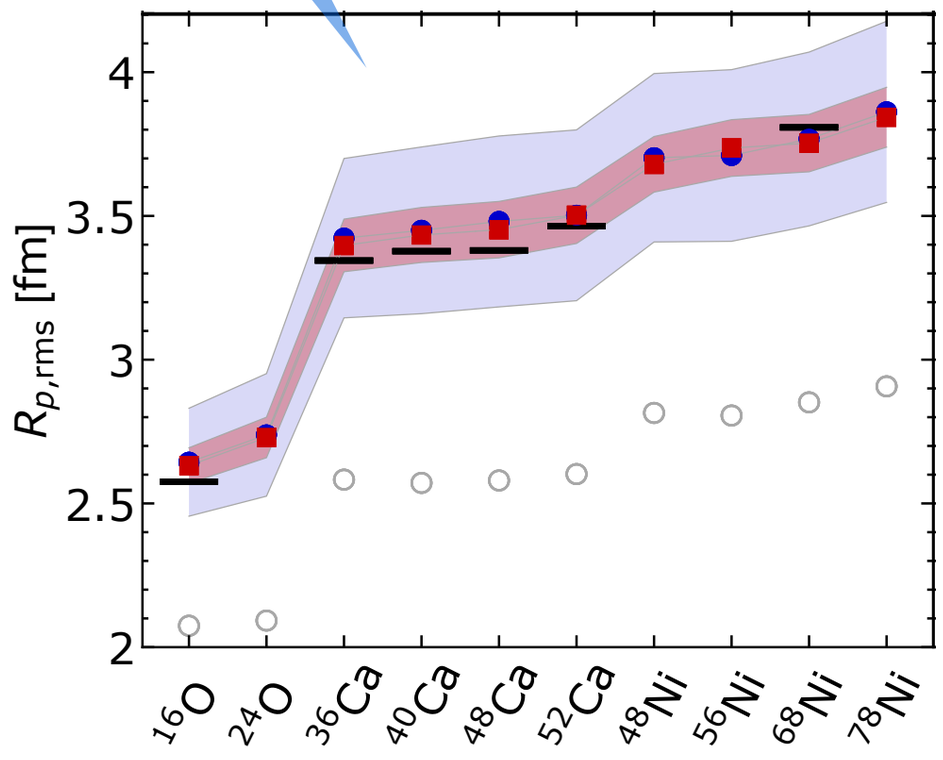
2015



[Somà *et al.*]

2020

[Hüther *et al.* 2020]



Rms deviations approaching phenomenological approaches

- Ground-state energies → rms deviation around 3 MeV (~ **1-1.5%**)

  (cf. ~1 MeV in energy density functionals)

- Charge radii → rms deviation around 0.02 fm (~ **0.5-1%**)

  (similar in energy density functionals)

Part 2

Exact many-body methods

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
- E_k^A → A-body energies of ground and excited states
- $|\Psi_k^A\rangle$ → A-body wave function → Other observables ← Expectation value of any operator

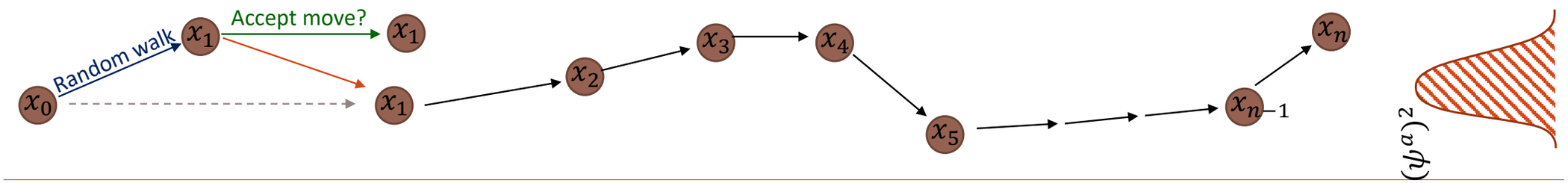
⊙ **Only input**

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

- ○ Given as a sum of many operators in momentum space (⊗ spin & isospin)
- ○ Transformed into basis of choice (e.g. harmonic oscillator)
- ○ Typically truncated at 3N level

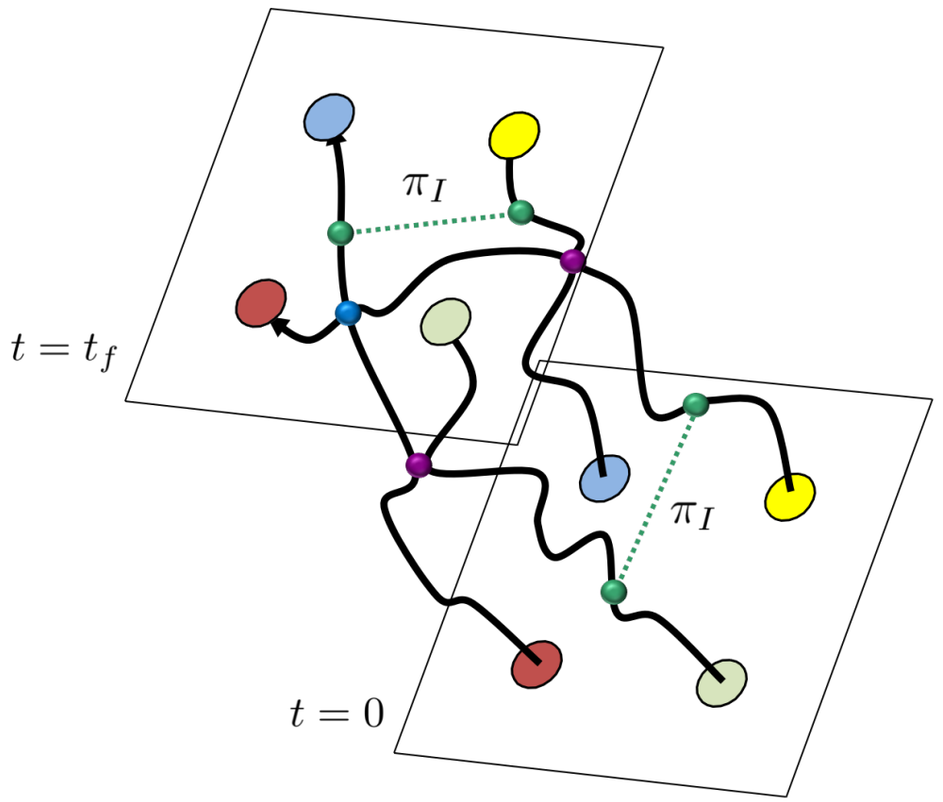
Coordinate-space vs configuration-space methods

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



Coordinate-space vs configuration-space methods

- **Coordinate-space methods**
  - Directly work with many-body wave function (e.g. Monte Carlo sampling)
  - Discretise the problem on a lattice → Nuclear Lattice Effective Field Theory



Coordinate-space vs configuration-space methods

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  - Directly work with many-body wave function (e.g. Monte Carlo sampling)
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✓ Flexible (any spatial configuration is accessible) + no intensive memory requirement

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

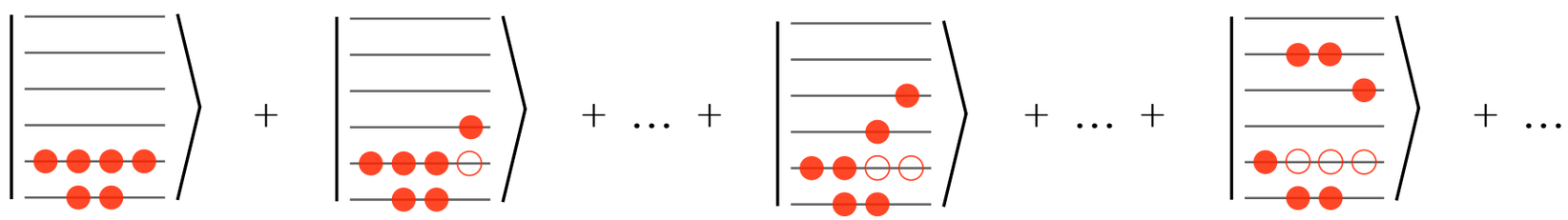
Coordinate-space vs configuration-space methods

- **Coordinate-space methods**
  - Directly work with many-body wave function (e.g. Monte Carlo sampling)
  - Discretise the problem on a lattice → Nuclear Lattice Effective Field Theory

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

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

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



✓ Universally applicable to any H + 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 $\mathcal{A} = \dfrac{1}{A!} \sum_{\pi} \mathrm{sgn}(\pi)\, P_\pi$

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

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

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

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

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

Model space truncations

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

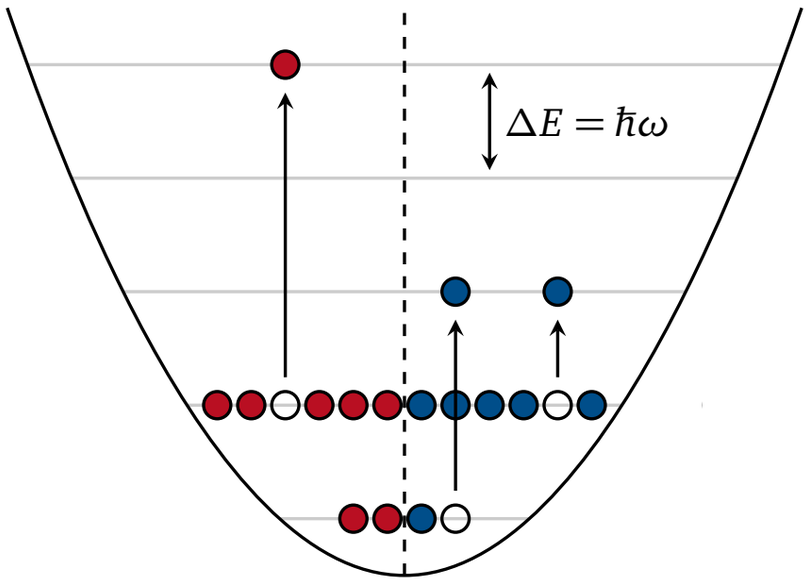
$$|\Psi_k\rangle = \sum_{i=1}^{\infty} C_i^{(k)} |\Phi_i\rangle \qquad \Rightarrow \qquad |\Psi_k(D)\rangle = \sum_{i=1}^{D} C_i^{(k)} |\Phi_i\rangle$$

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 $N_{\mathbf{max}}$)

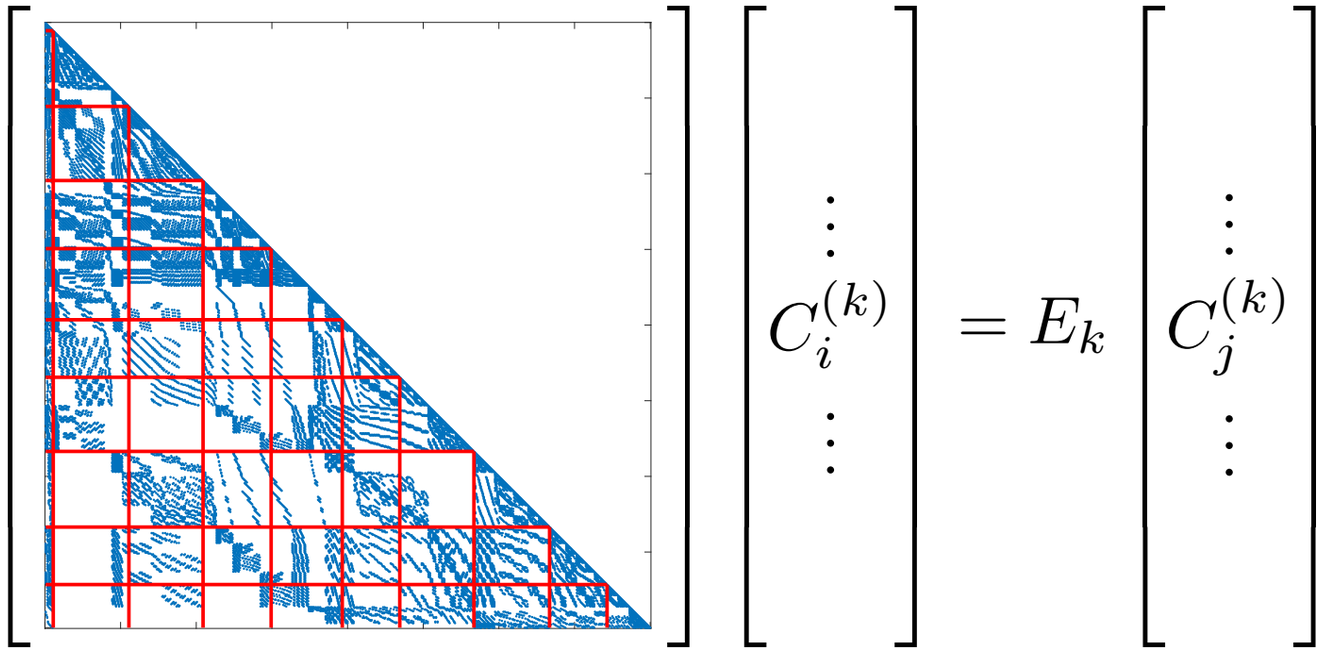


Example: $N_{\mathbf{max}} = 6$

[*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 $\left(\begin{array}{c} n \\ A \end{array} \right) = \frac{n!}{(n-A)!\,A!}$

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

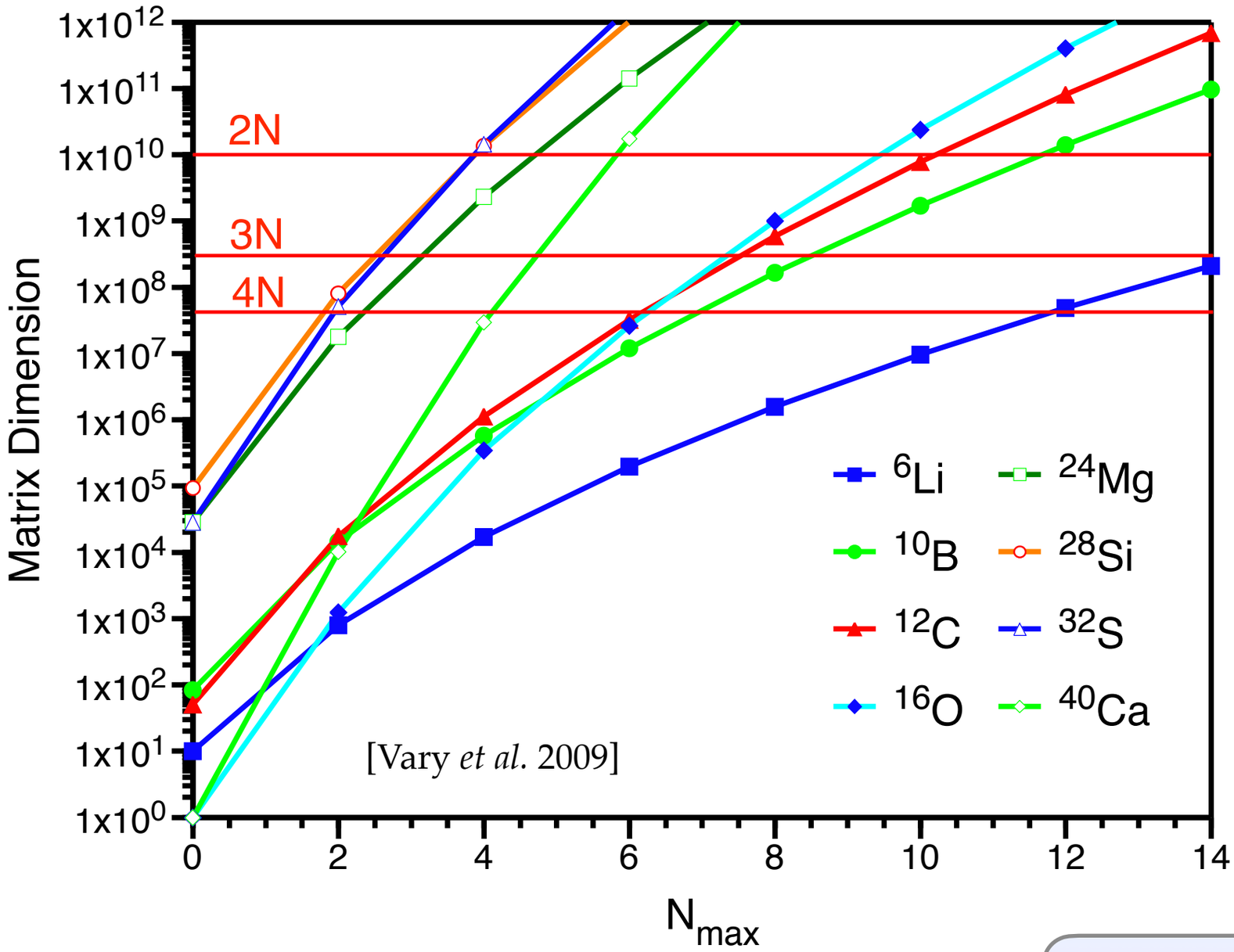
$$\left(\begin{array}{c} 40 \\ 8 \end{array} \right) = \frac{40!}{(40-8)!\,8!} \approx 8 \cdot 10^7 \quad \text{for protons} \quad \text{x} \quad \left(\begin{array}{c} 40 \\ 8 \end{array} \right) = \frac{40!}{(40-8)!\,8!} \approx 8 \cdot 10^7 \quad \text{for neutrons}$$

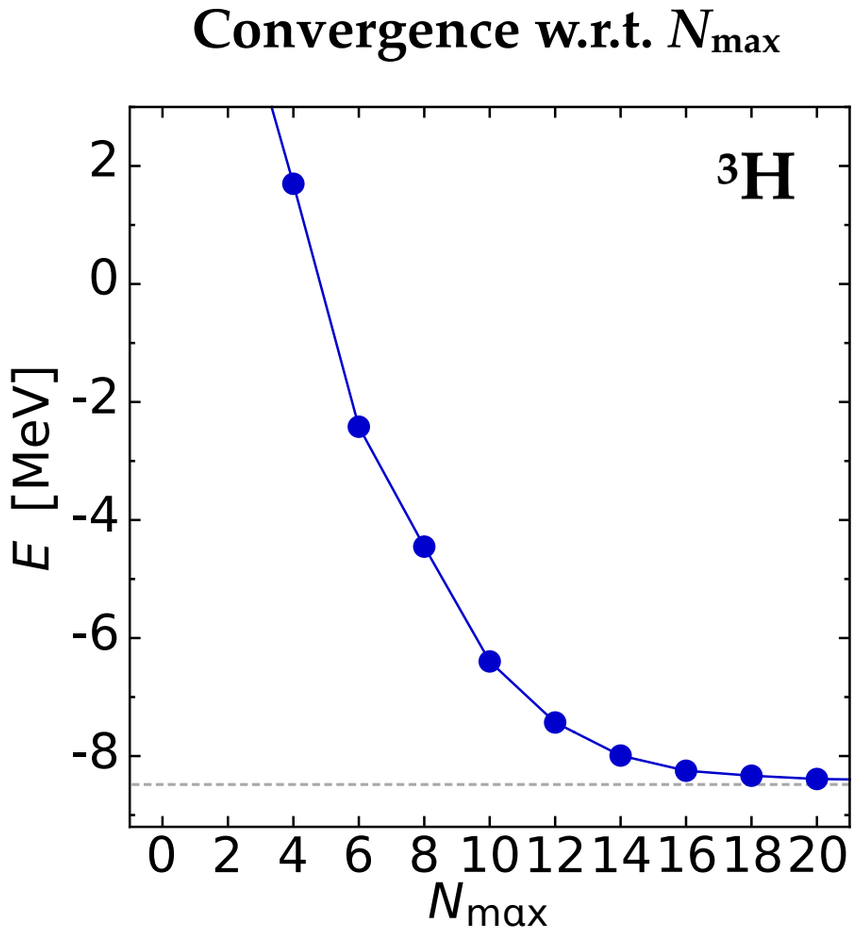
  - ➪ Total of D = $6 \cdot 10^{15}$ Slater determinants
  - ➪ Number of non-zero matrix elements (*NN* only!) scales as $D^{1.2}$ → ~ 10^{18} non-zero entries
  - ➪ Size in memory beyond EB → well beyond current capabilities

- **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)



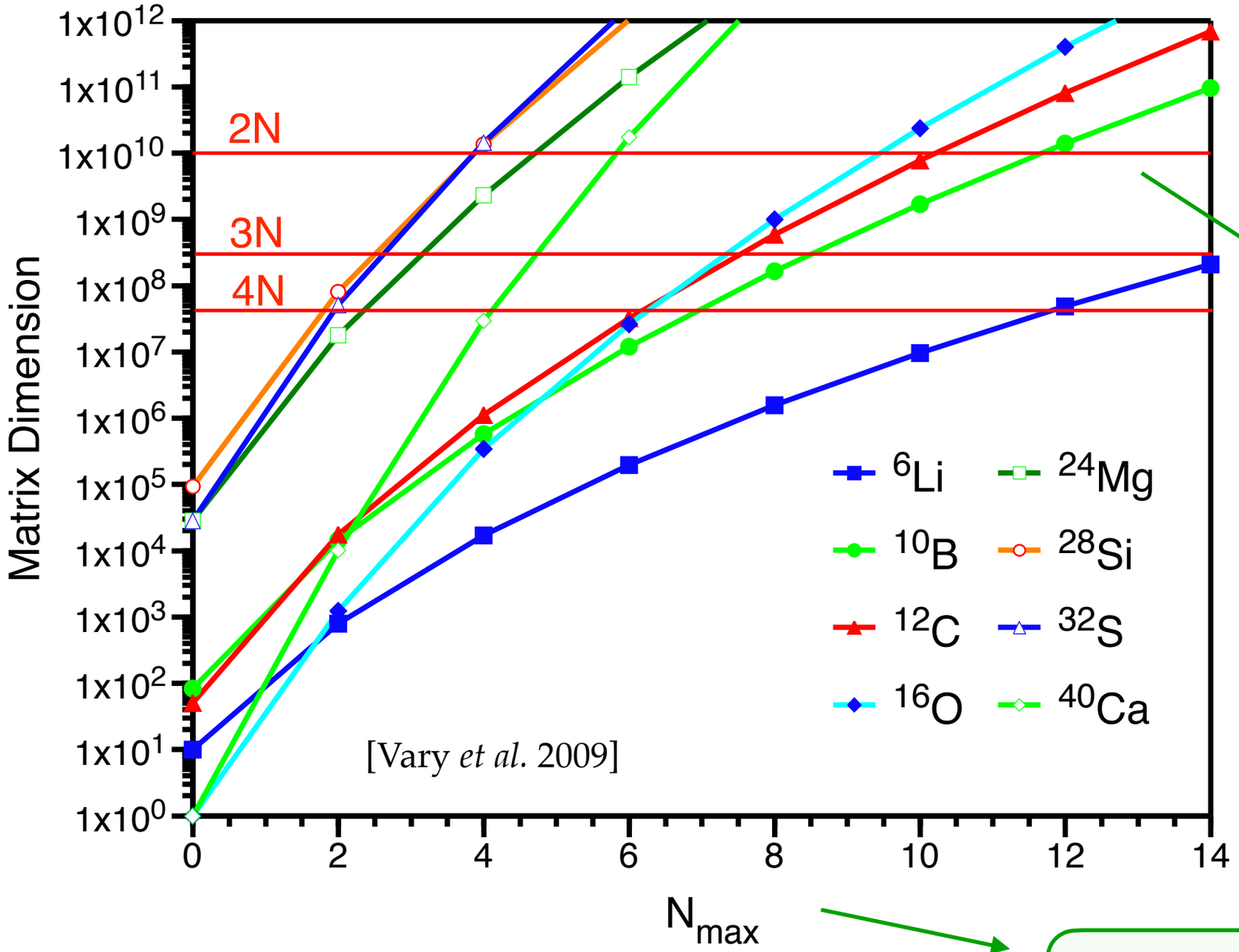


➪ Computational limits quickly reached

NCSM dimensionality

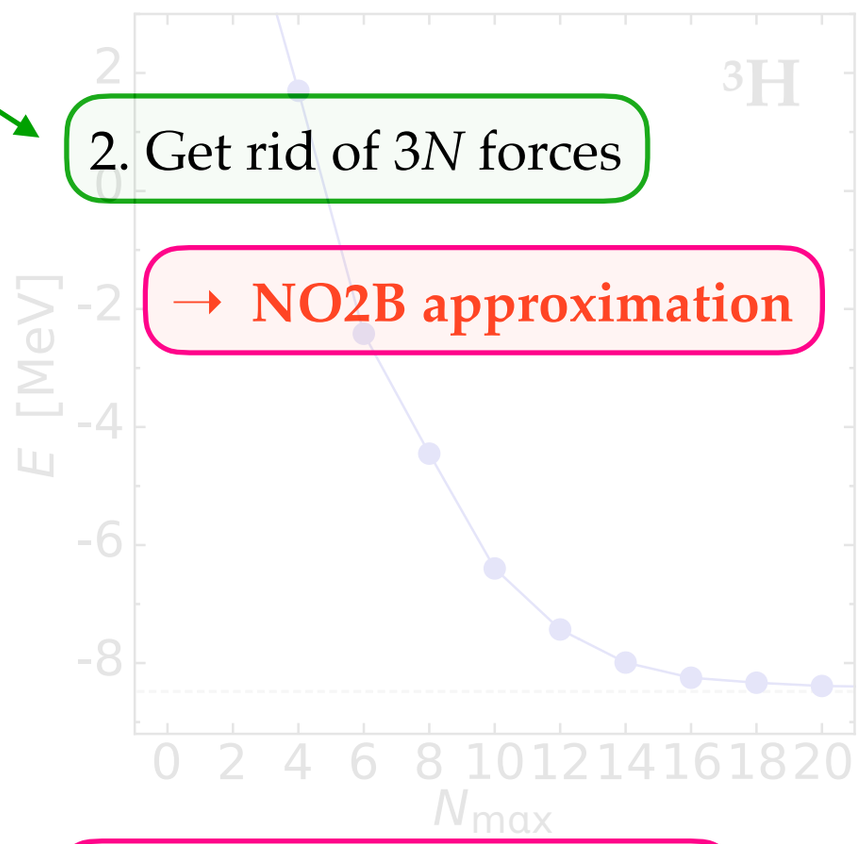
3. Get rid of some matrix elements

→ **Importance truncation**



2. Get rid of 3*N* forces

→ **NO2B approximation**



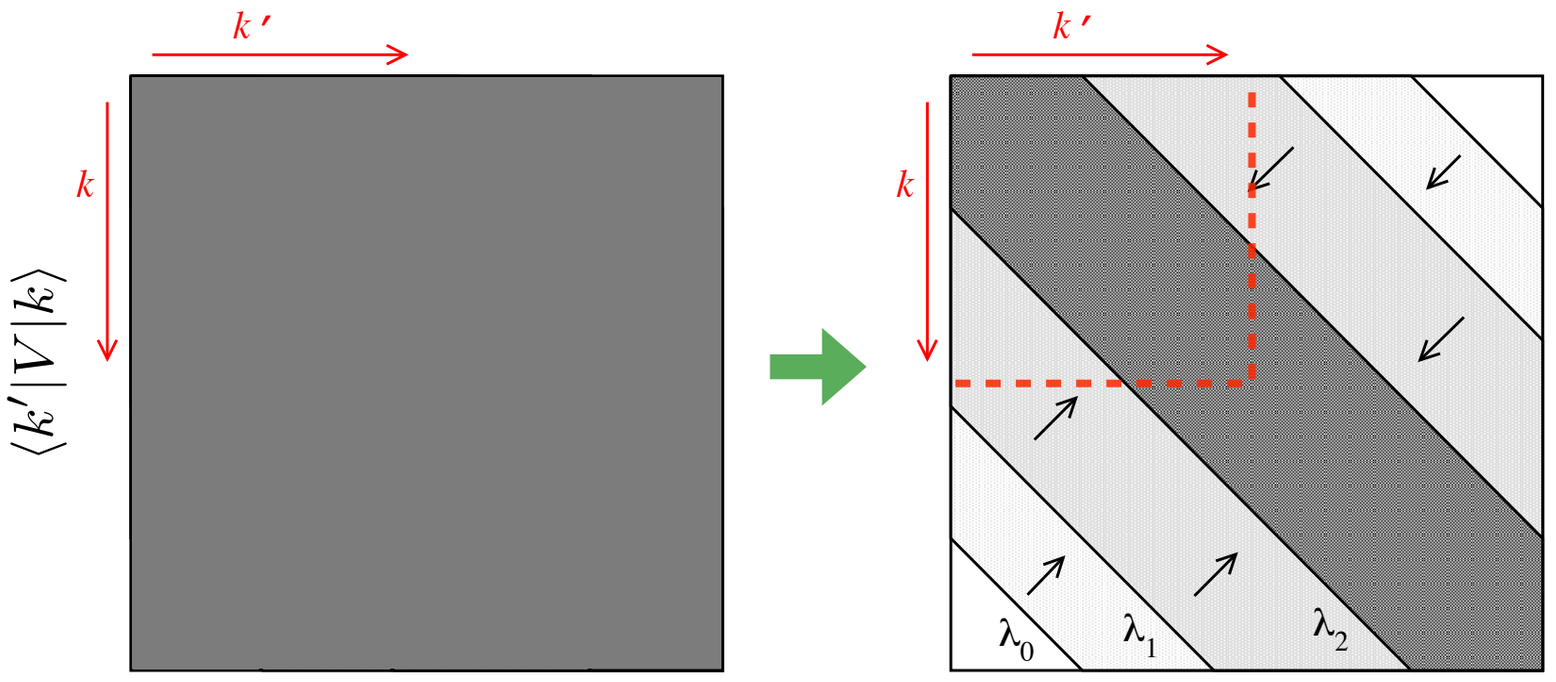
→ **SRG transformations**

1. Improve $N_{\max}$ convergence

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**



→ Decouple low- and high-momenta

→ Can work in small Hilbert space

→ Less correlated wave functions

→ Observables unchanged!

$$U^\dagger H U U^\dagger |\Psi\rangle = E U^\dagger |\Psi\rangle$$

$$\tilde{H}|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle$$

Short-range correlations & "low-momentum" interactions

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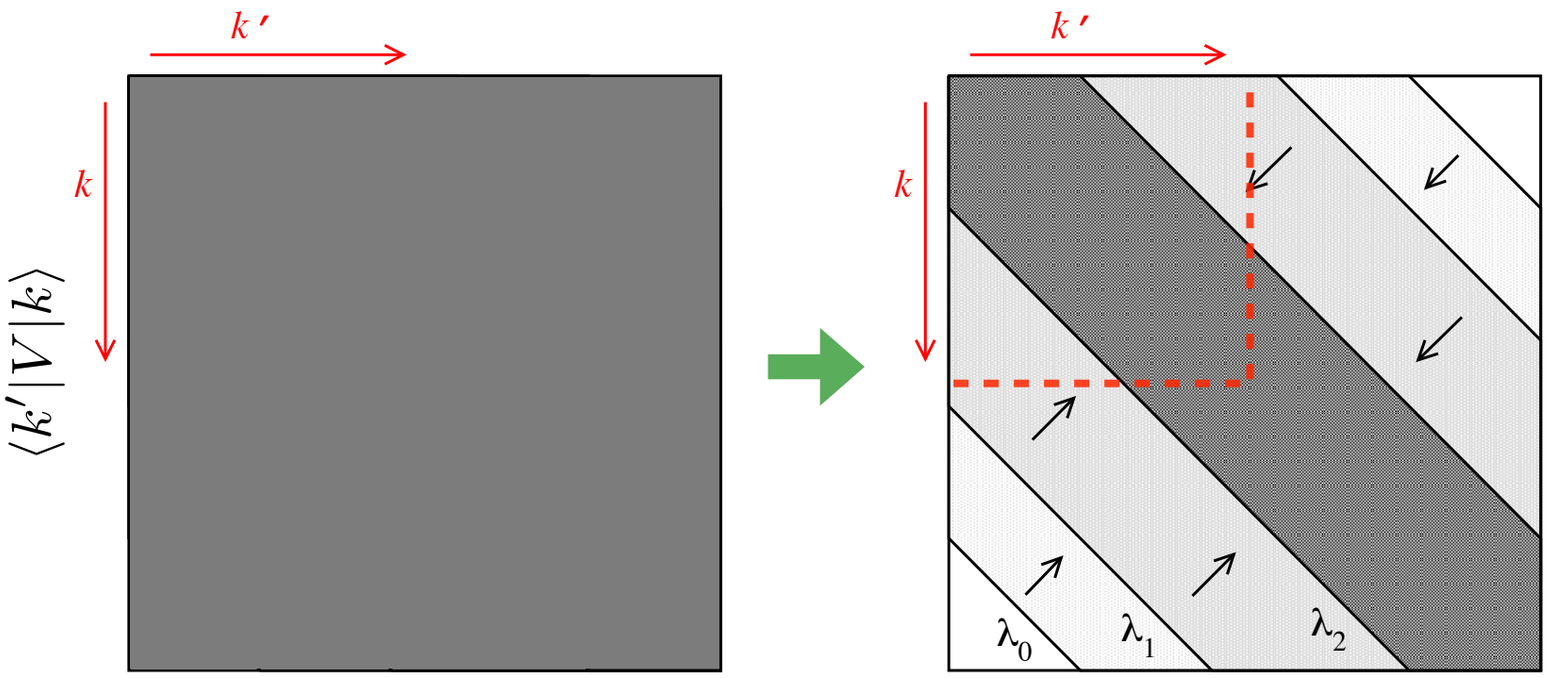


→ Decouple low- and high-momenta

→ Can work in small Hilbert space

→ Less correlated wave functions

→ Observables unchanged!

→ Many-body forces generated

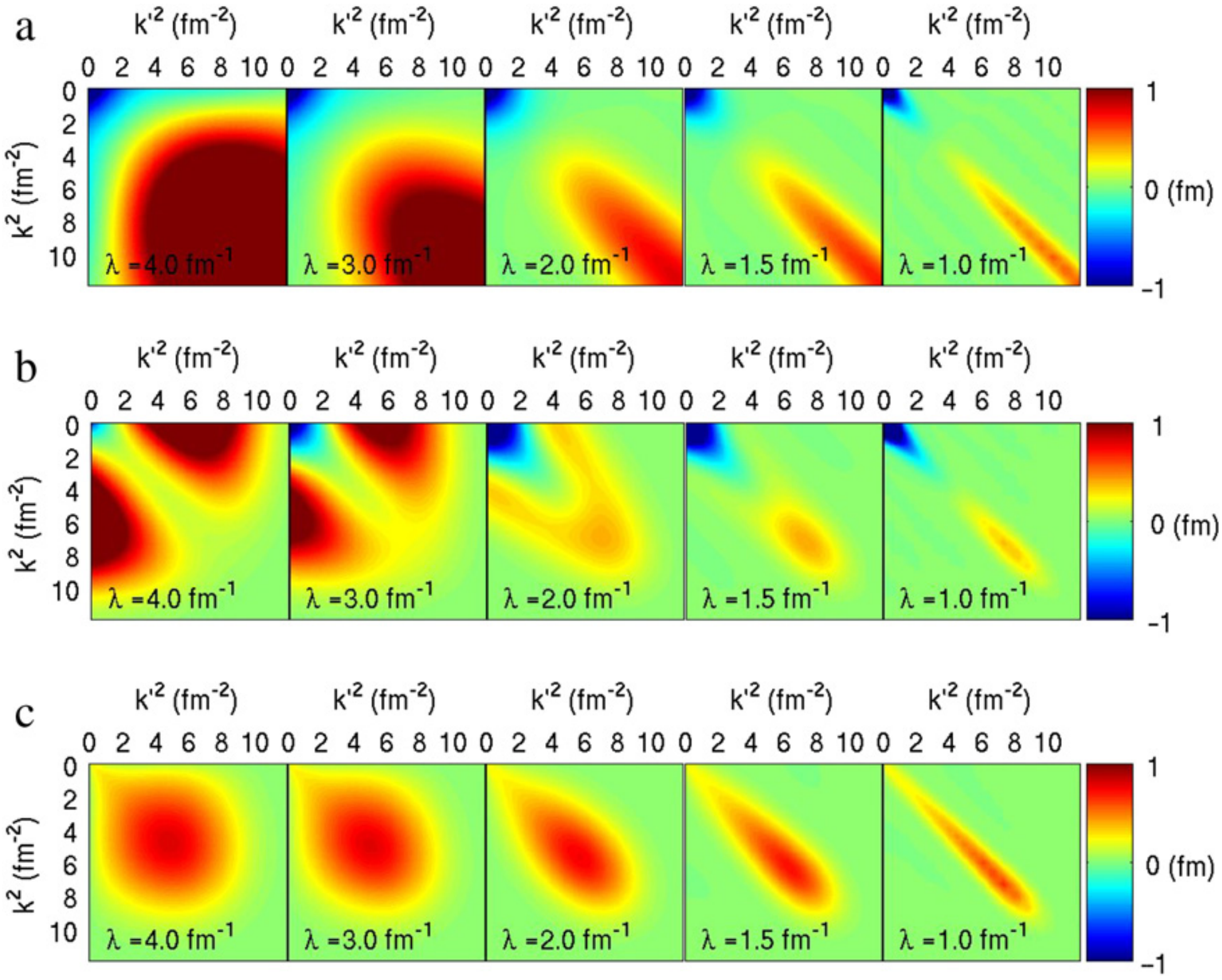
➪ **Similarity renormalisation group (SRG) transformation**

A matter of resolution

[figures from K. Hebeler]

SRG transformation

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



$^1S_0$

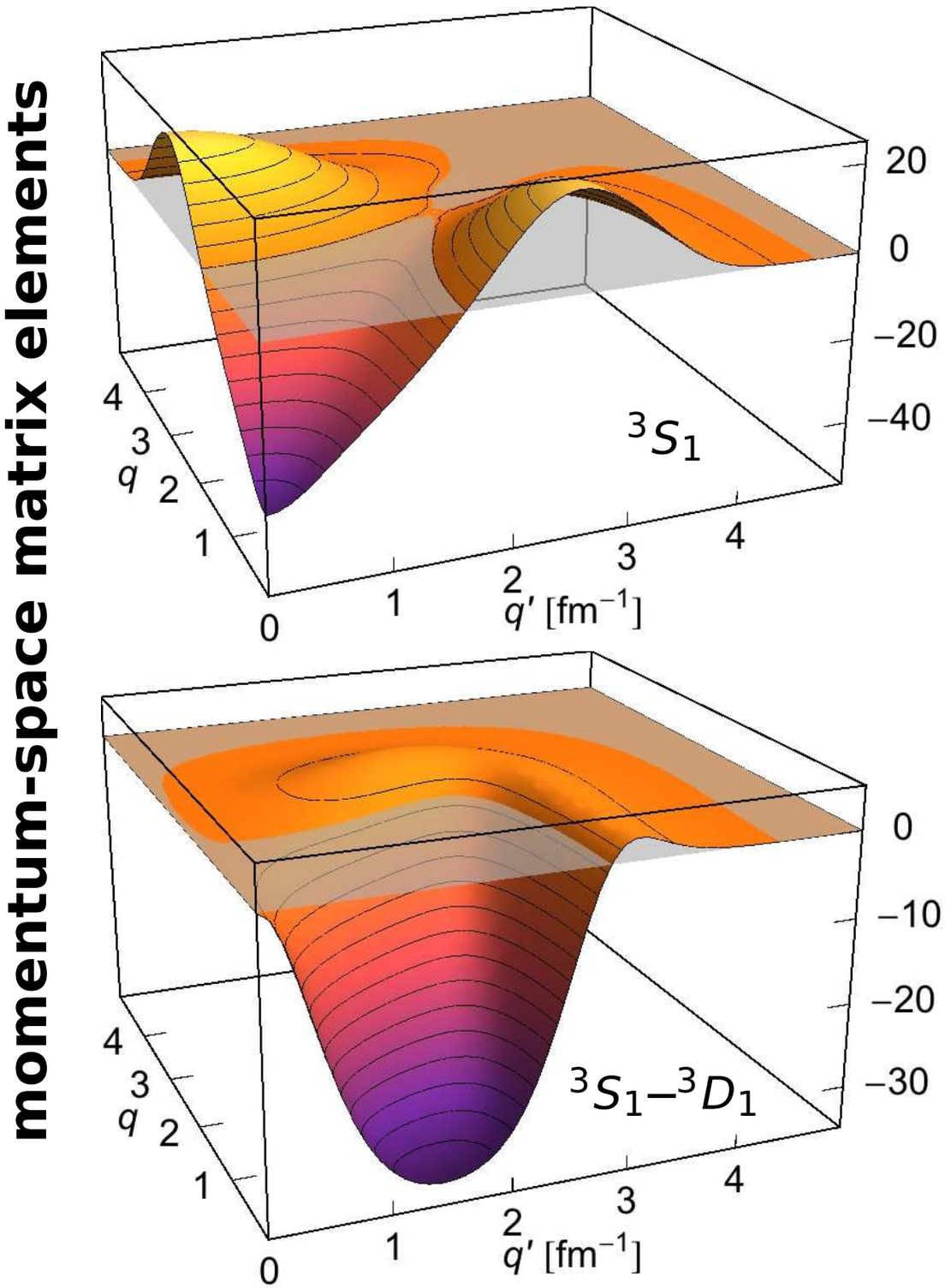
$^3S_1$

$^1P_1$

[Bogner *et al.* 2010]

SRG transformation

[*Figures*: R. Roth]

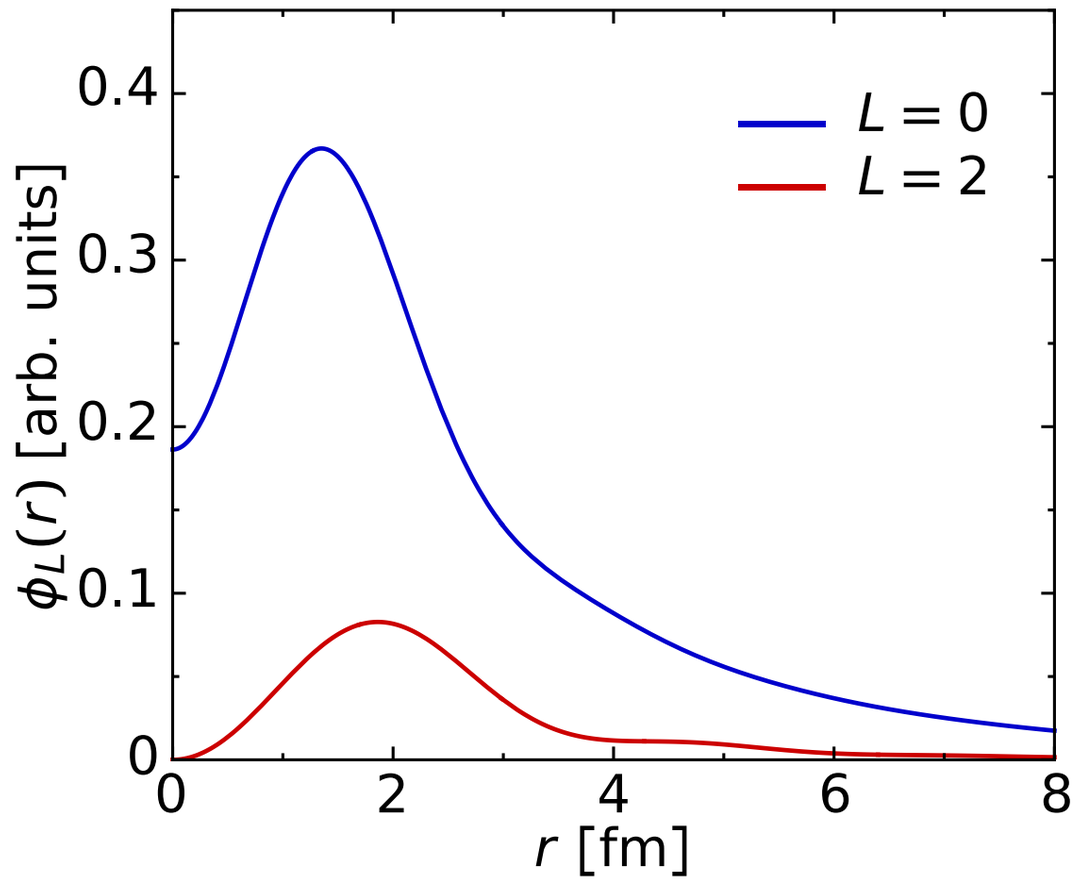


chiral NN

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

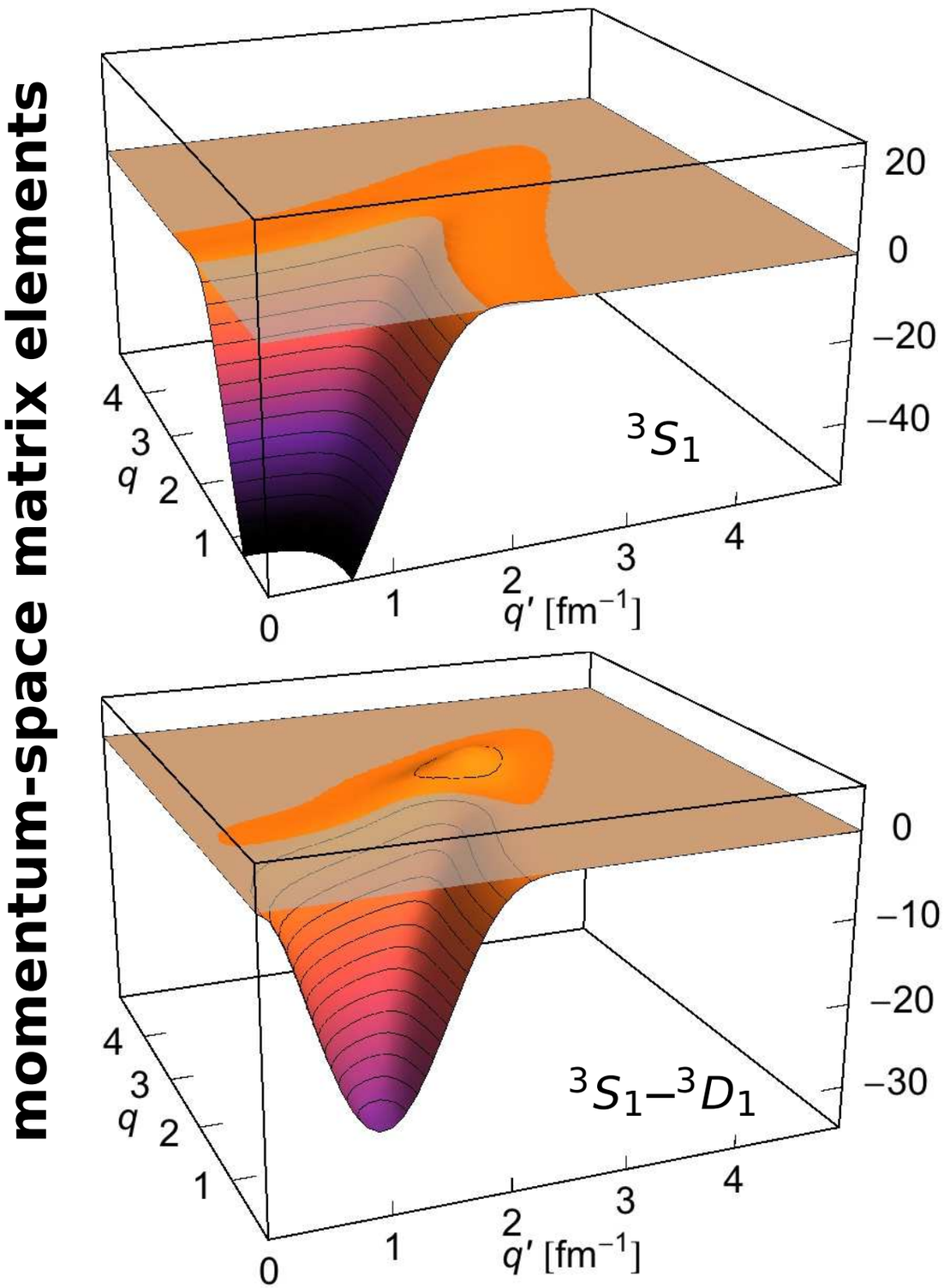
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG transformation

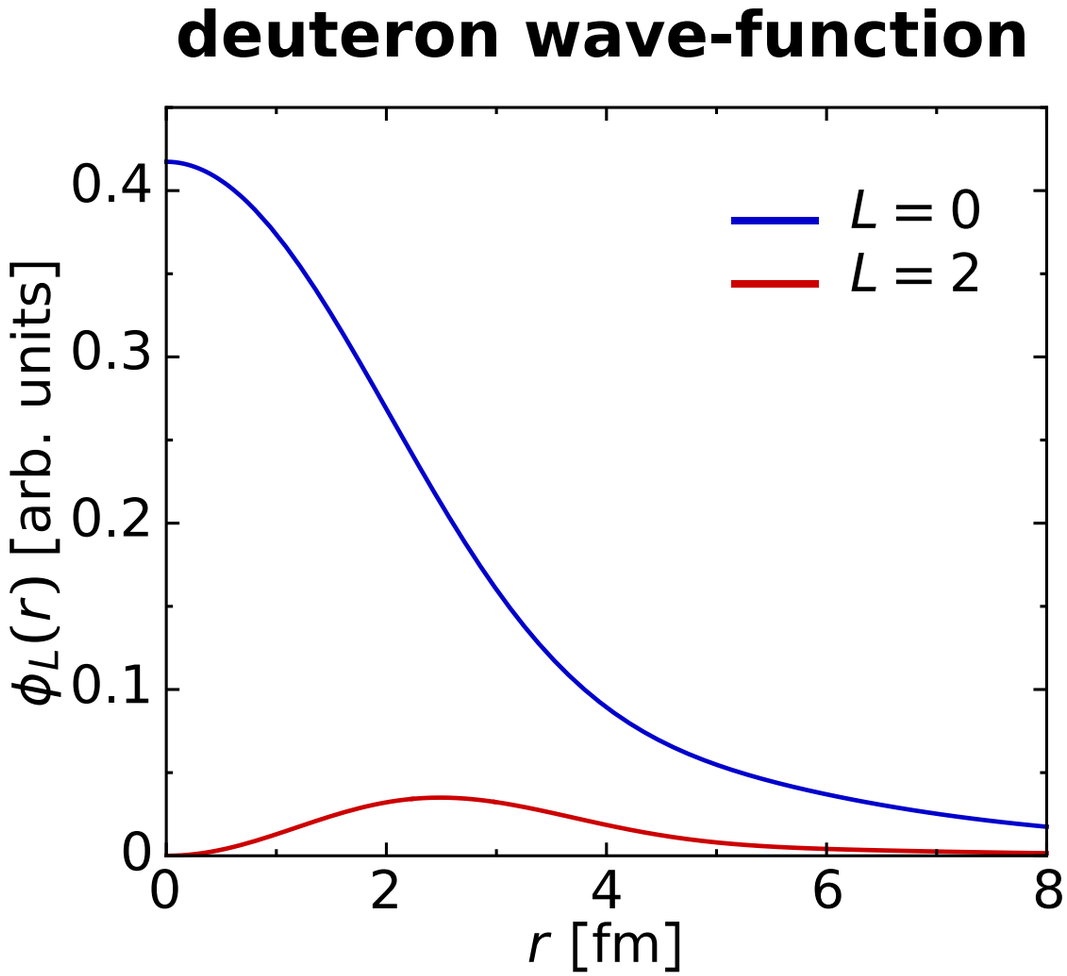
[*Figures*: R. Roth]



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

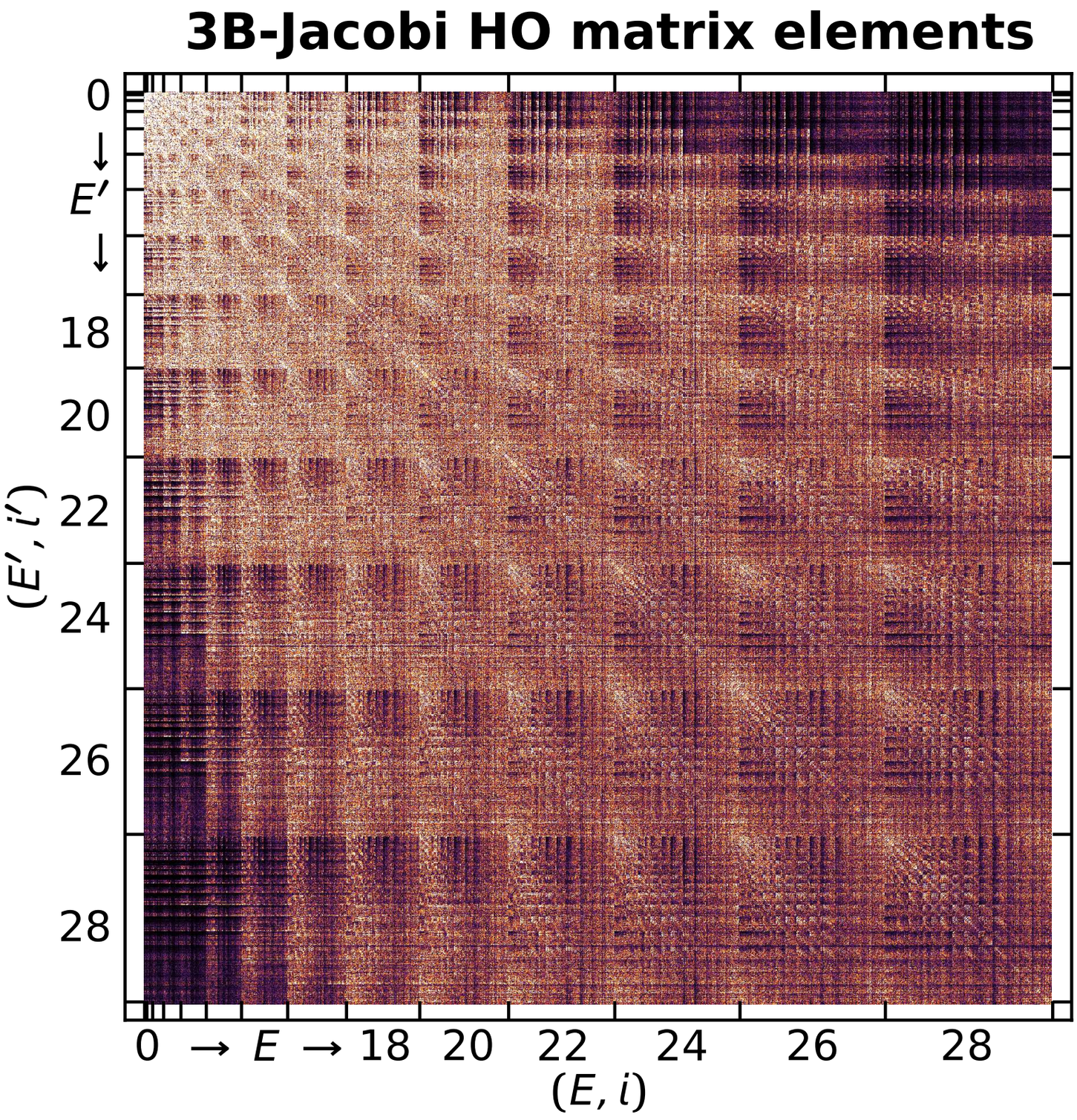
$\Lambda = 1.58\,\mathrm{fm}^{-1}$

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



SRG transformation

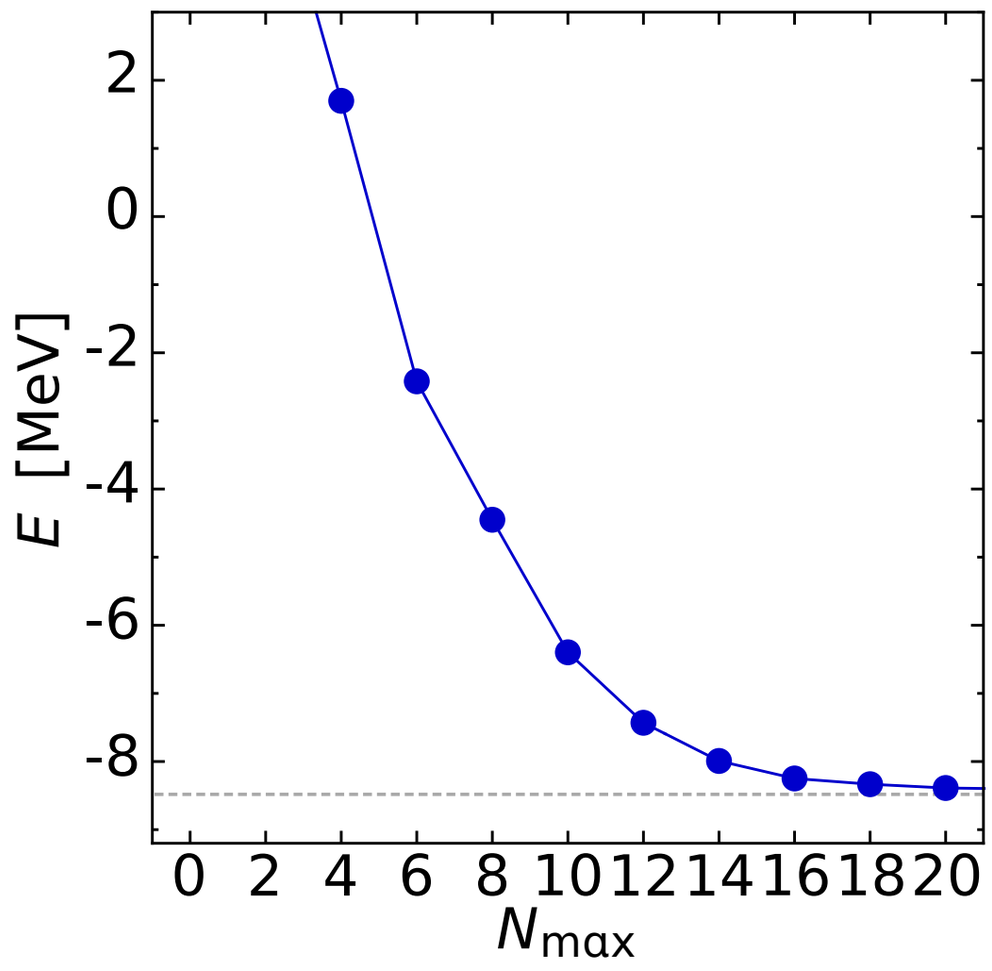
[*Figures*: R. Roth]



chiral NN+3N

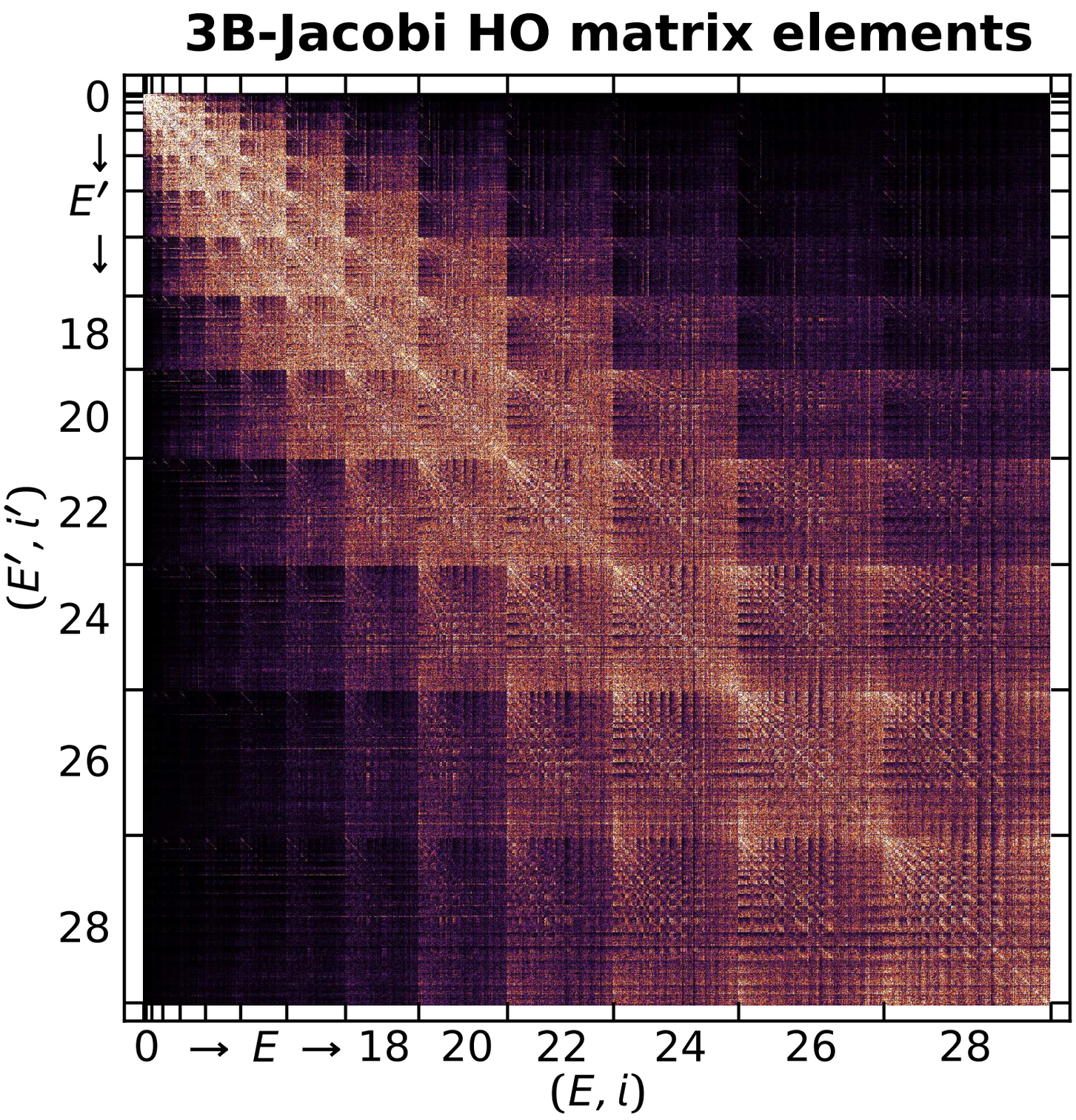
N^{3}LO + N^{2}LO, triton-fit, 500 MeV

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



SRG transformation

[*Figures*: R. Roth]



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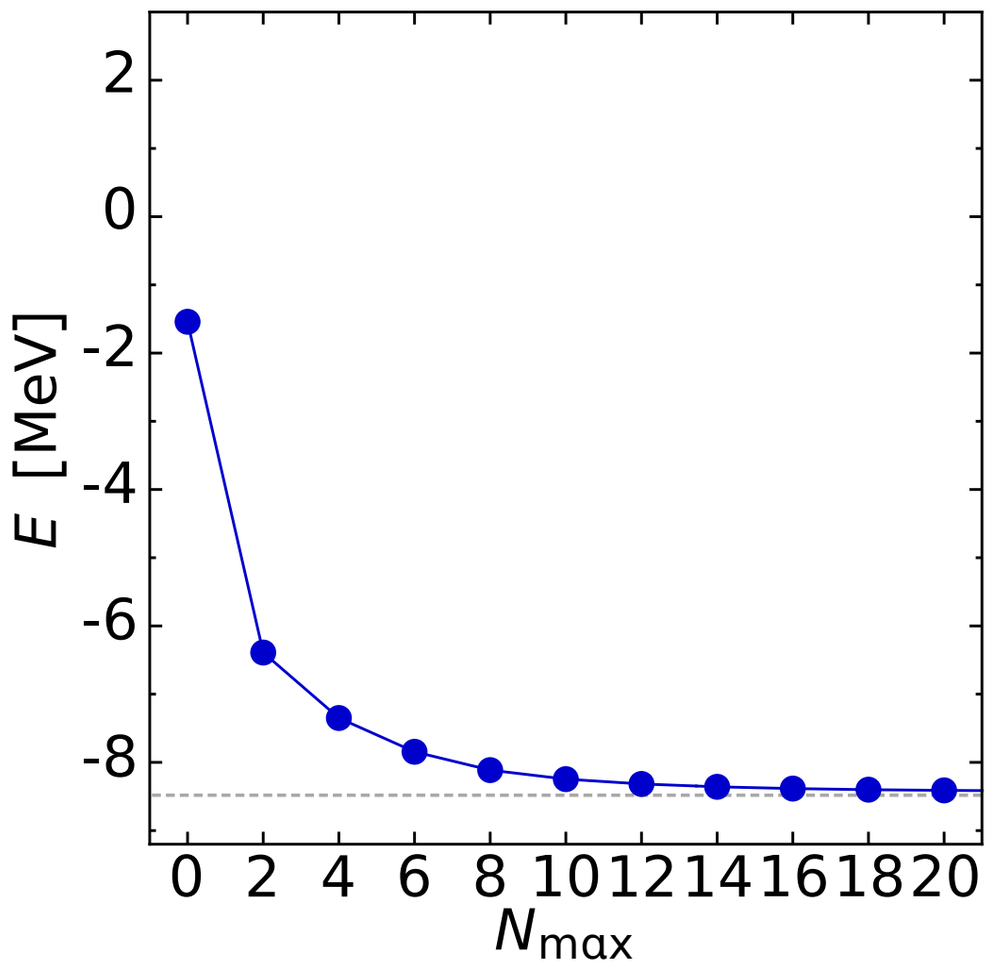
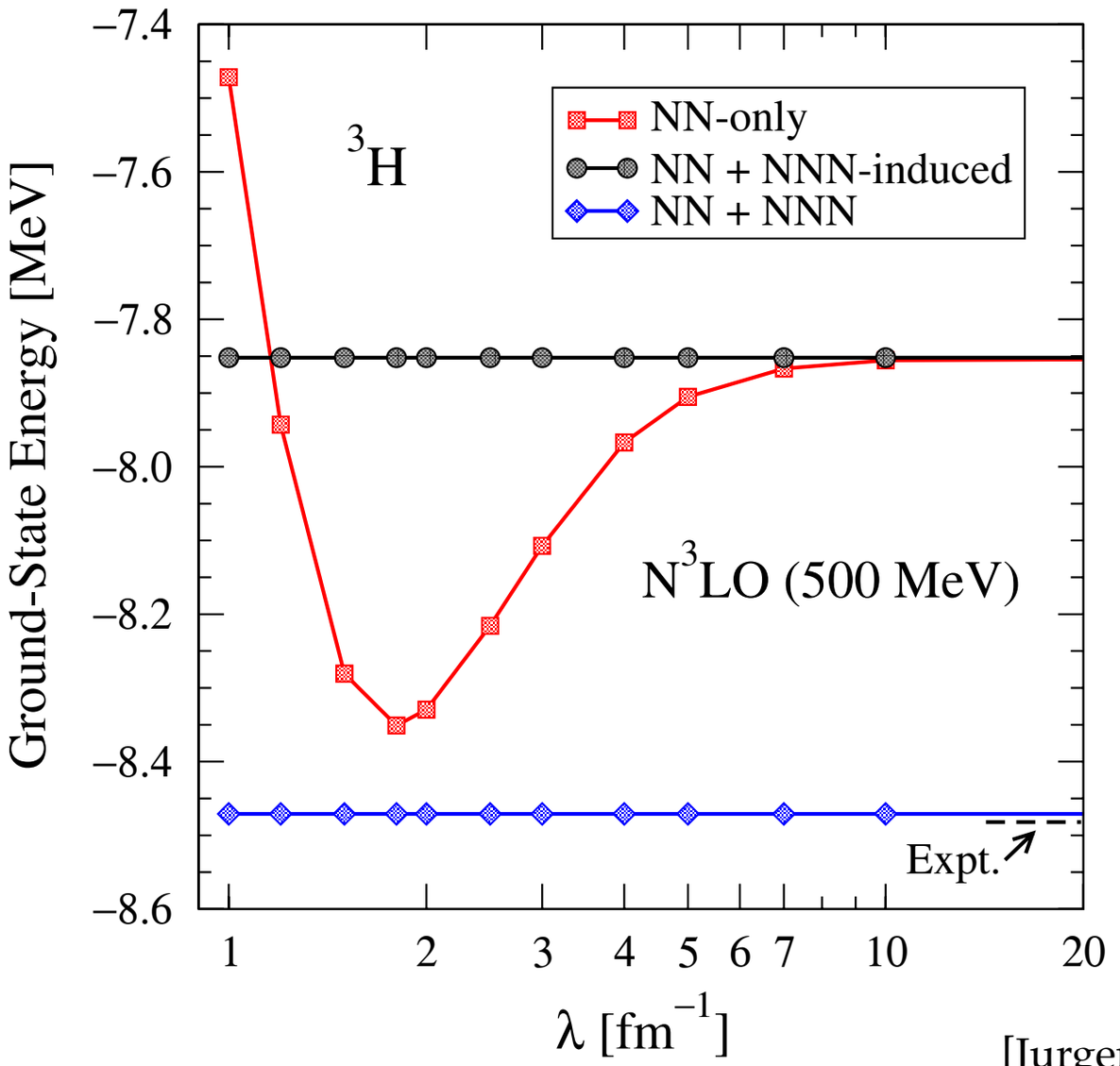
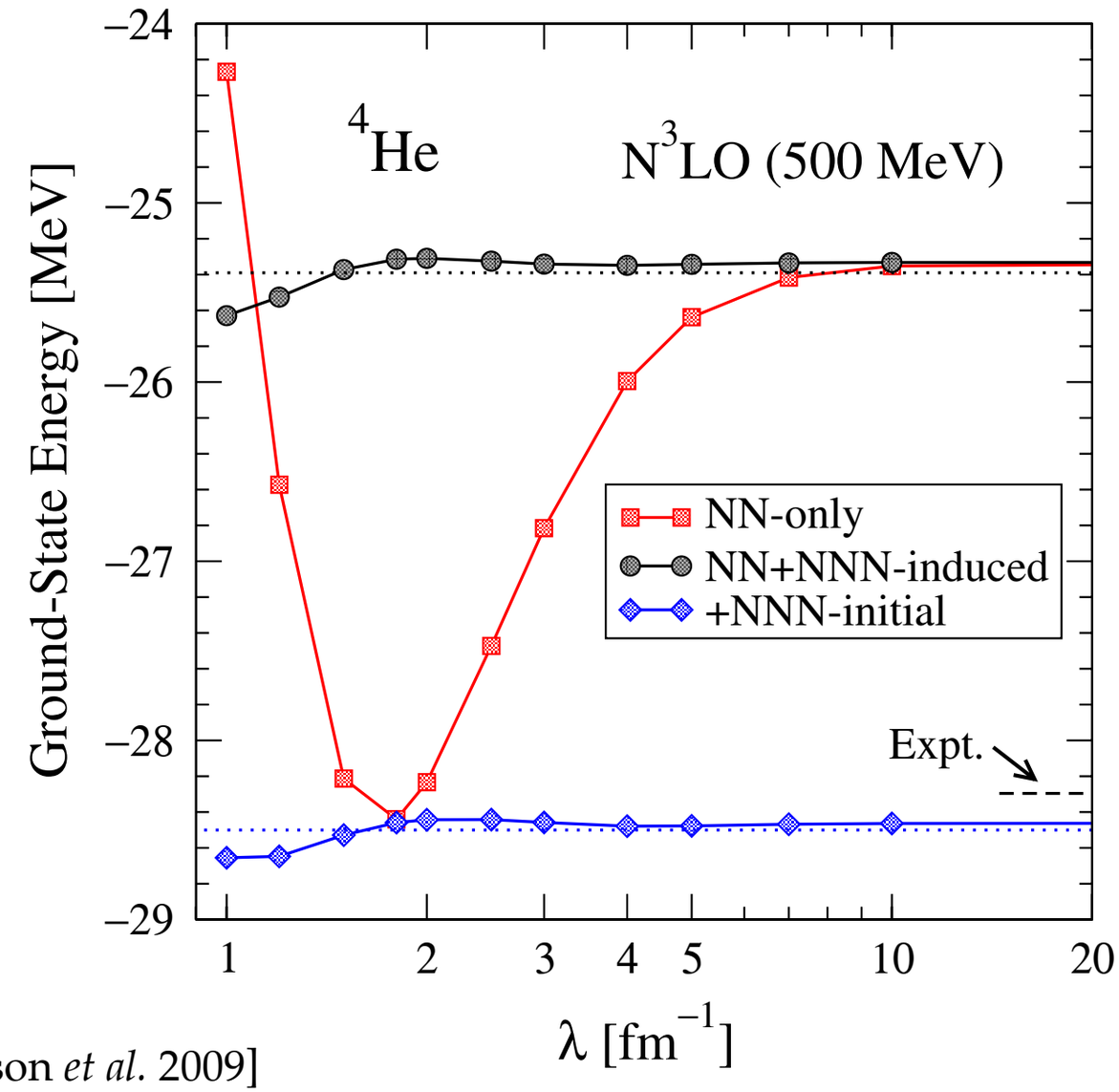


SRG in *A*-body systems

⊙ **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

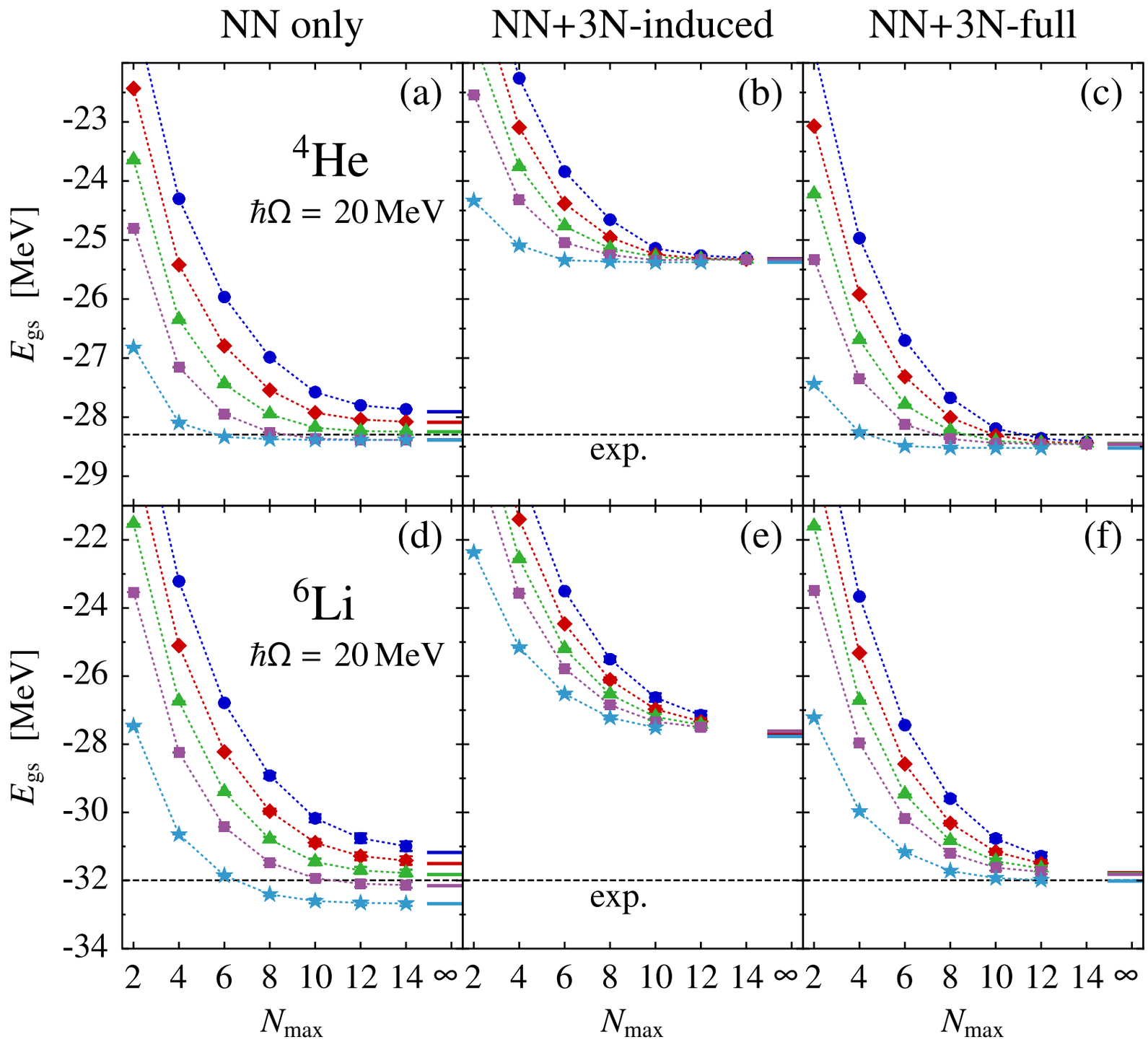
SRG in *A*-body systems

⊙ **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

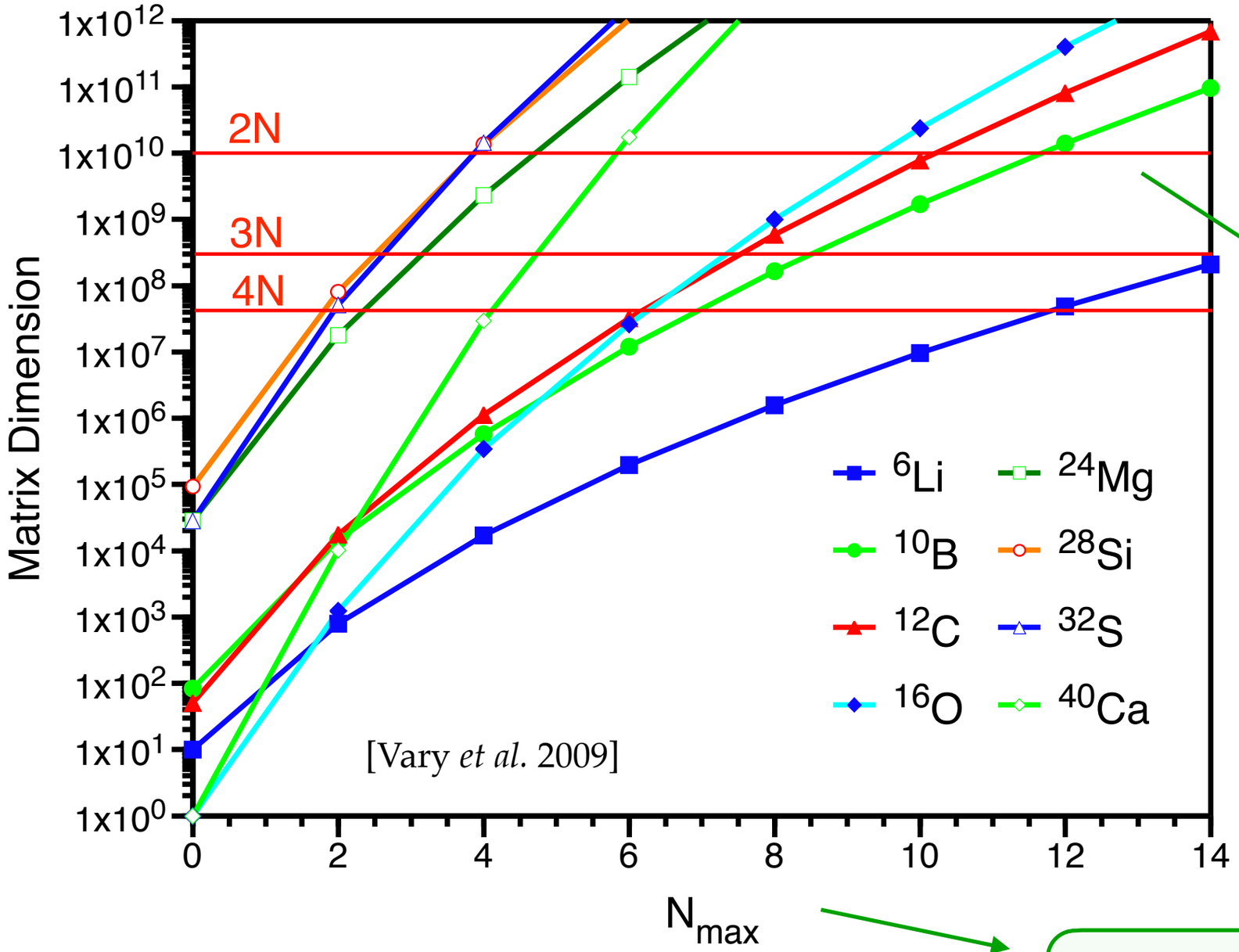


[Roth *et al.* 2011]

NCSM dimensionality

3. Get rid of some matrix elements

→ **Importance truncation**



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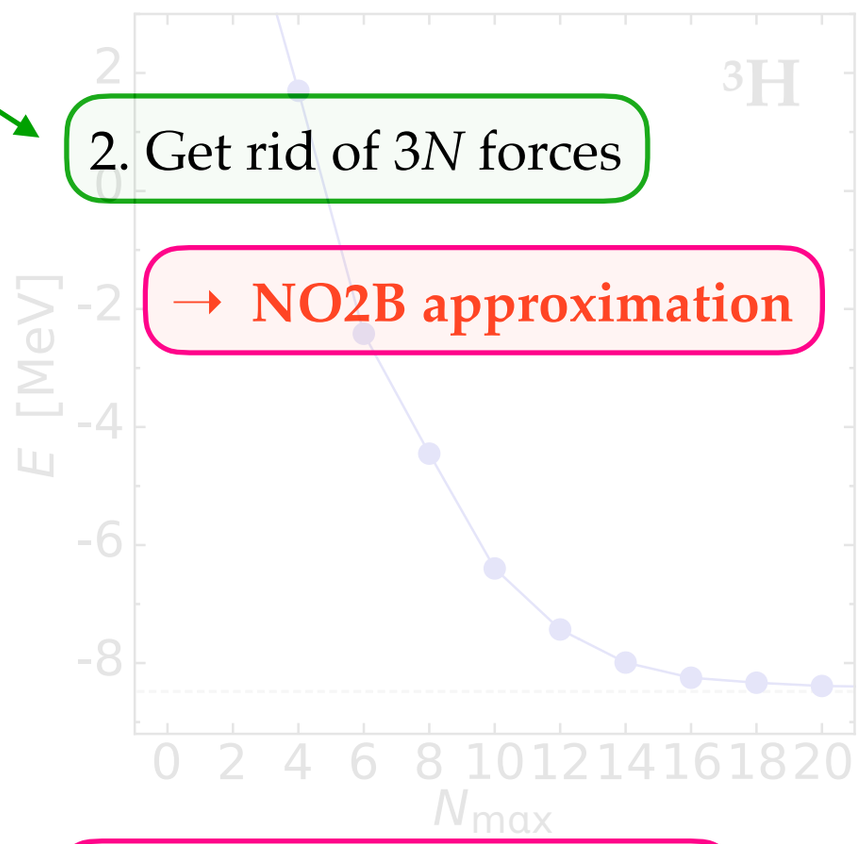


→ **SRG transformations**

1. Improve $N_{\max}$ convergence

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

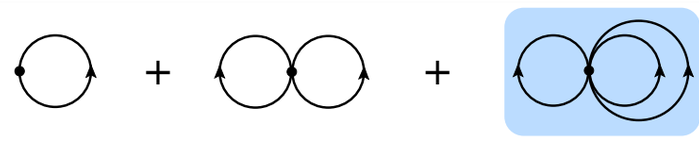
Normal-ordered 2-body approximation (NO2B)

→ Discard residual 3N operator

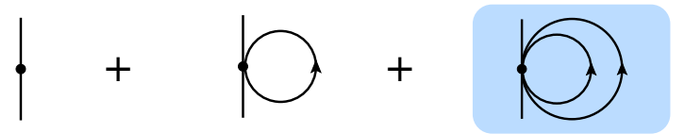
Normal-ordered two-body approximation

⊙ **Normal-ordered matrix elements**

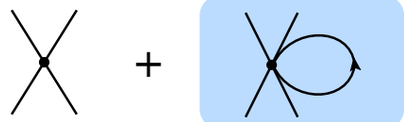
$$h^{(0)} = \sum_i t_{ii}\, n_i + \frac{1}{2}\sum_{ij} v_{ijij}\, n_i n_j + \frac{1}{6}\sum_{ijk} w_{ijkijk}\, n_i n_j n_k =$$



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



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



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

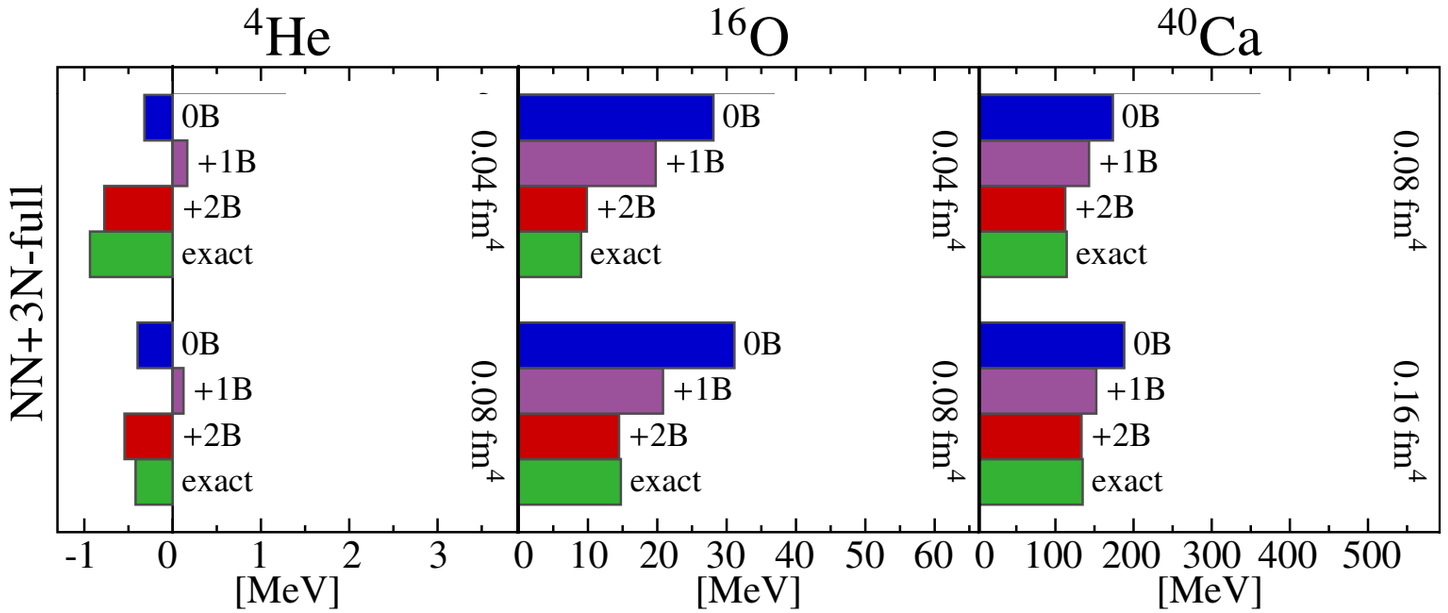
Normal-ordered 2-body approximation (NO2B)

→ Discard residual 3N operator

⊙ **Benchmarked** in light nuclei

- 1-3% error
- Comparable to other errors

[Roth *et al.* 2012]



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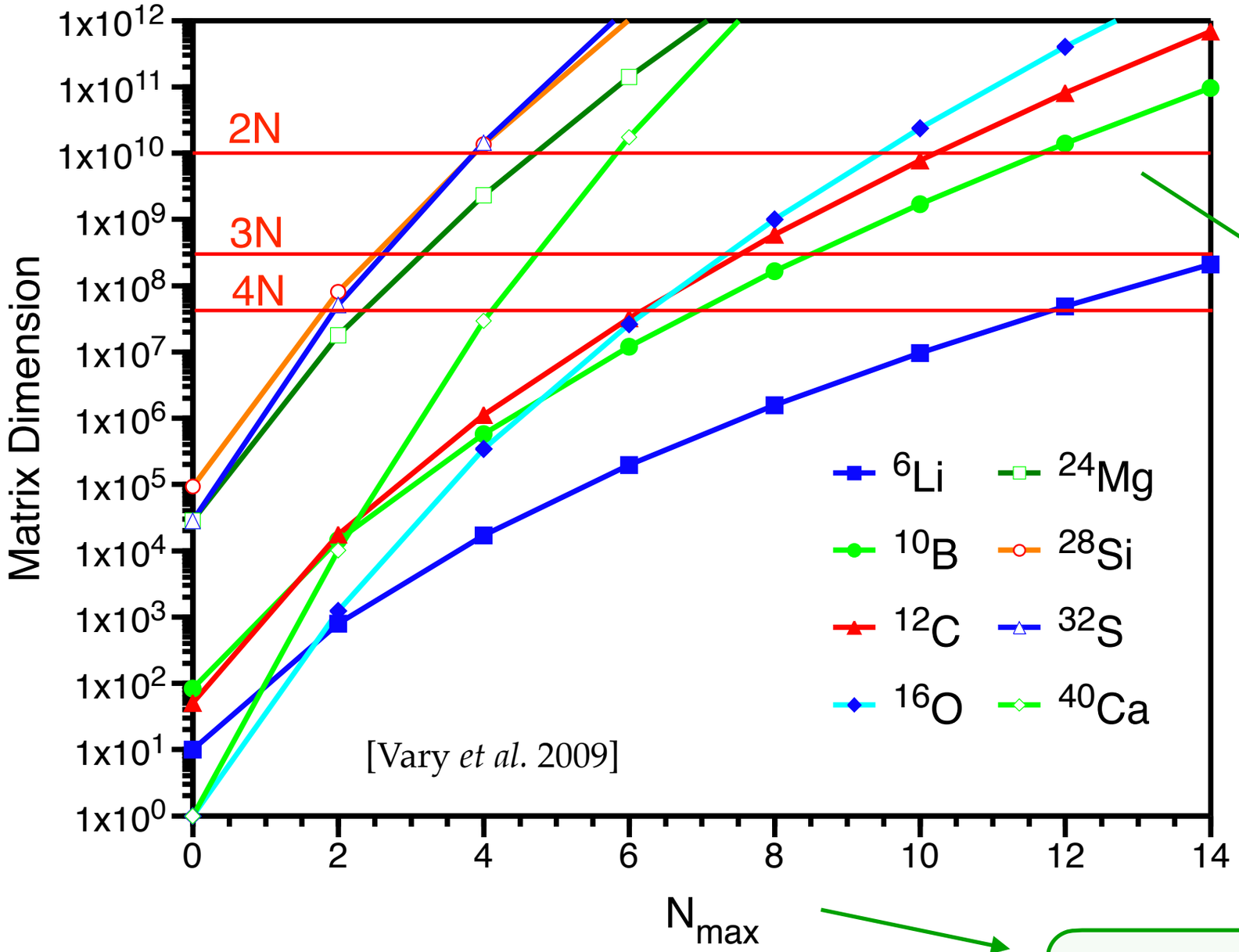

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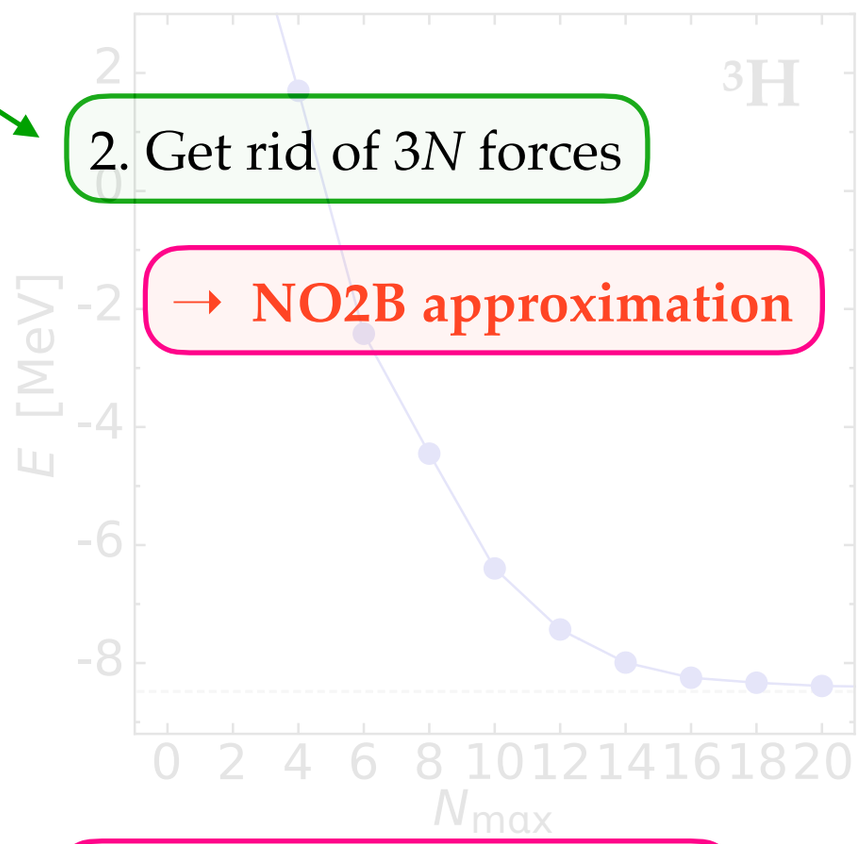


→ **SRG transformations**

1. Improve $N_{\max}$ convergence

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 $\quad |\kappa_\nu| \geq \kappa_{\min}$

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

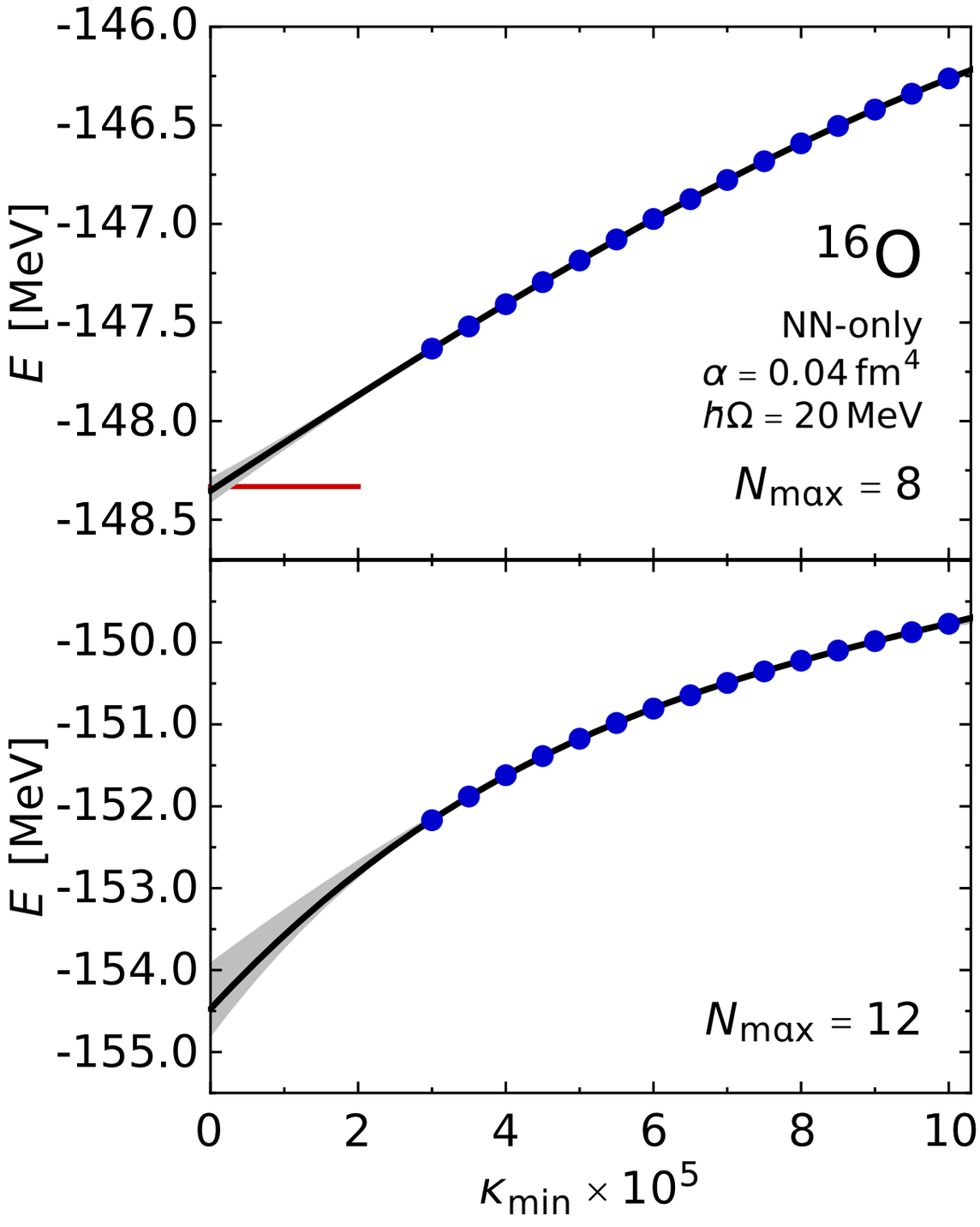
    - Typical tool of choice: **many-body perturbation theory**

  - In the limit of null threshold one must recover the original (exact) problem

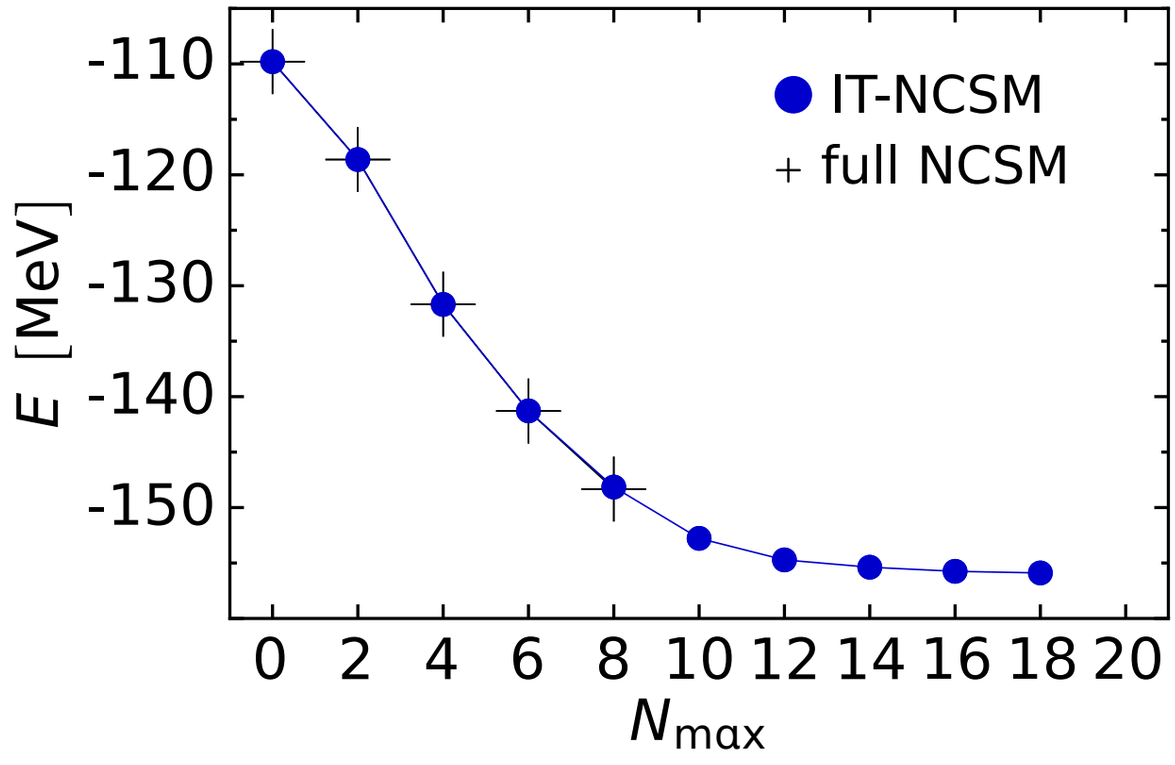
    - Smooth behaviour desirable in order to **perform extrapolations**

Importance truncation

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

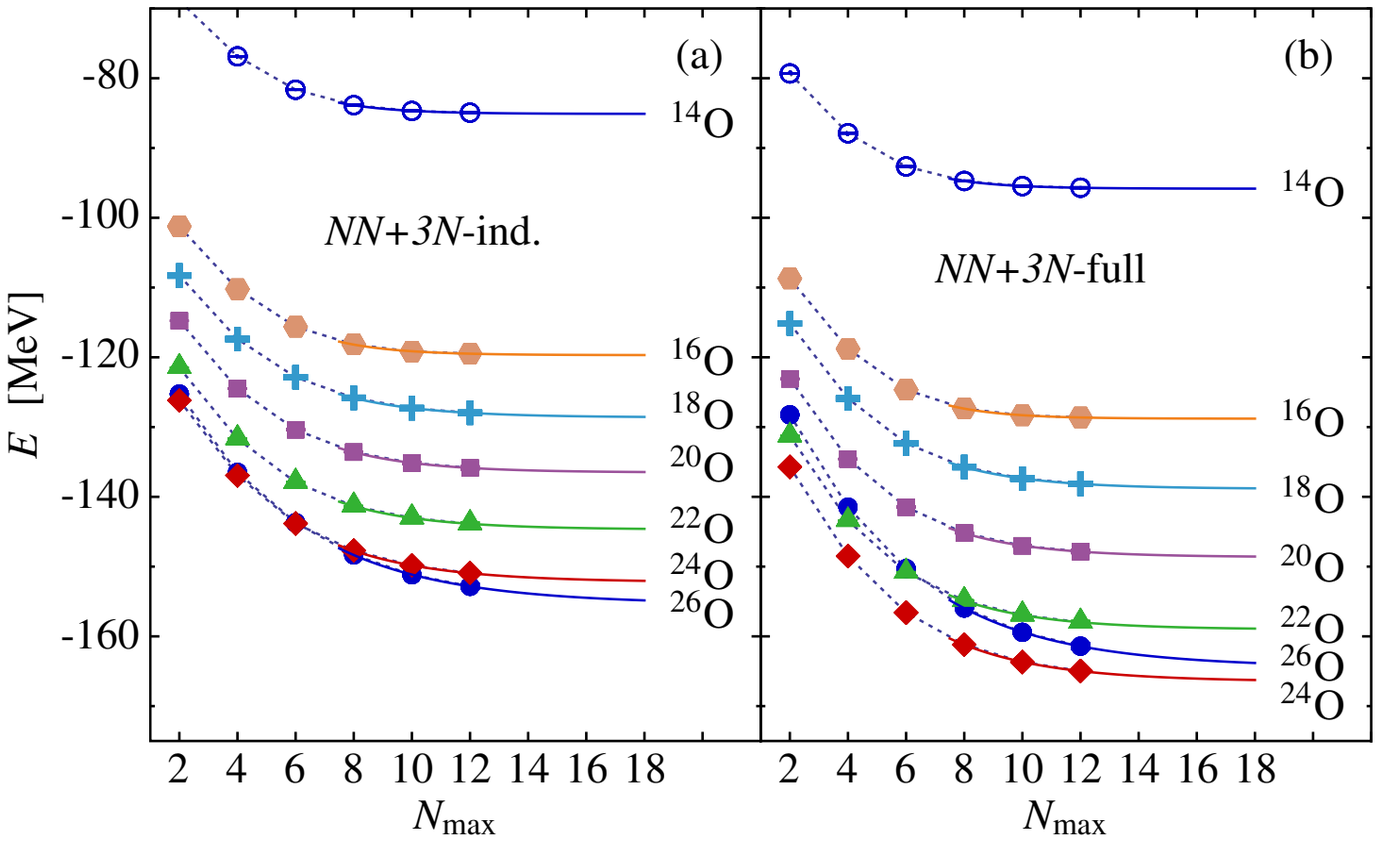


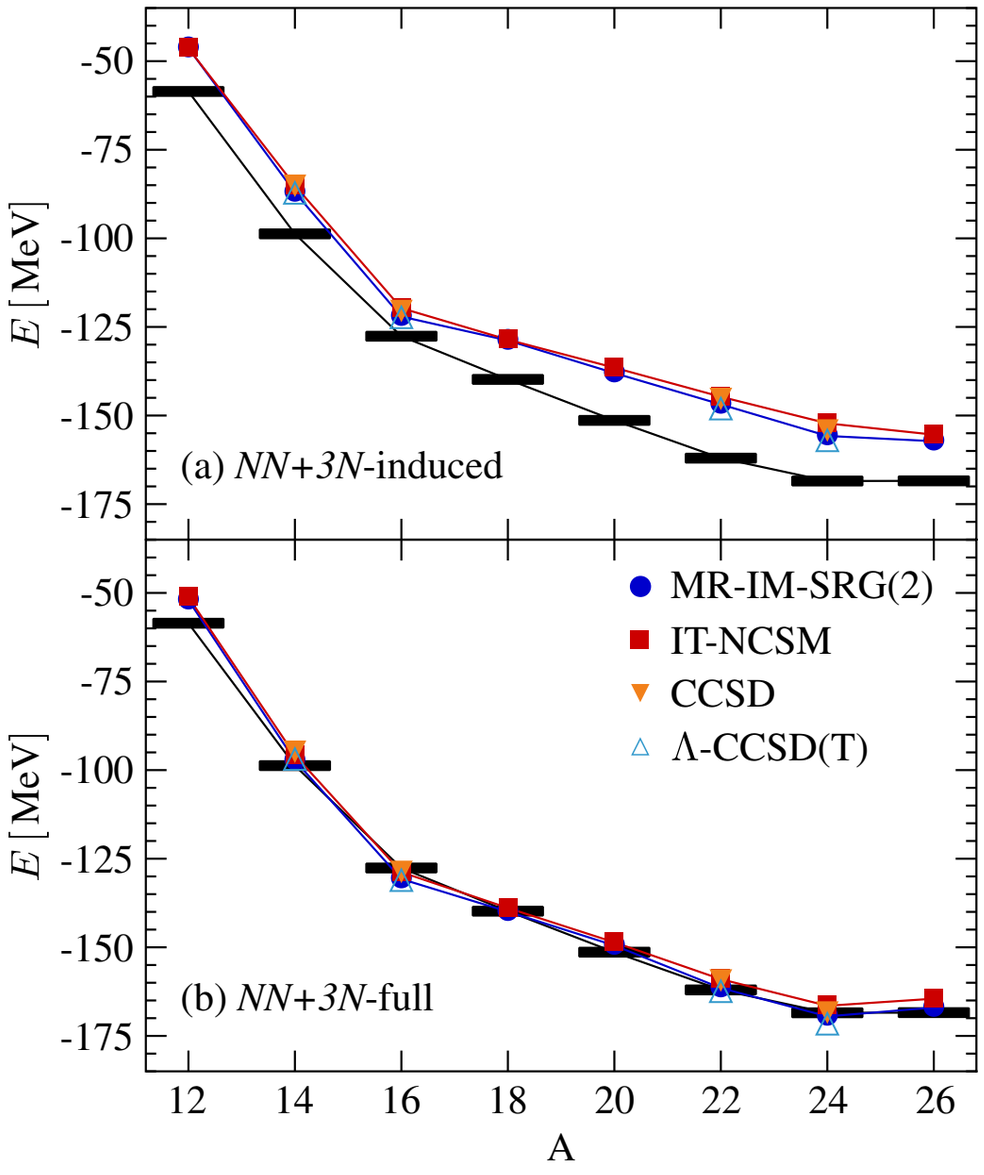
- Smooth threshold dependence
- Extrapolation to un-truncated result
- Uncertainty quantification from fit
- Benchmarks possible for for small $N_{\max}$



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]

Part 3

Expansion many-body methods for closed-shell nuclei

Correlation expansion methods: the idea

- The goal is always to solve $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$
- Idea: write the exact ground-state wave function as

$$|\Psi_0^A\rangle = \Omega_0|\phi_0\rangle$$

wave operator / correlation operator — **reference state**

➪ Expansion in terms of **particle-hole excitations**

then **expand** and **truncate** Ω_0

➪ Before truncation, the expansion is **exact**

➪ After truncation, **cost reduced** from e^N to N^α with $\alpha \geq 4$

- **Reference state**
  - Must be simple enough (such that it can be computed easily and exactly)
  - Must be rich enough (such that it is a suitable starting point for the expansion)
  - Obtained by

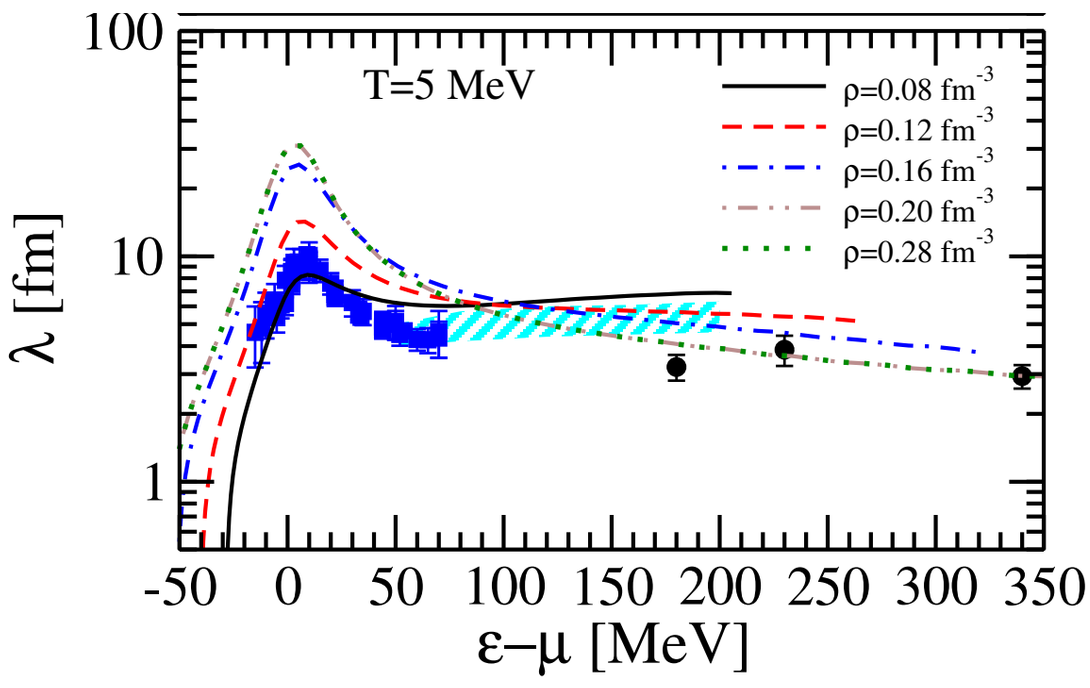
1) Splitting $H = H_0 + H_1$ 2) Solving for H_0 (**one-body** operator) $H_0|\phi_k\rangle = \epsilon_k|\phi_k\rangle$

Mean field

- **Independent-particle** picture
  - One-body potential: $H_0 = \sum_{i=1}^{A} h_0(i) \quad \rightarrow \quad H_0|\phi_k\rangle = \epsilon_k|\phi_k\rangle$ ⟹ $h_0|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \quad \forall i$

    A-body problem ⟹ A one-body problems
  - Build Slater determinant $|\phi_0\rangle = \prod_{i=1}^{A} a^\dagger_{\alpha_i}|0\rangle$
  - Nucleons move independently inside a (one-body) potential well or ***mean field***

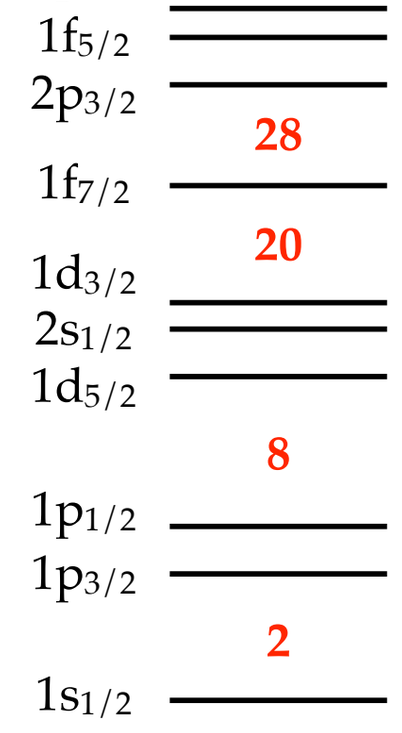
- **Does an independent-particle picture make any sense at all?**
  - Range of nuclear interaction ≈ Inter-particle distance in nuclei ~ 2 fm
  - However, it looks like it actually does make sense



✓ Fermi statistics helps out

✓ **Large mean free path** λ

[Rios & Somà 2012; Lopez *et al.* 2014]



✓ Success of nuclear **shell model**

Effective or phenomenological models

Energy density functionals

$$H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$$

Compensate for correlations in H

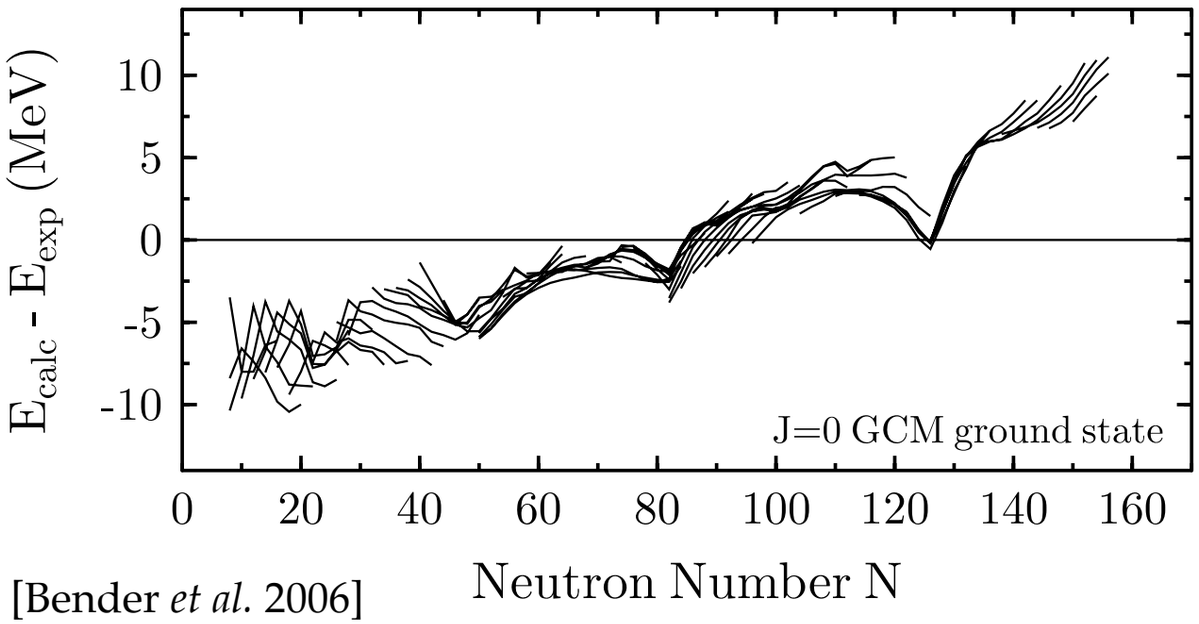
Phenomenological fit

Simplified w.f.

(Beyond) mean field

✓ Low cost → Access whole nuclear chart

✗ Unclear how to improve (systematically)



[Bender *et al.* 2006]

Interacting shell model

$$H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$$

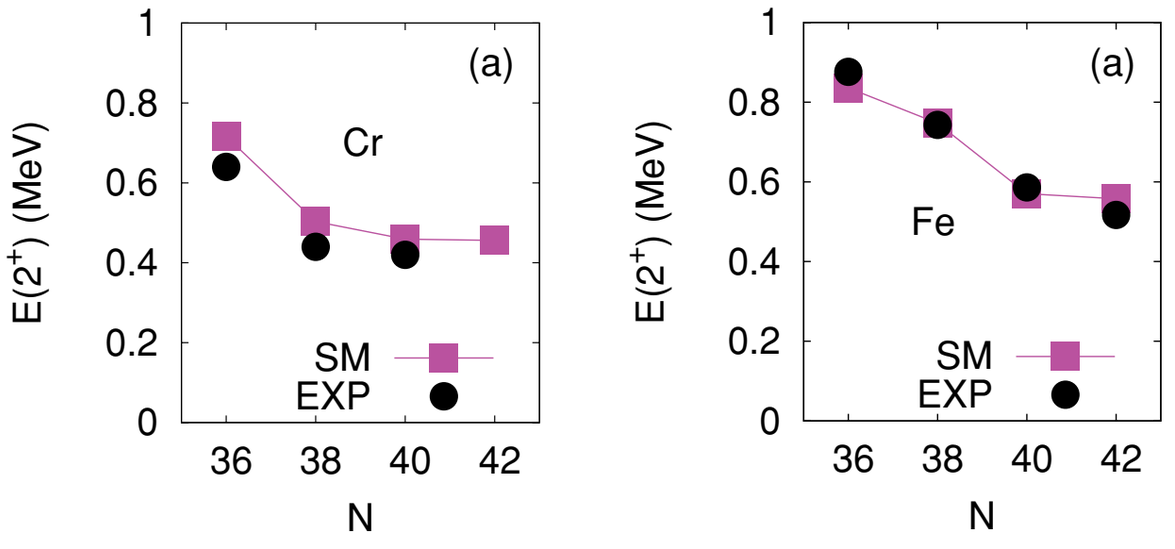
Compensate for correlations in H

Phenomenological fit

Full (CI) w.f., but in **valence space**

✓ Very accurate locally in the nuclear chart

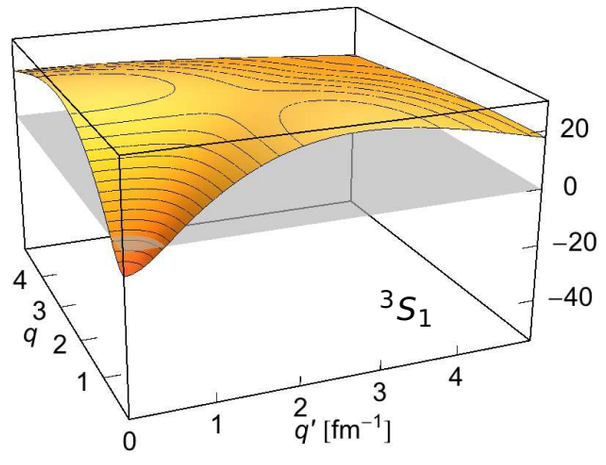
✗ Limited predictive power + scaling

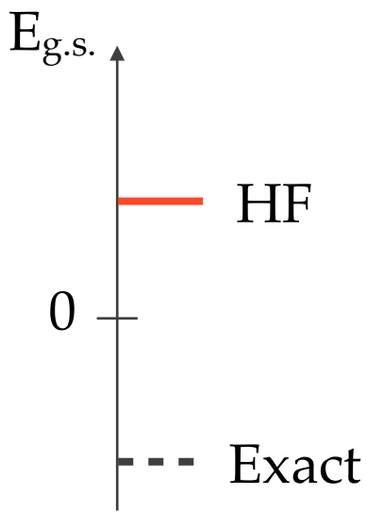


[Lenzi *et al.* 2010]

Hartree-Fock with ab initio interactions

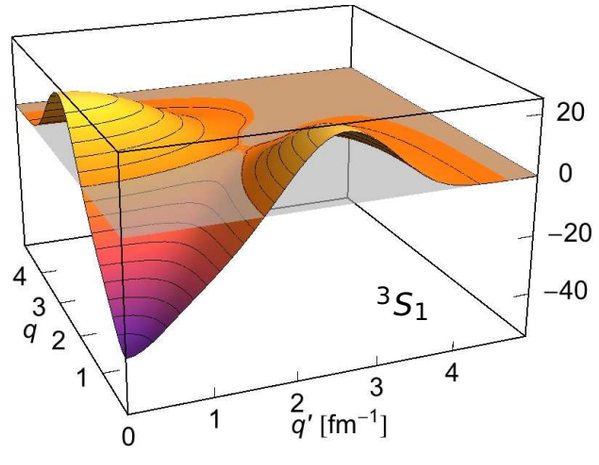
OBE potentials

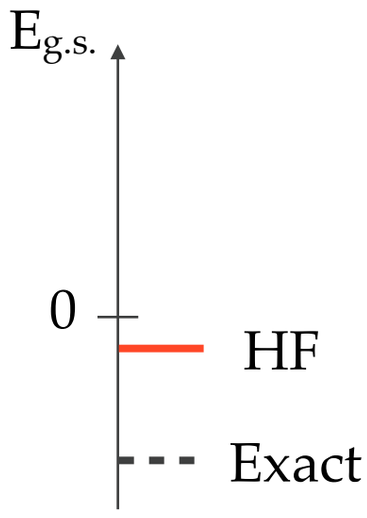




Expansion **problematic**:
full diagonalisation needed

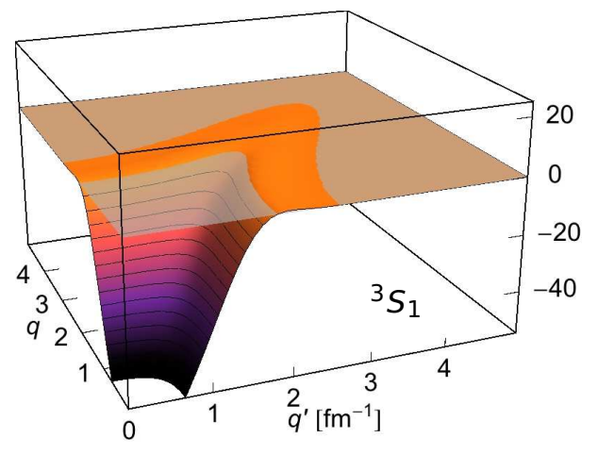
Chiral potentials

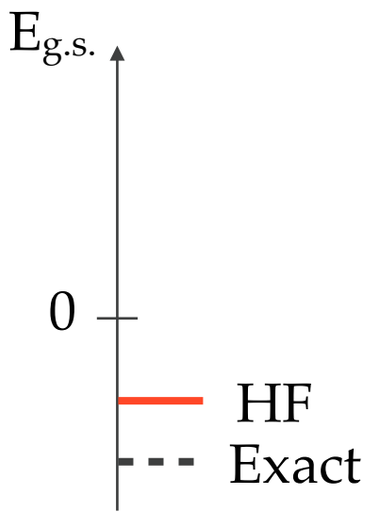




Expansion **possible**, but
problem non-perturbative

SRG potentials



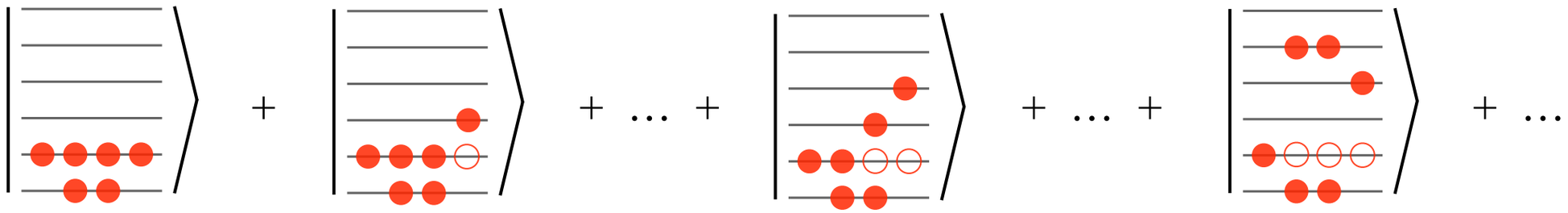


Expansion **simple**: even
perturbation theory works!

Correlation expansion: perturbative approach

⊙ **Expansion of the exact wave function**

$$|\Psi_0^A\rangle =$$



Ref 1p1h 2p2h 3p3h

➪ **Perturbative** methods: expansion coefficients computed **independently**

⊙ Standard **many-body perturbation theory (MBPT)**

- ○ Simple expressions for E at low orders
- ○ Non-iterative calculation
- ○ Polynomial scaling $O(N^\alpha) \rightarrow O(N^4)$ at MBPT(2) level

$$E^{(2)} = \frac{1}{4} \sum_{ab}^{>\epsilon_F} \sum_{ij}^{<\epsilon_F} \frac{\langle ab|W|ij\rangle\langle ij|W|ab\rangle}{(\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j)}$$

Many-body perturbation theory

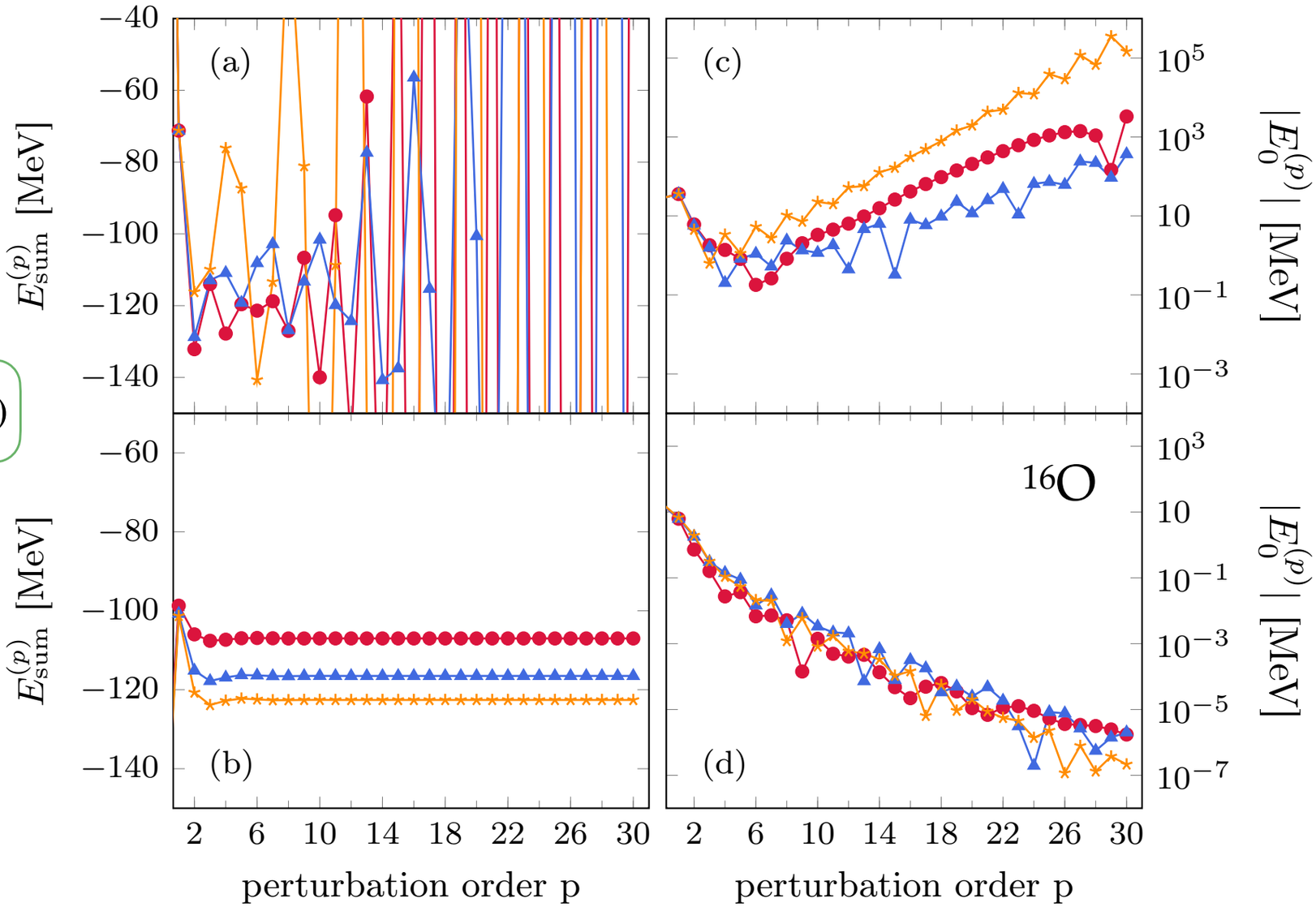
⊙ Convergence of MBPT series

○ Convergence of the series can be tested up to high orders in small basis (recursive scheme)

HO reference

$N_{\max}$ = 2 (●), 4 (▲) and 6 (★)

HF reference



[Tichai *et al.* 2016]

➪ Importance of using the right reference

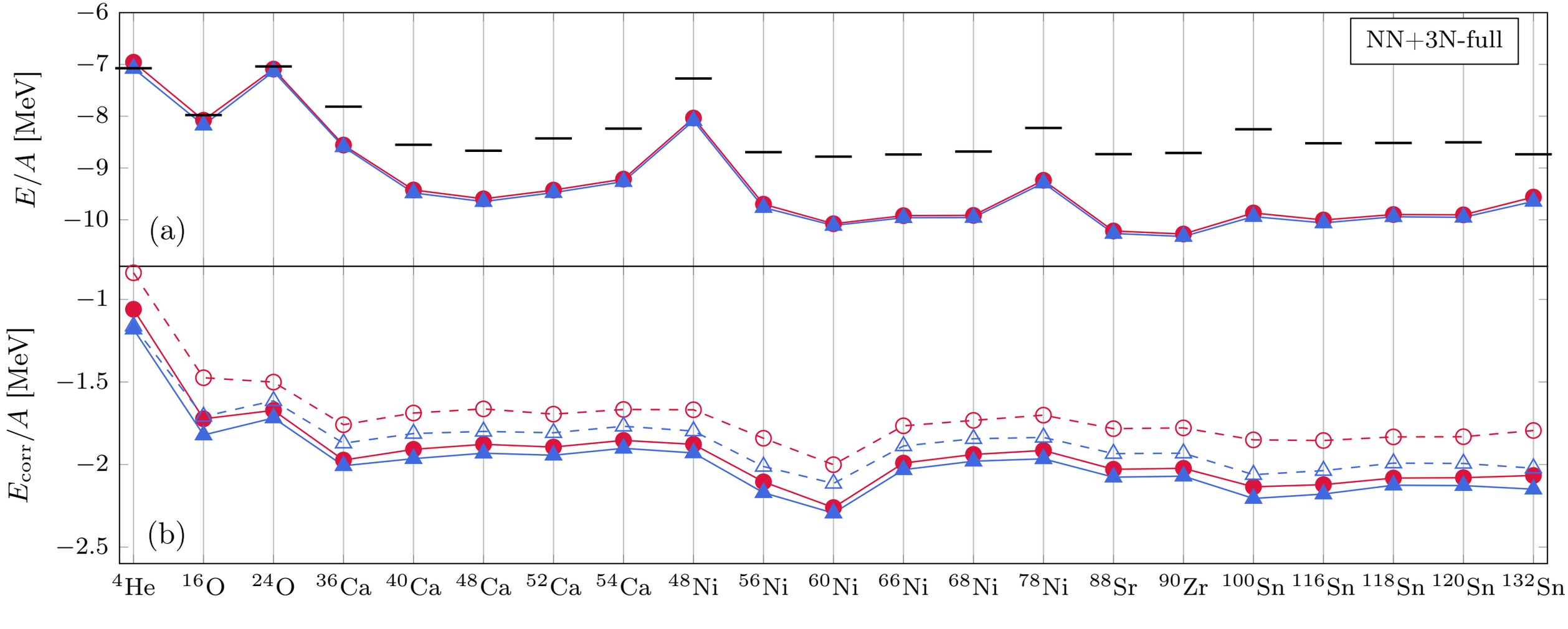
➪ Resummation schemes possible (e.g. Padé, eigenvector continuation, …)

Many-body perturbation theory

- **Reach**
  - Calculations currently possible up to mass $A \sim 100$ (and beyond)
- **Benchmark** [Tichai *et al.* 2016]
  - Accuracy competitive with coupled cluster calculations (non-perturbative and more costly)

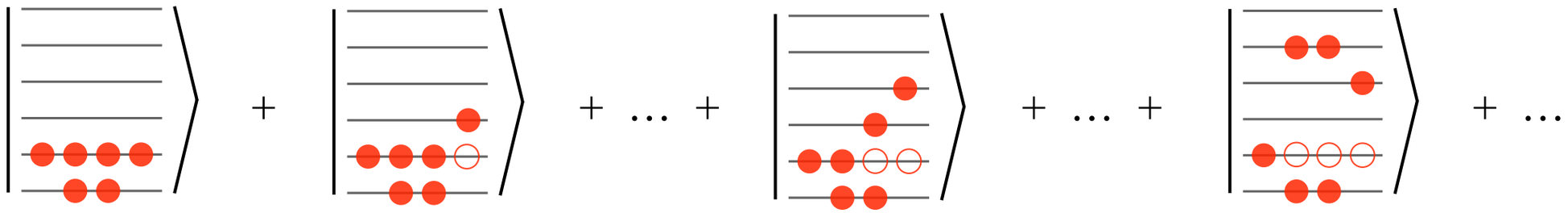
MBPT $E_0^{(2)}$ (○) $E_0^{(2)} + E_0^{(3)}$ (●)

Coupled cluster CCSD (△) CR-CC(2,3) (▲)



Correlation expansion: non-perturbative approach

⊙ **Expansion of the exact wave function**

$$|\Psi_0^A\rangle =$$  $$+ \ \ldots \ +$$ $$+ \ \ldots \ +$$ $$+ \ \ldots$$

Ref 1p1h 2p2h 3p3h

➪ **Perturbative** methods: expansion coefficients computed **independently**

➪ **Non-perturbative** methods: expansion coefficients computed **self-consistently**

⊙ Examples of non-perturbative approaches

○ **Coupled-cluster theory (CC)**

➪ Exponential ansatz for the wave function $|\Psi_{CC}\rangle = e^T |\Phi\rangle$

○ **In-medium similarity renormalisation group (IMSRG)**

➪ SRG evolution for H normal-ordered w.r.t. to a reference Slater determinant

○ **Self-consistent Green's function (SCGF)** [next slide]

Green's function techniques

⊙ The goal is to solve the ***A*-body Schrödinger equation**

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

⊙ Instead of working with the full A-body wave function $|\Psi_k^A\rangle$, rewrite the Schrödinger equation in terms of **1-, 2-, …. *A*-body objects** G_1=G, G_2, … G_A (**Green's functions**)

➟ A-1 coupled equations

⊙ 1-, 2-, …. A-body Green's functions yield **expectation values of 1-, 2-, …. *A*-body operators**

➟ In practice, one usually needs 1- and/or 2-body GFs (~ 1- & 2-body density matrices)

⊙ One-body Green's function obtained by solving **Dyson equation** (derived from Schrödinger eq.)

$$G = G^{(0)} + G^{(0)}\,\Sigma\,G$$

unperturbed Green's function

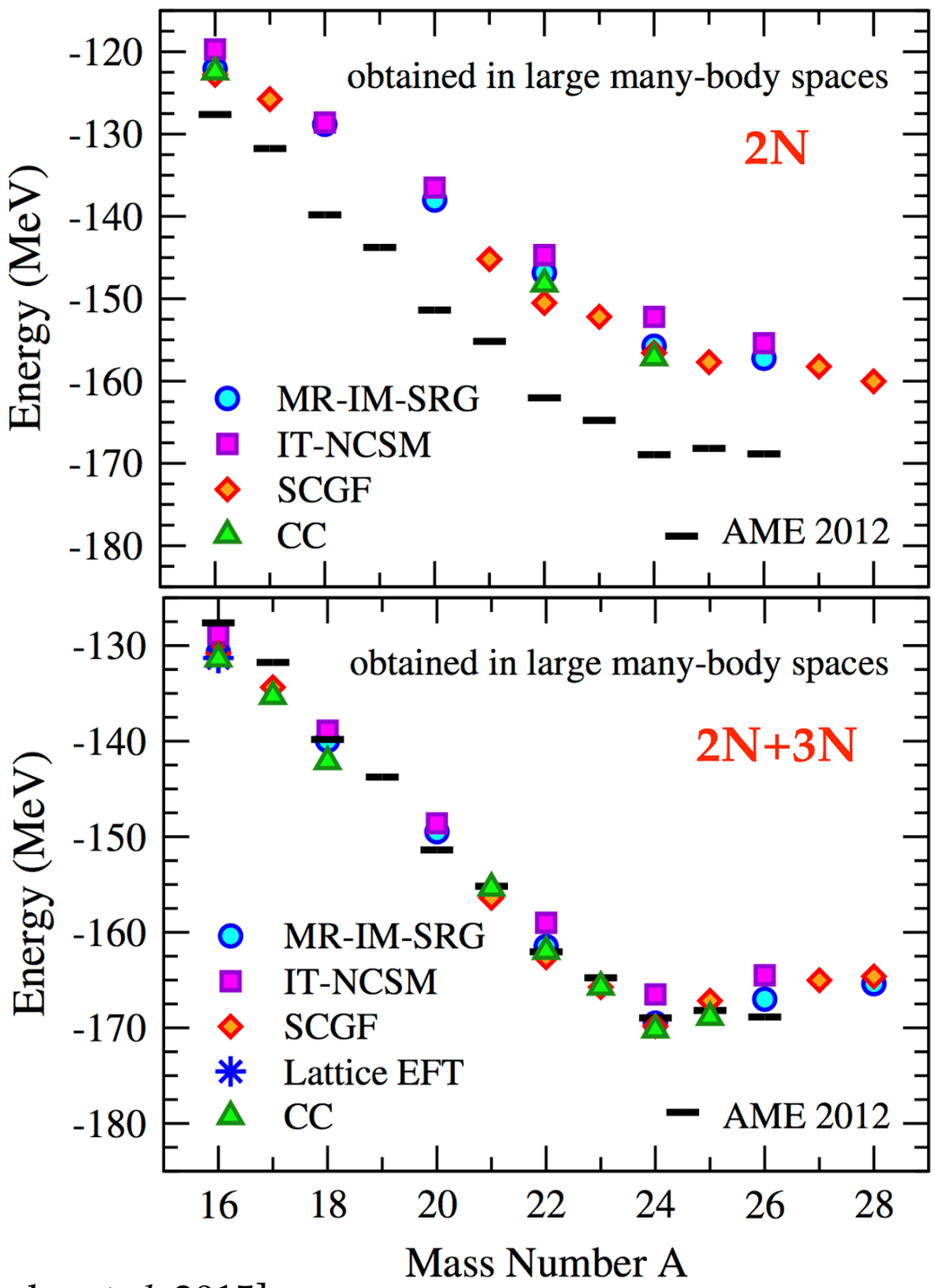
many-body effects contained in the **self-energy** Σ

⊙ Bonus: one-body Green's function contains information about ***A*±1 excitation energy spectra**

➟ Spectral or **Lehmann representation** of the Green's function

Benchmarks

Oxygen binding energies



[Hebeler *et al.* 2015]

⊙ **Convergence of many-body results**

- ○ Different strategies to solve $H\Psi=E\Psi$
- ○ Same input Hamiltonian (except lattice EFT)
- ○ **All methods agree within 5%**

⊙ **Physics of oxygen isotopes**

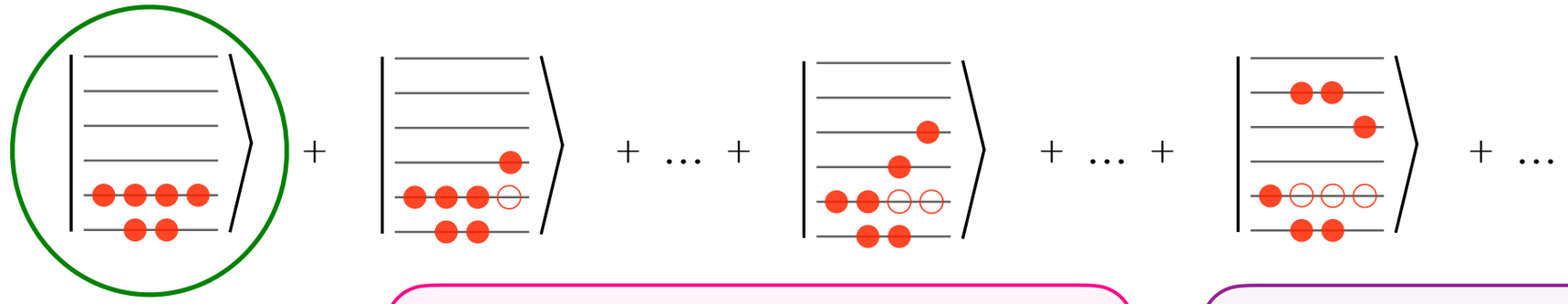
- ○ Energy trend reproduced by 2N+3N results
- ○ **Correct drip line only with 3N forces**

Part 4

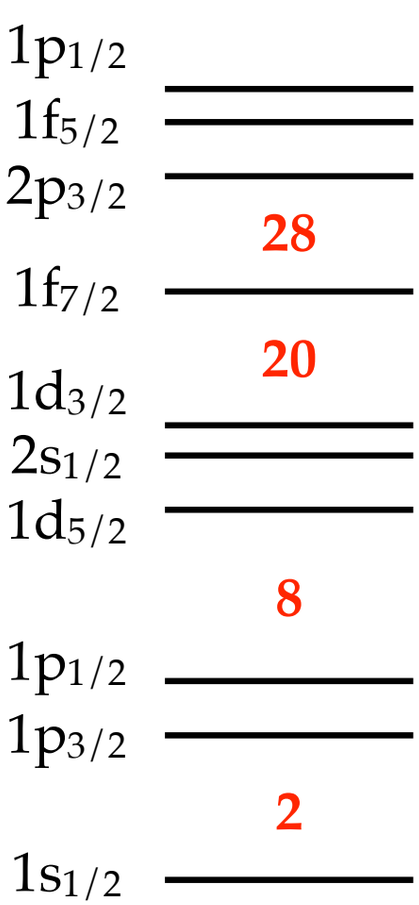
Expansion many-body methods for open-shell nuclei

Closed- vs. open-shell systems

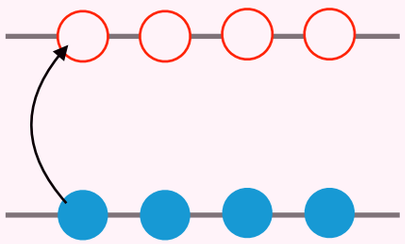
⊙ In practice: expand on Slater determinant basis → particle-hole (ph) expansion



Ref. state varies with N & Z



Nucleons **entirely** fill levels below a magic number



Closed-shell systems

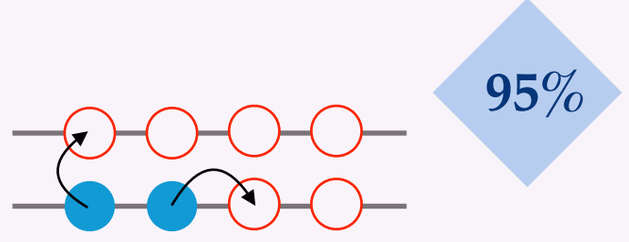
↓

Larger energy gap,
excitations hindered,
enhanced stability

↓

Weakly correlated,
clear ph hierarchy,
expansion **well defined**

Nucleons **partially** fill levels below a magic number



Open-shell systems

↓

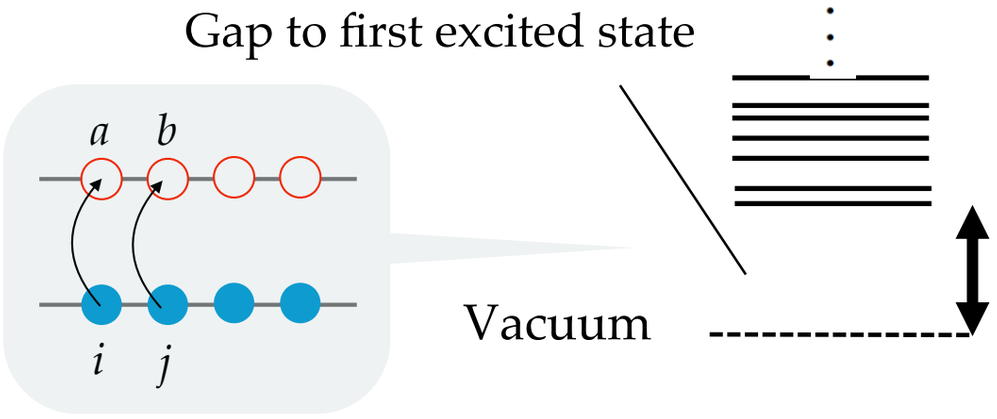
Smaller (→ 0) energy gap,
excitations enabled,
lesser stability

↓

Strongly correlated,
no ph hierarchy,
expansion **ill defined**

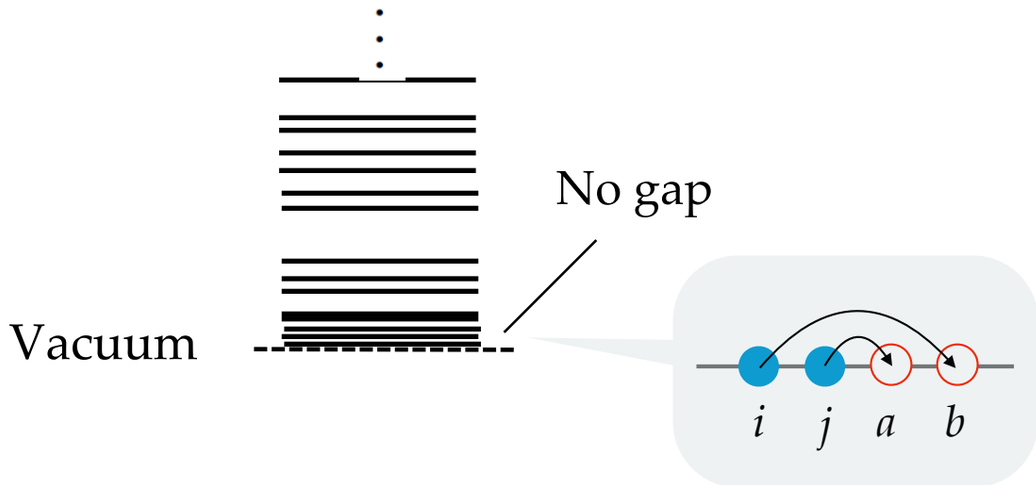
Breakdown of ph expansion

Closed-shell



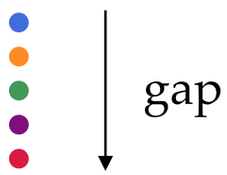
$$\Delta E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{4}\sum_{ijab}\frac{|h^{(2)}_{ijab}|^2}{e_a + e_b - e_i - e_j} > 0$$

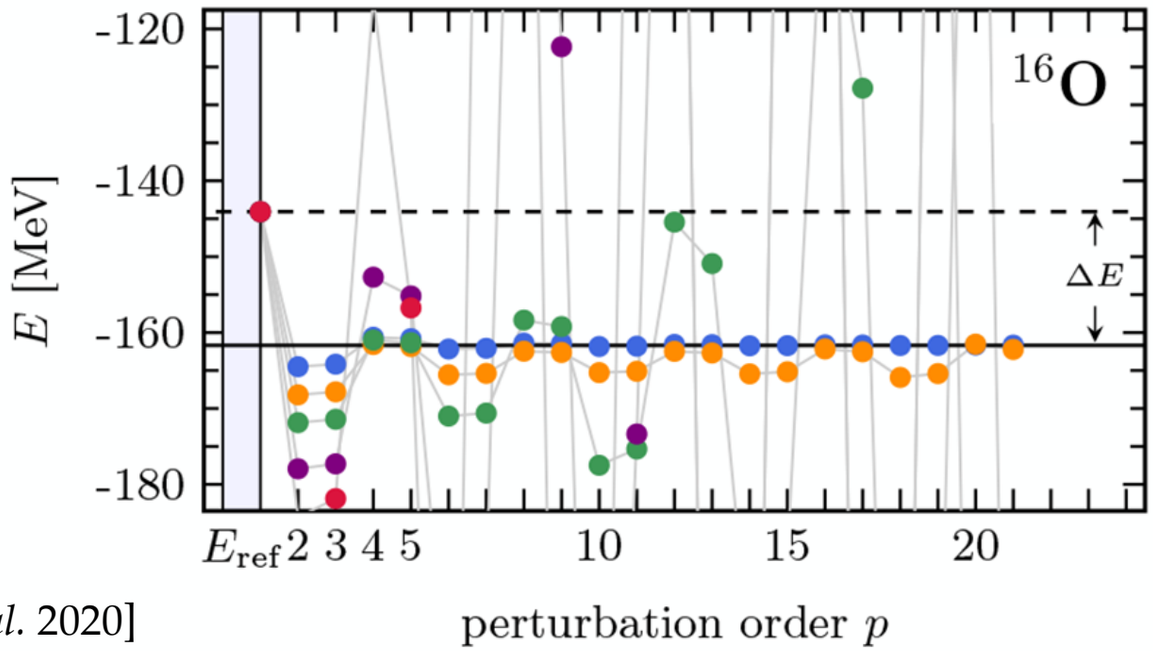
Open-shell



$$\Delta E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{4}\sum_{ijab}\frac{|h^{(2)}_{ijab}|^2}{e_a + e_b - e_i - e_j} = 0$$

- Breakdown of ph expansion evident already in MBPT(2) expressions
- Can be explicitly demonstrated by artificially decreasing the gap in ^{16}O

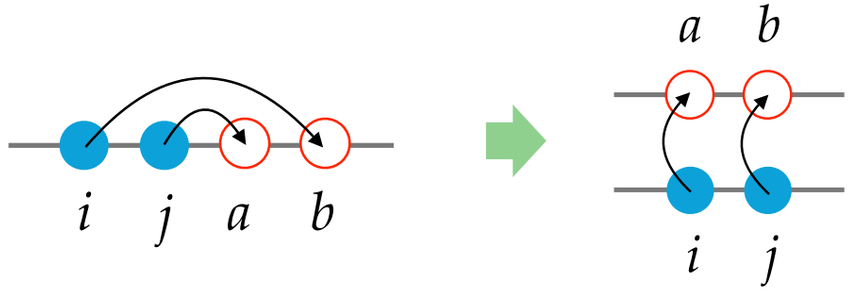




[Tichai *et al.* 2020]

Symmetry breaking

⊙ Idea: reopen gap via **symmetry breaking**



⊙ Which symmetries?

- ○ $G_{\mathbf{Ham}} \rightarrow$ symmetries of H usually dictated by QCD + general principles
- ○ $G_{\mathbf{wf}} \rightarrow$ symmetries of w.f. depend on a given ansatz
- ○ $G_{\mathbf{bas}} \rightarrow$ eigenfunctions of a given operator with certain symmetries (e.g. HO Hamiltonian)

Usually one chooses $G_{\mathbf{Ham}} = G_{\mathbf{wf}} = G_{\mathbf{bas}}$

Symmetry breaking $\rightarrow$ $G_{\mathbf{Ham}} \neq G_{\mathbf{wf}}$

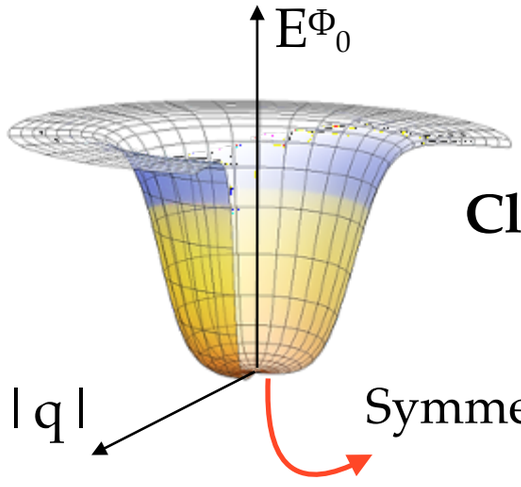
⊙ Why should it help?

- ○ Variational space of w.f. is **enlarged**
- ○ Degeneracy is **lifted** by deformation $\rightarrow$ Particle-hole expansion again well defined
- ○ We know it works from **experience** (collective model, energy density functionals)

Symmetry breaking

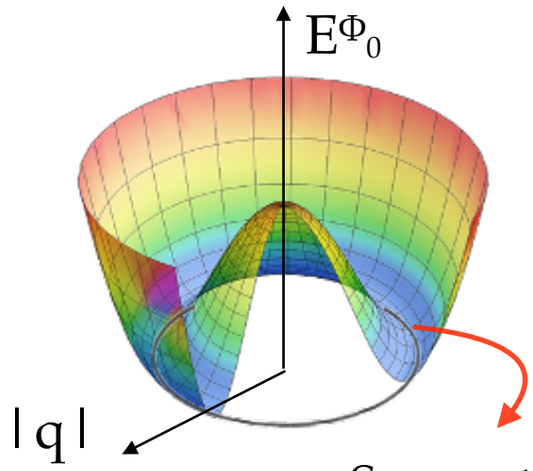
⊙ **Allowing w.f. to break symmetries is an efficient way to account for strong correlations**

Order parameter $\langle \Phi_0 | Q | \Phi_0 \rangle = q \equiv |q| e^{i \arg(q)}$



Closed-shell systems

Symmetry-conserving minimum



Open-shell systems

Symmetry-breaking minimum

<u>Which symmetry for which type of correlation?</u>

Physical symmetry	*Group*	*Correlations*
Rotational inv.	SU(2)	Deformation
Particle-number	$U(1)_N$ x $U(1)_Z$	Superfluidity

Singly open-shell ➪ Sufficient to **break U(1)**

Doubly open-shell ➪ Necessary to **break SU(2)**

✓ **Advantage:** polynomially-scaling (N^α) method that can tackle strongly correlated systems

✗ **Prices to pay:**

1) $N_{\text{sym-breaking}} > N_{\text{sym-conserving}}$

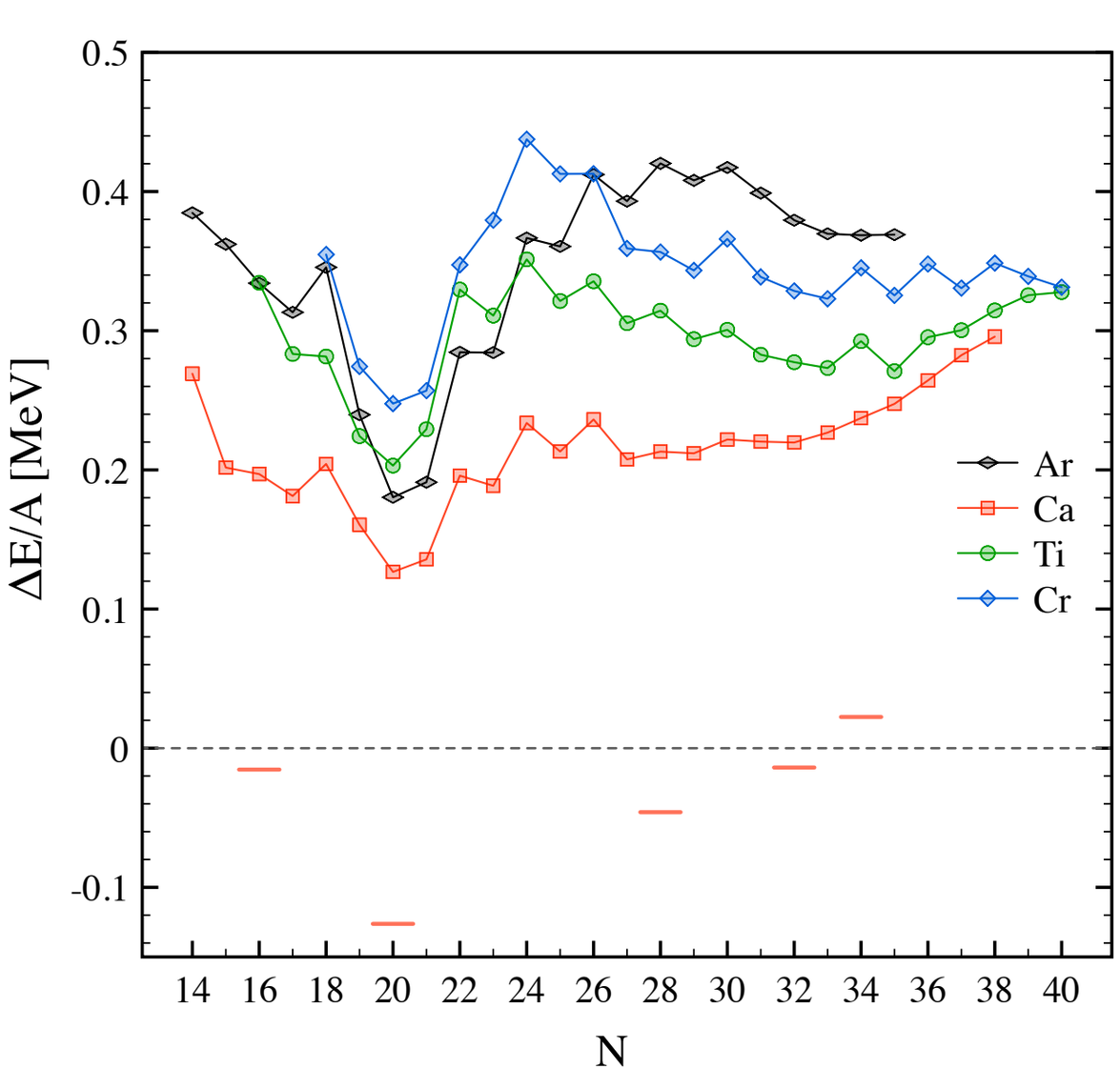
2) Symmetries must be eventually **restored** in finite systems

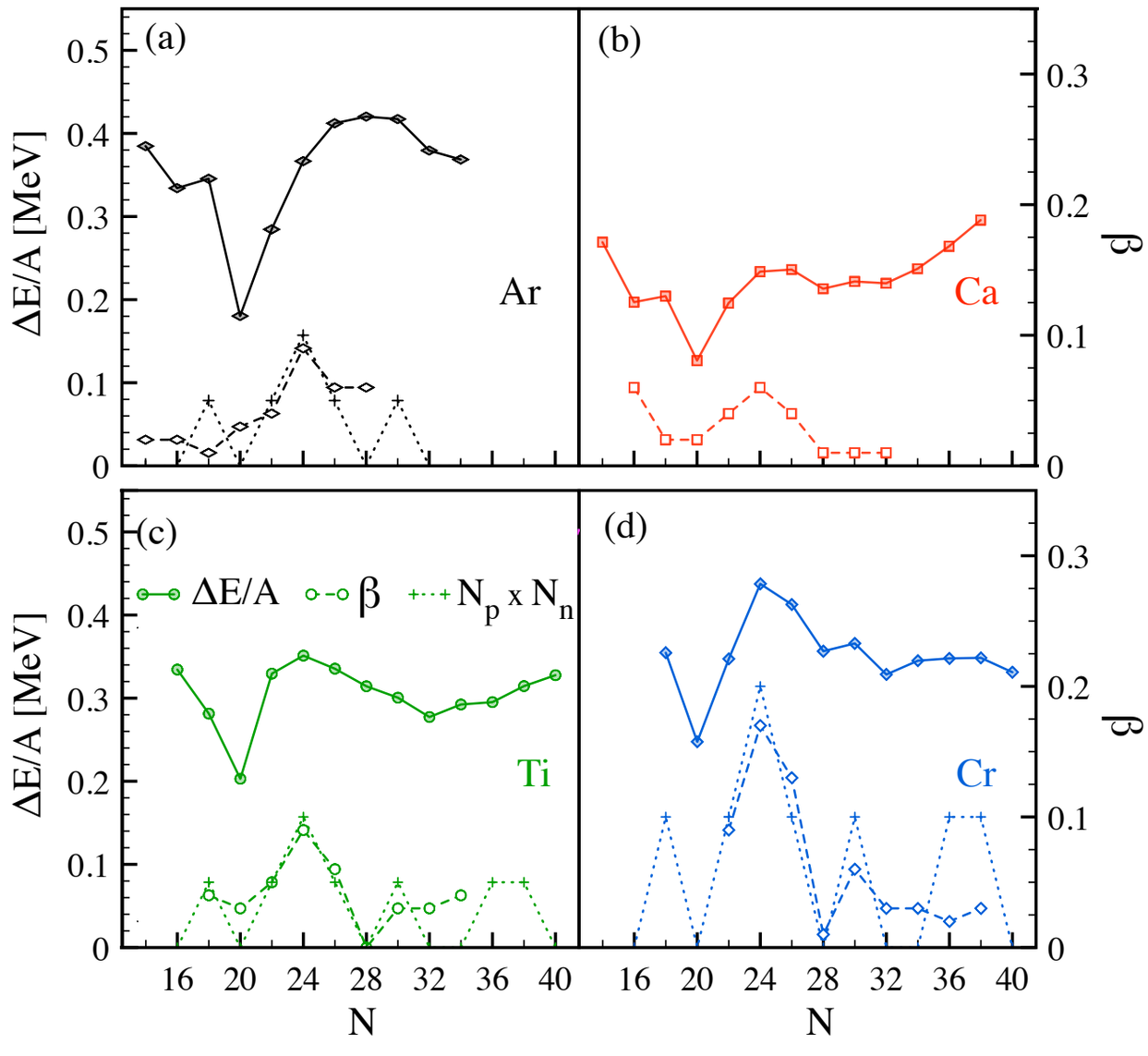
Symmetry breaking

- **Example: U(1)-breaking SCGF calculations**

  [Somà *et al.* 2021]

  - Description deteriorates when going away from singly open-shell
  - Correlation with (expected) deformation observed





Partition, expand, project

⊙ Partition, then expand & project

1. Compute symmetry-breaking ref. state

$$|\Theta^0\rangle = |\Phi(q_{\min})\rangle \longrightarrow H = H_0 + H_1$$

2. Expand in H_1

3. Restore broken symmetries

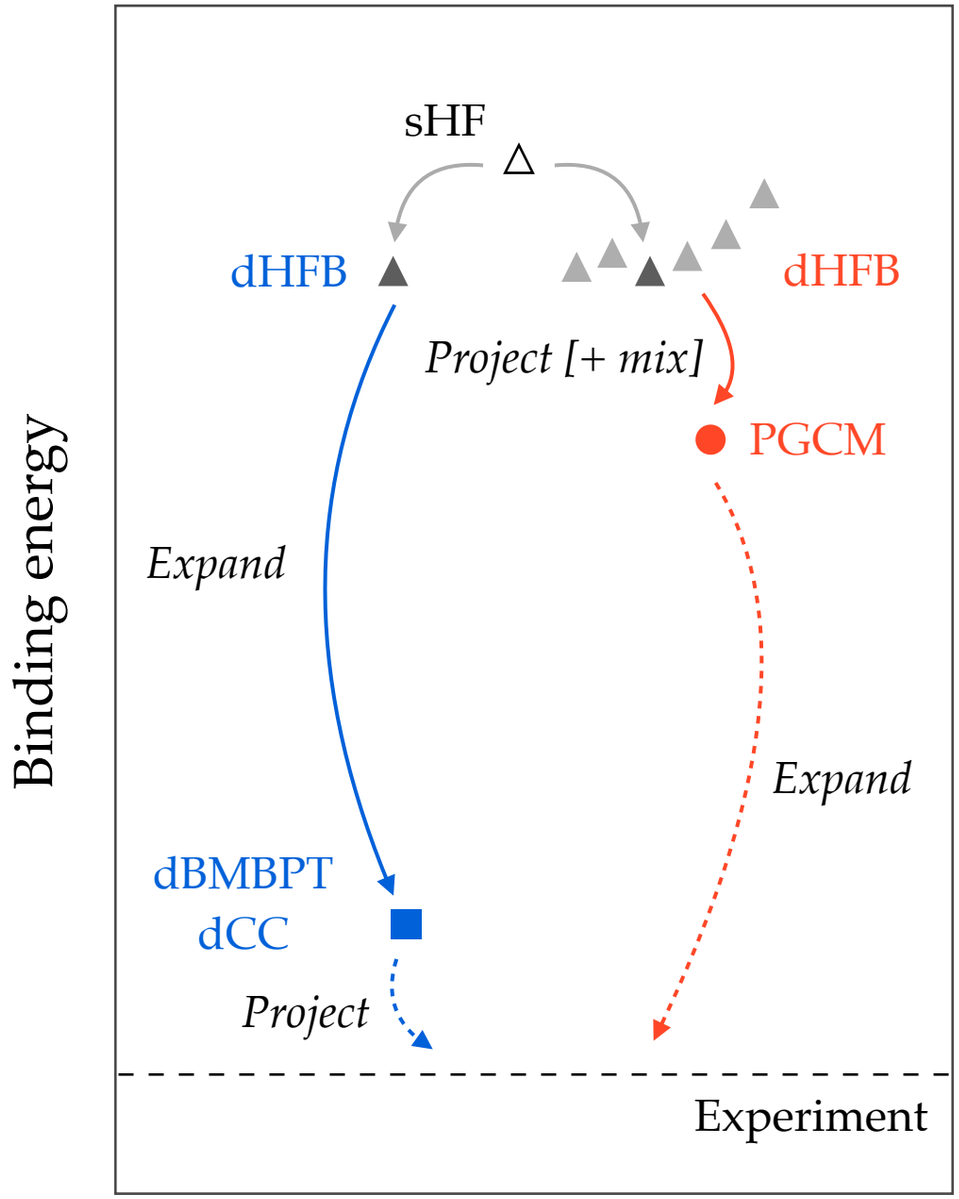
⊙ Partition & project, then expand

1. Compute symmetry-breaking states [at many q]

2. Restore symmetries [+ q-mixing (PGCM)]

$$|\Theta^0\rangle = \sum_q f(q)\, P\, |\Phi(q)\rangle \longrightarrow H = H_0 + H_1$$

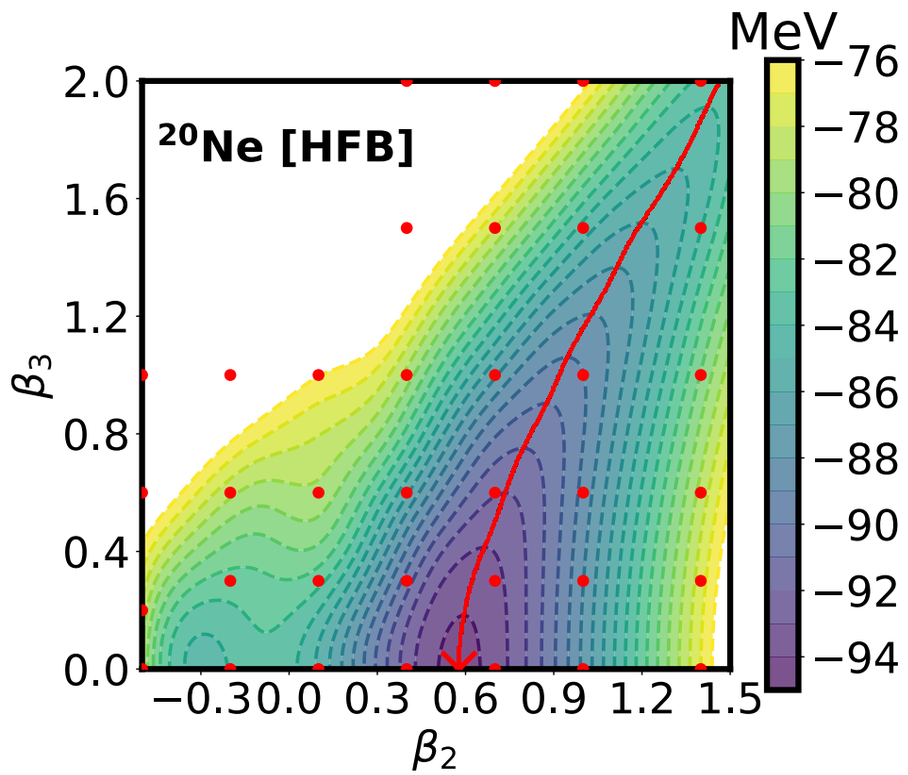
3. Expand in H_1



Each step scales polynomially!

^{20}Ne

1. Constrained HFB

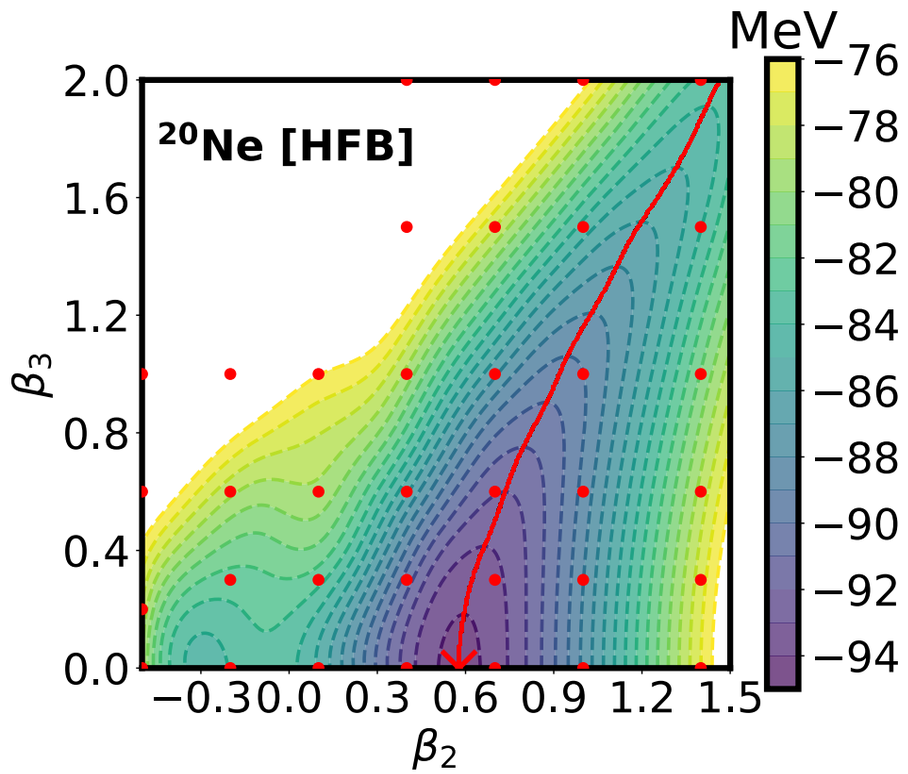


- **Constrained HFB calculations**
  - Maps total energy surface (TES)
  - Minimum at strongly deformed configuration
  - TES soft along the octupole direction

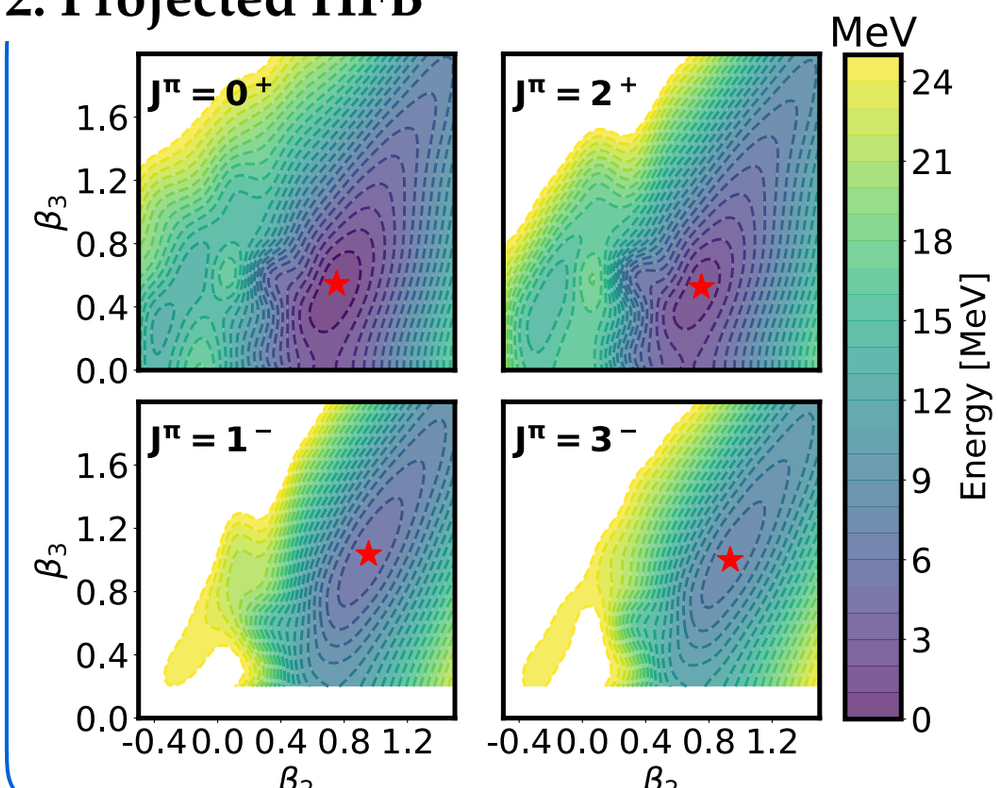
[Frosini *et al.* 2022]

^{20}Ne

1. Constrained HFB



2. Projected HFB

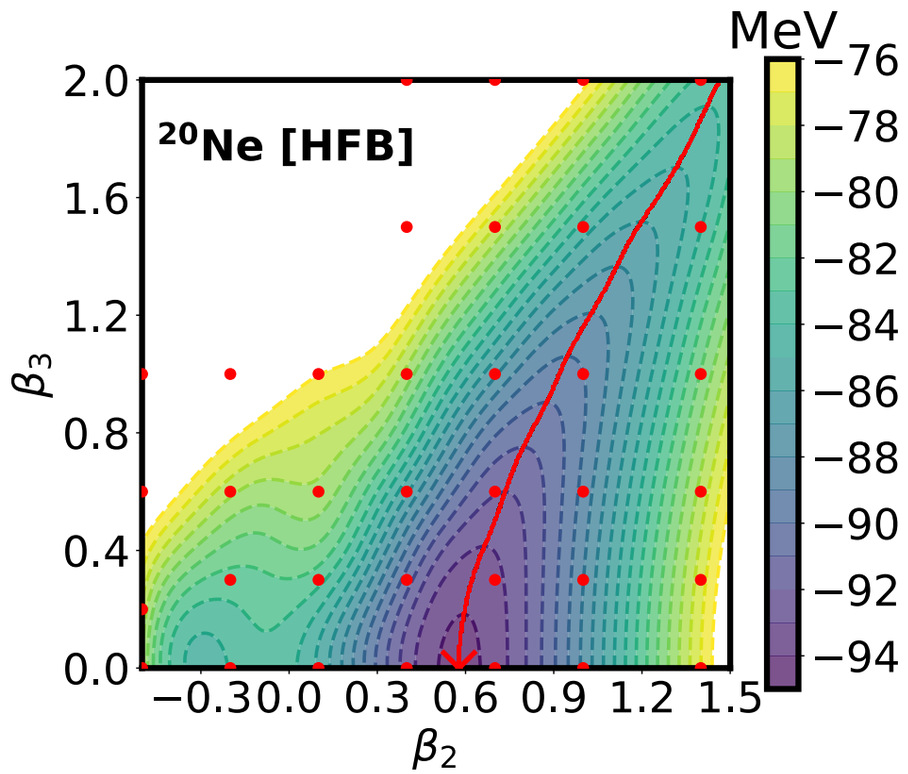


- **Projected HFB calculations**
  - Projections favour deformed configurations
  - Negative parity states accessed
  - Provide input for computing PGCM state

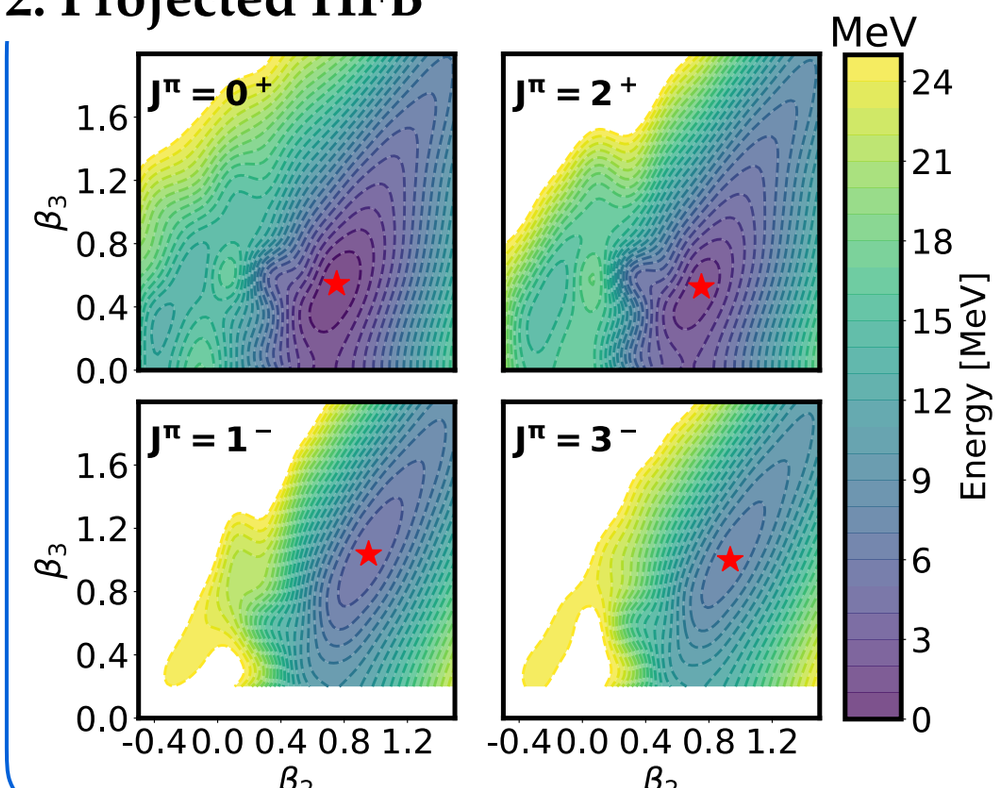
[Frosini *et al.* 2022]

^{20}Ne

1. Constrained HFB



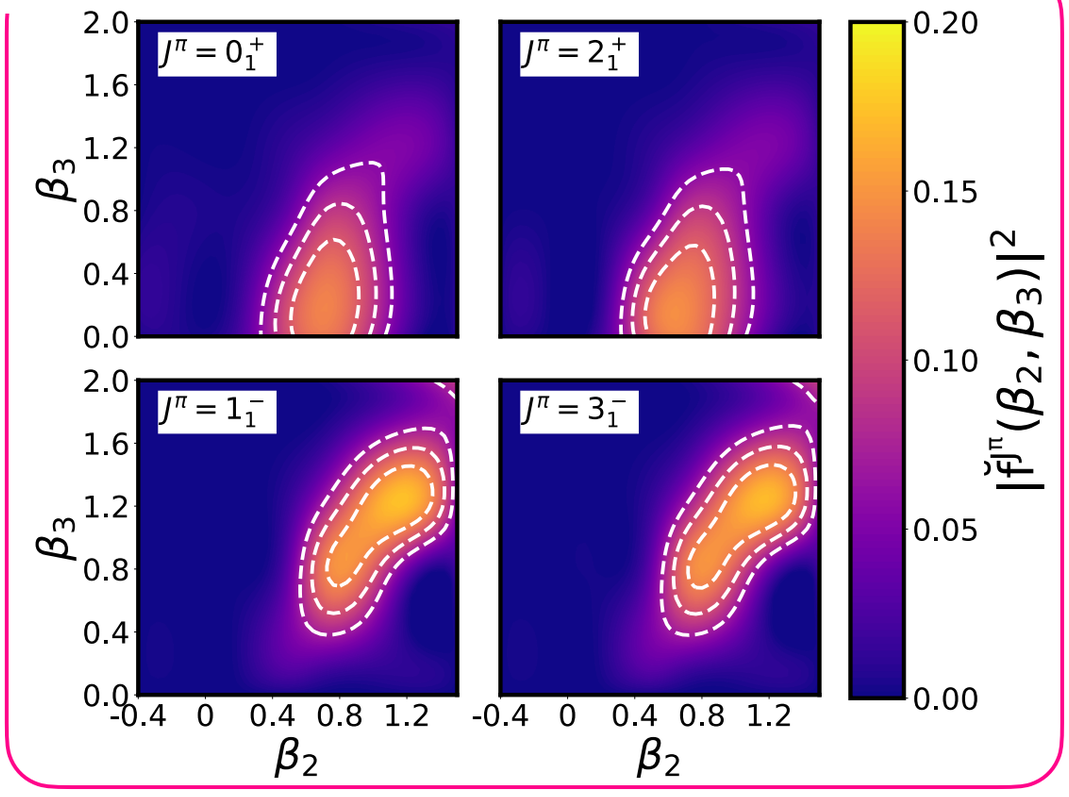
2. Projected HFB



- **PGCM mixing**
  - Collective q.f. → admixture of PHFB states
  - Significant shape fluctuations
  - Negative parities mix more deformations

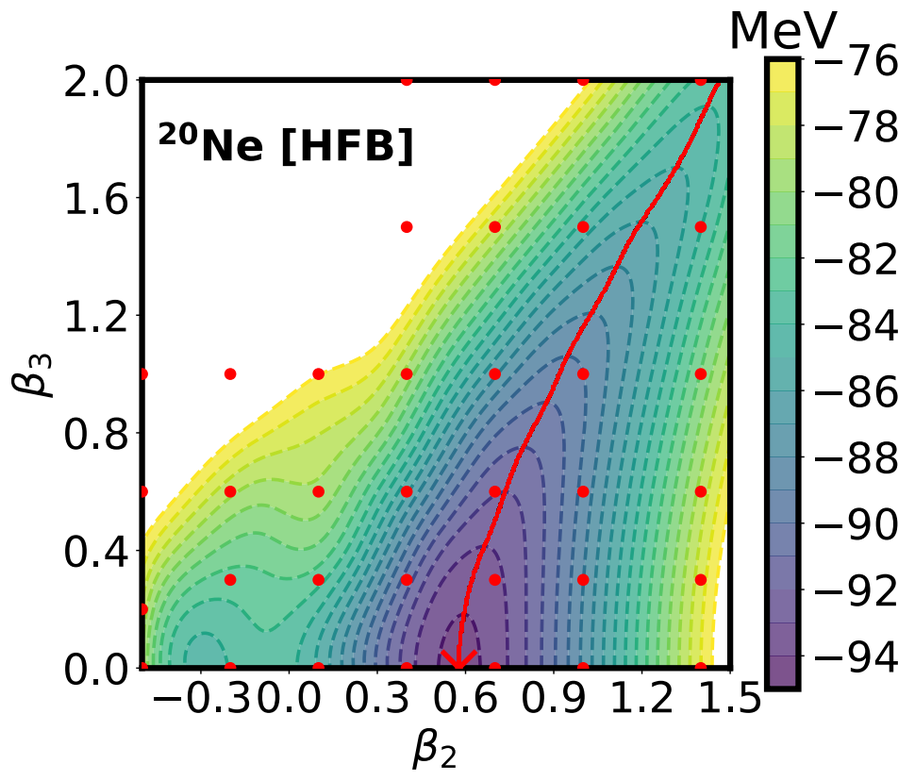
[Frosini *et al.* 2022]

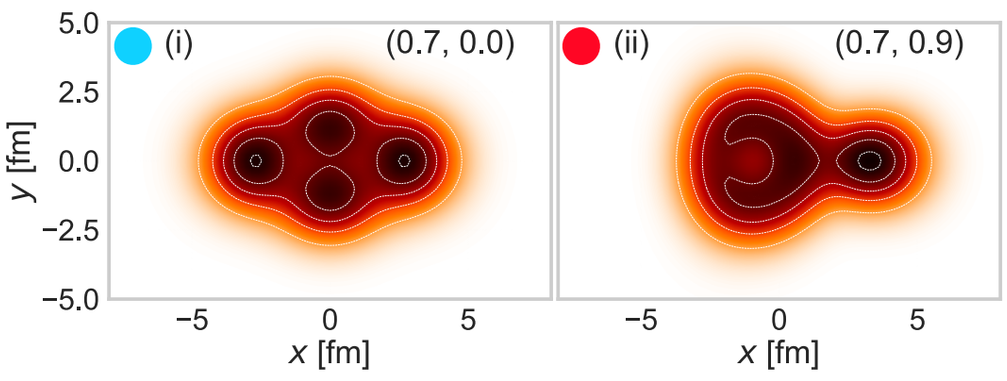
3. PGCM

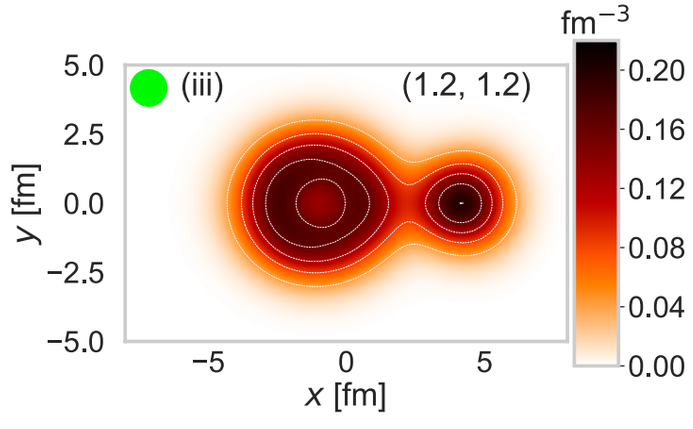


^{20}Ne

1. Constrained HFB

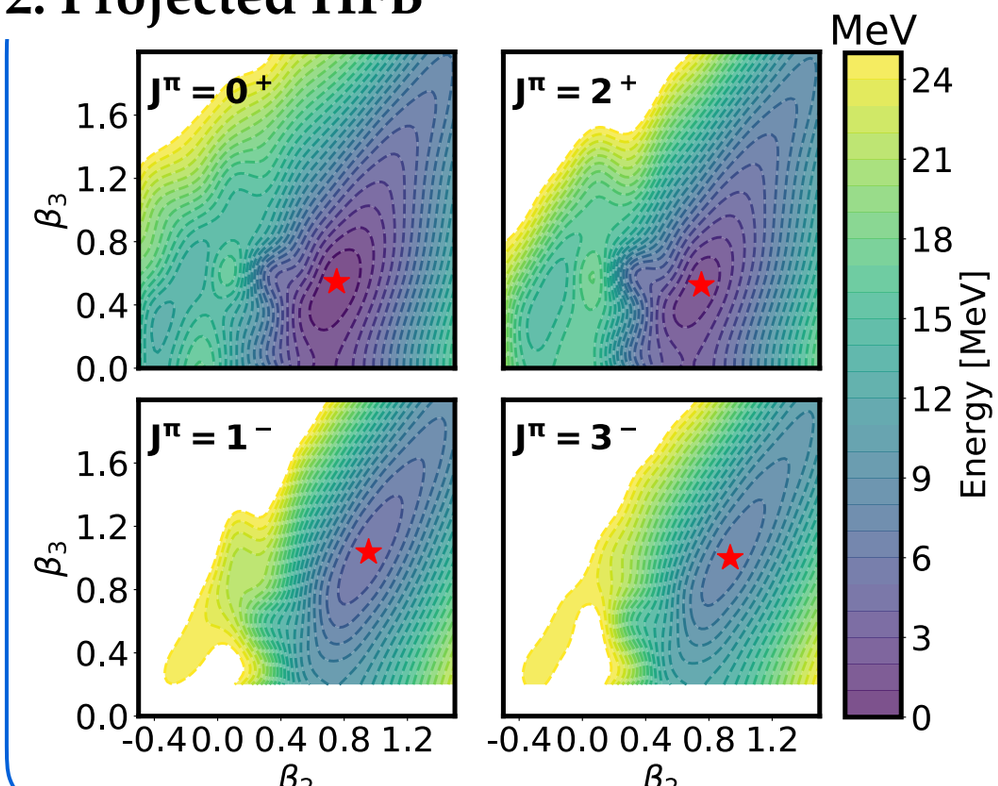




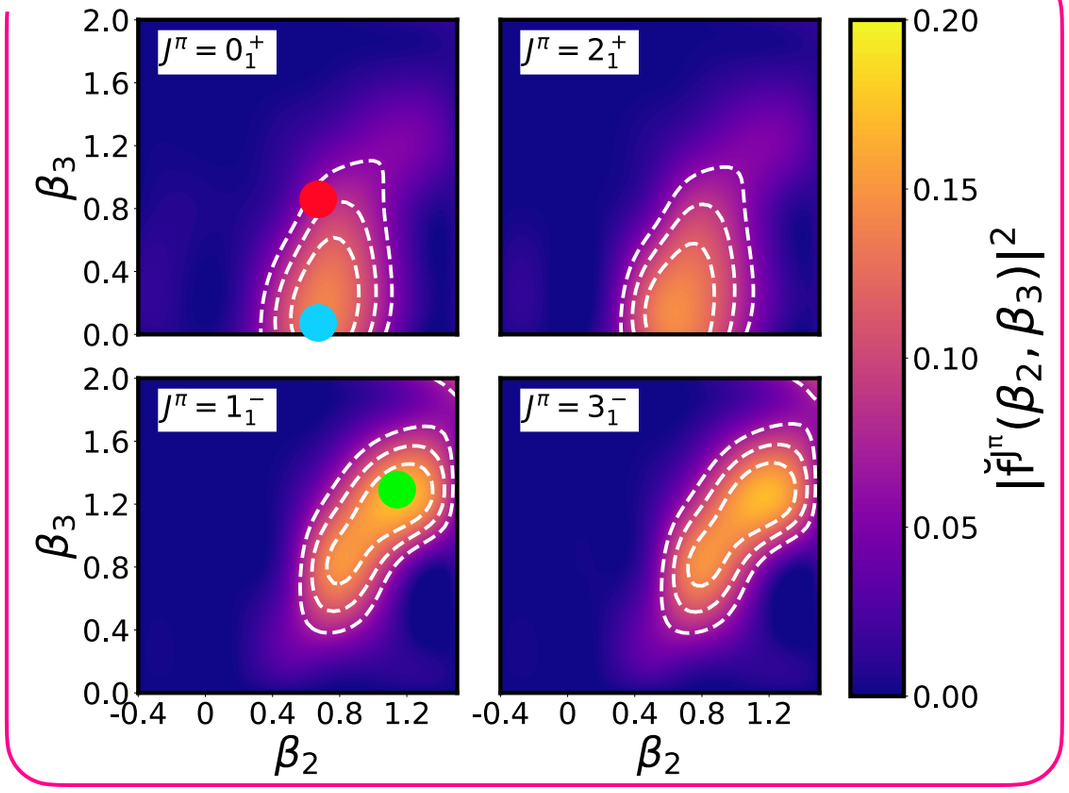


[Frosini *et al.* 2022]

2. Projected HFB

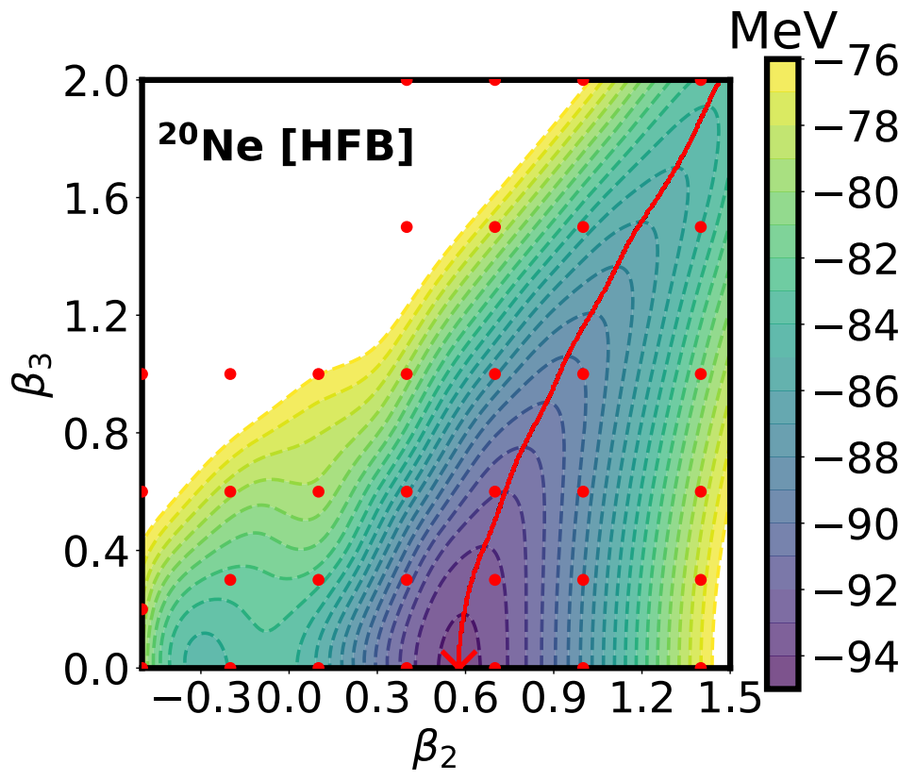


3. PGCM

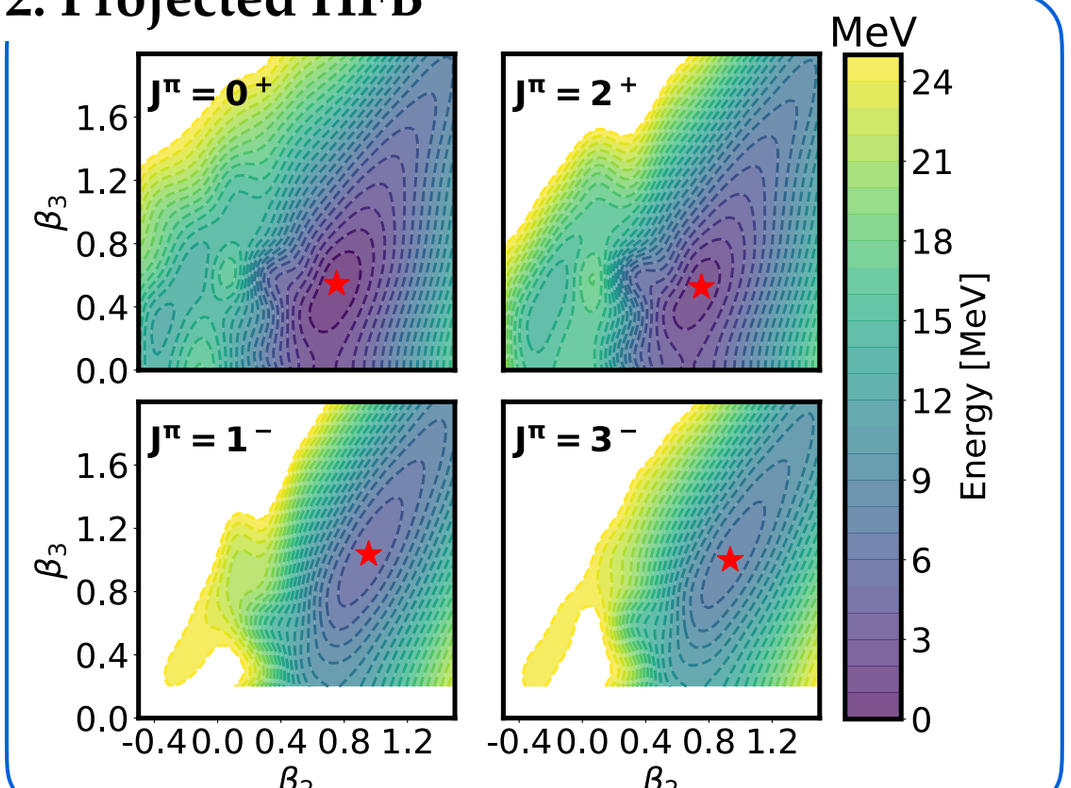


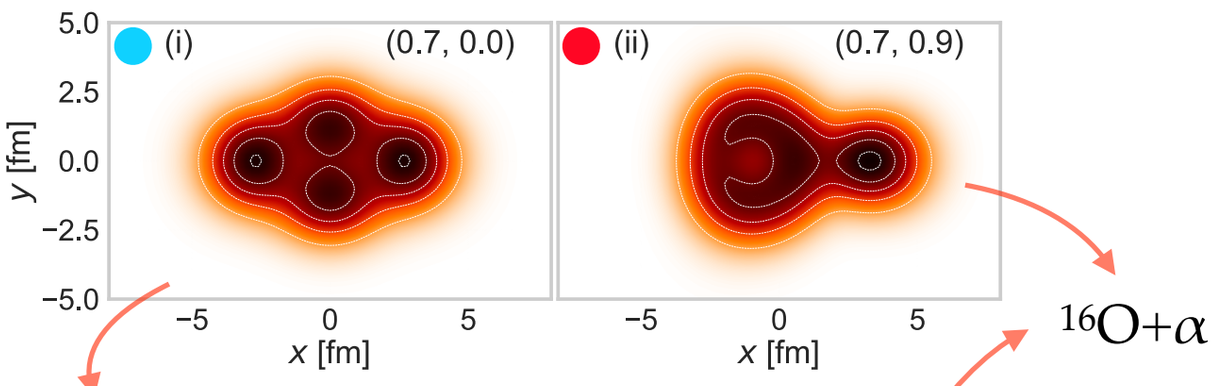
^{20}Ne

1. Constrained HFB



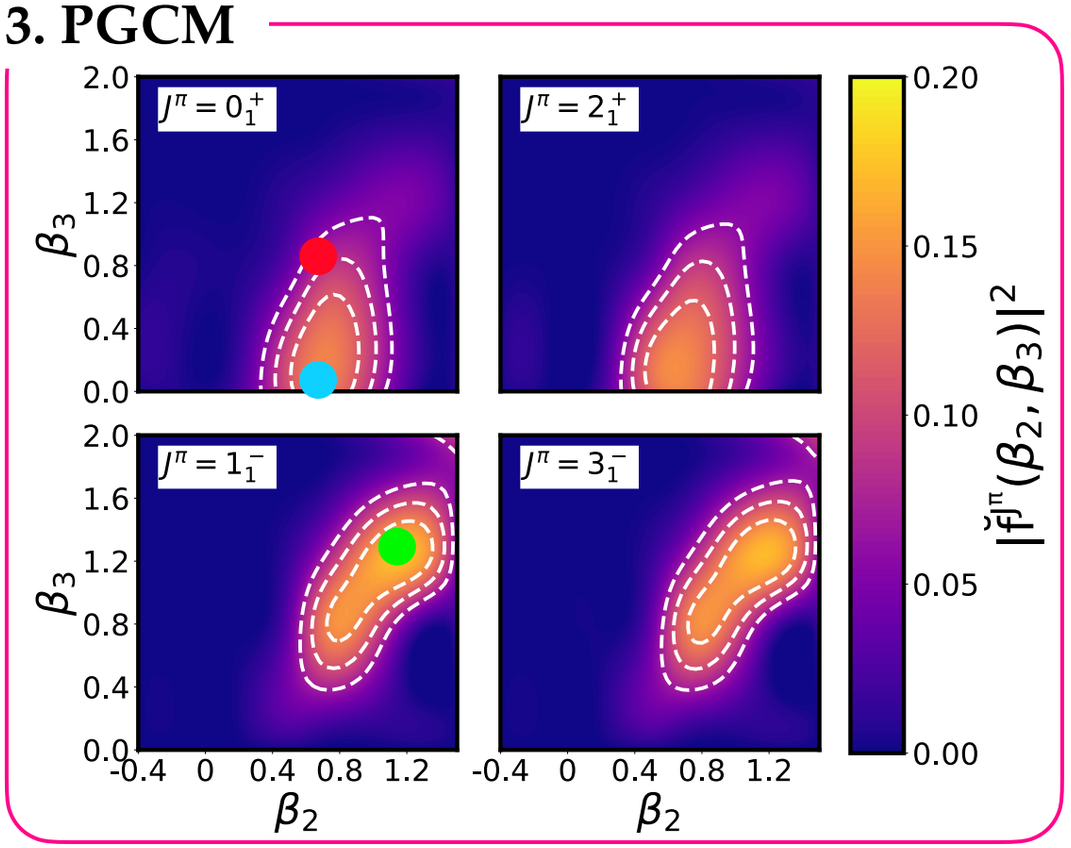
2. Projected HFB





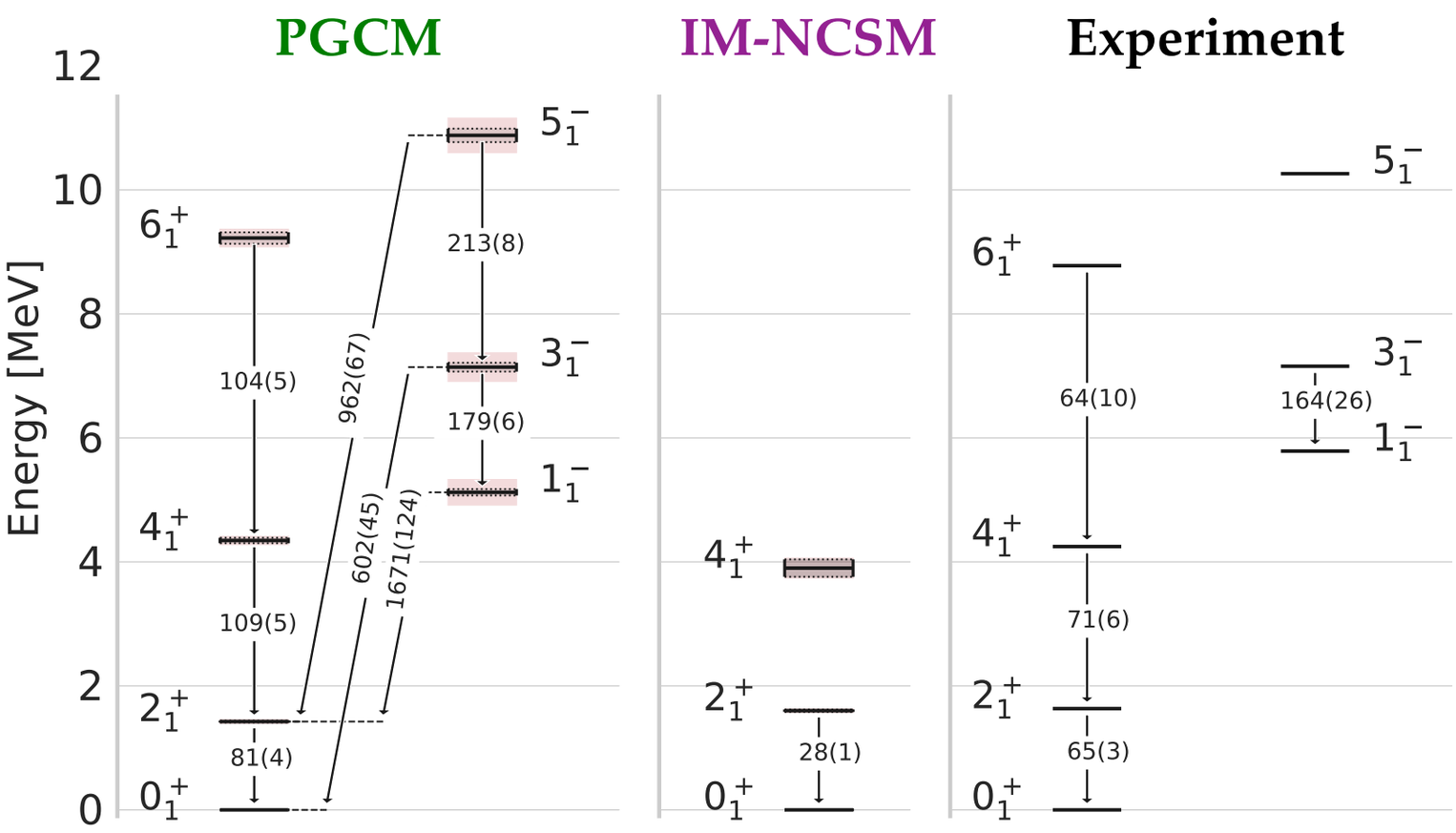
[Frosini *et al.* 2022]

3. PGCM

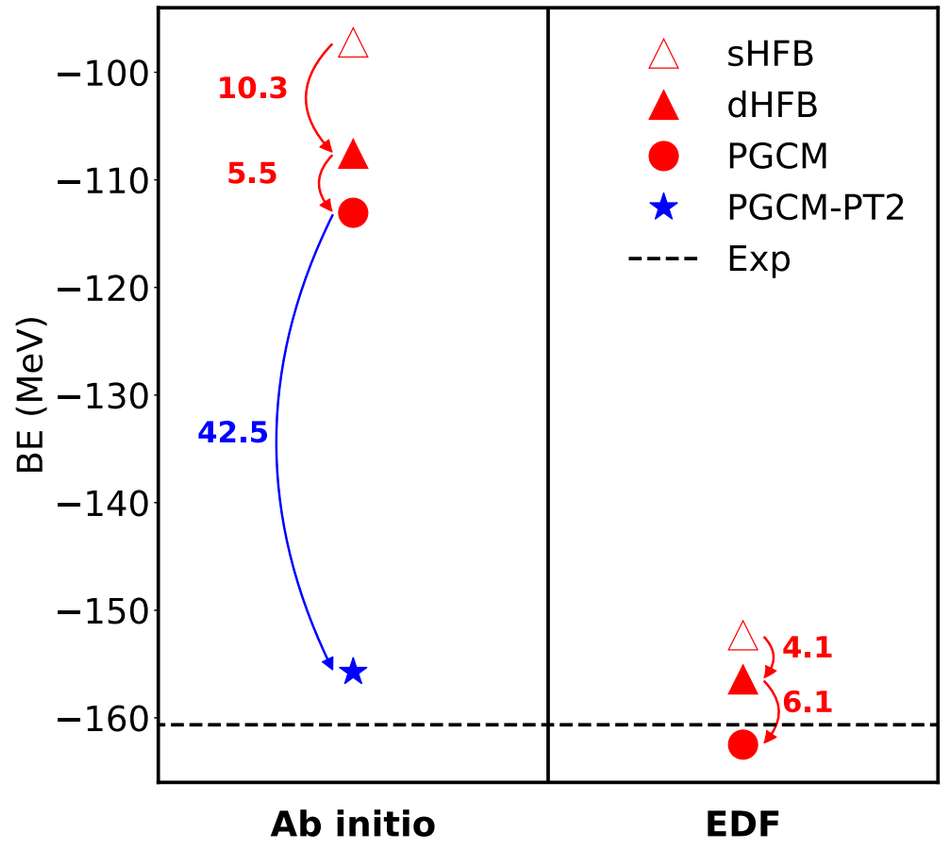


^{20}Ne

Excitation spectrum



Binding energy



- (Rotational) excitation spectrum emerges in both (symmetry-breaking and -conserving) approaches
- Symmetry-breaking approach achieves it at a much smaller cost
- **Relative** energies reproduced at PGCM level
- Dynamical correlations (PT correction) needed for **absolute** energies

[Frosini *et al.* 2022]

Revisiting EDF and shell model

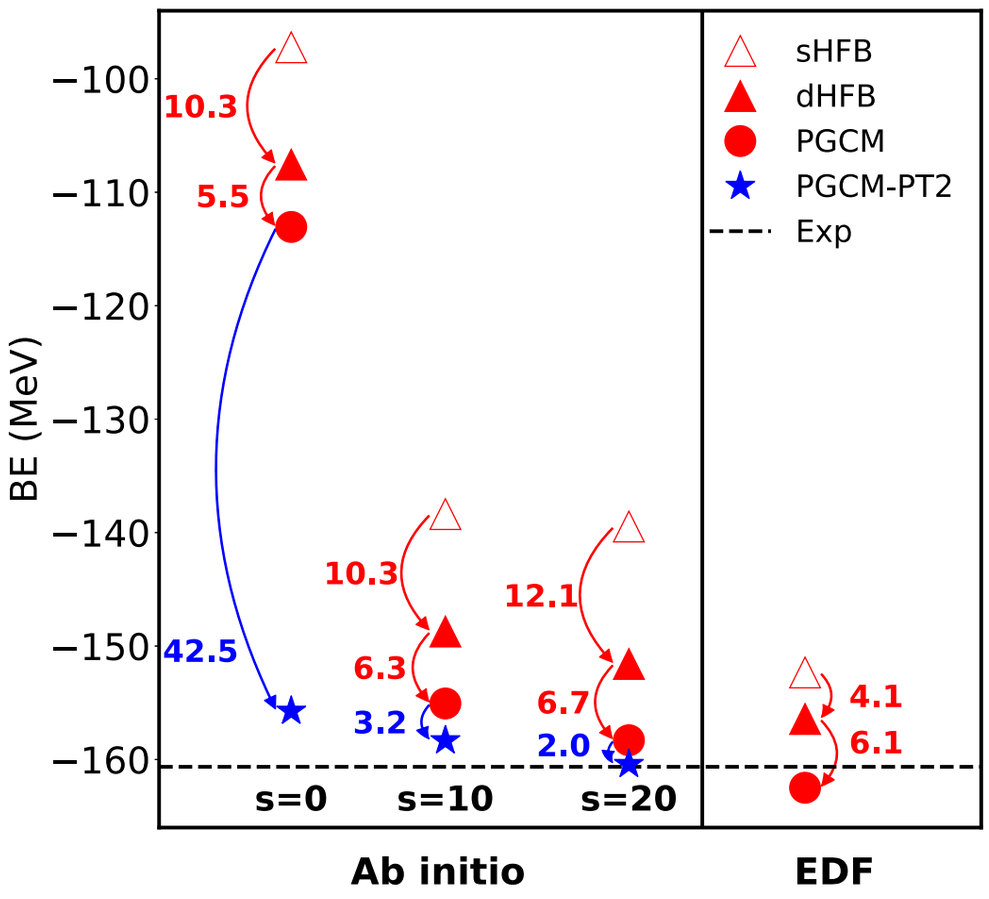
Energy density functionals

$$H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$$

Derive ab initio effective H

Simplified w.f.

(Beyond) mean field



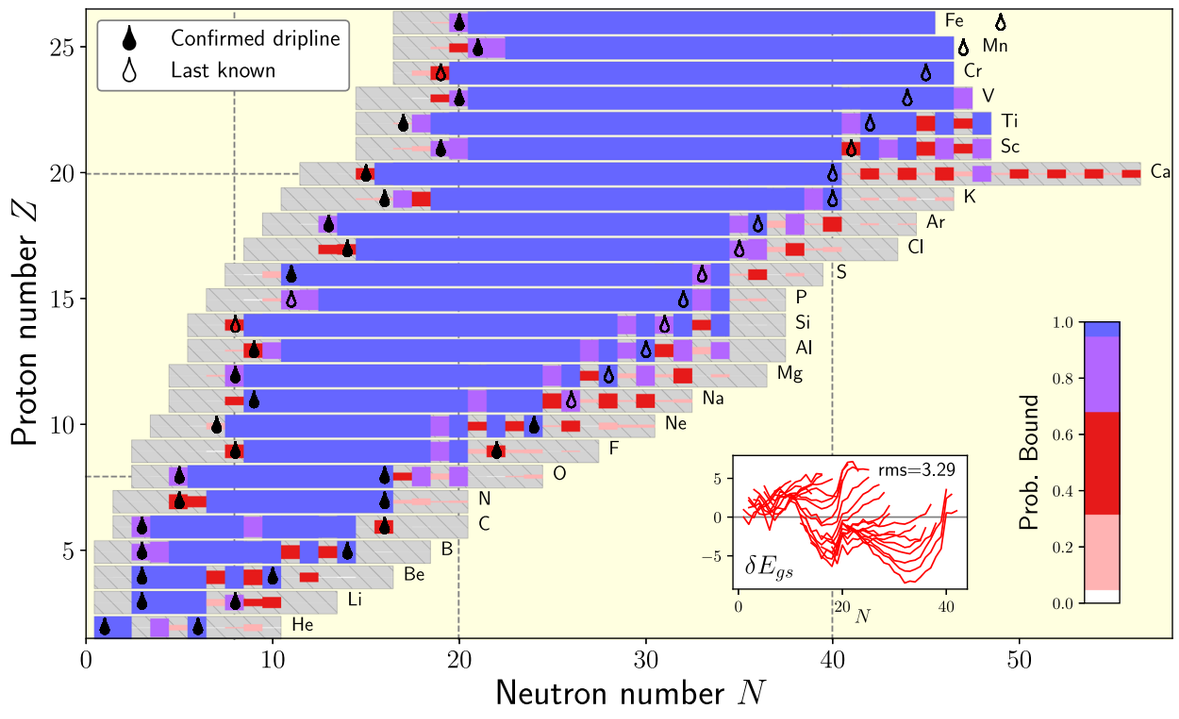
[Duguet *et al.* 2022]

Interacting shell model

$$H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$$

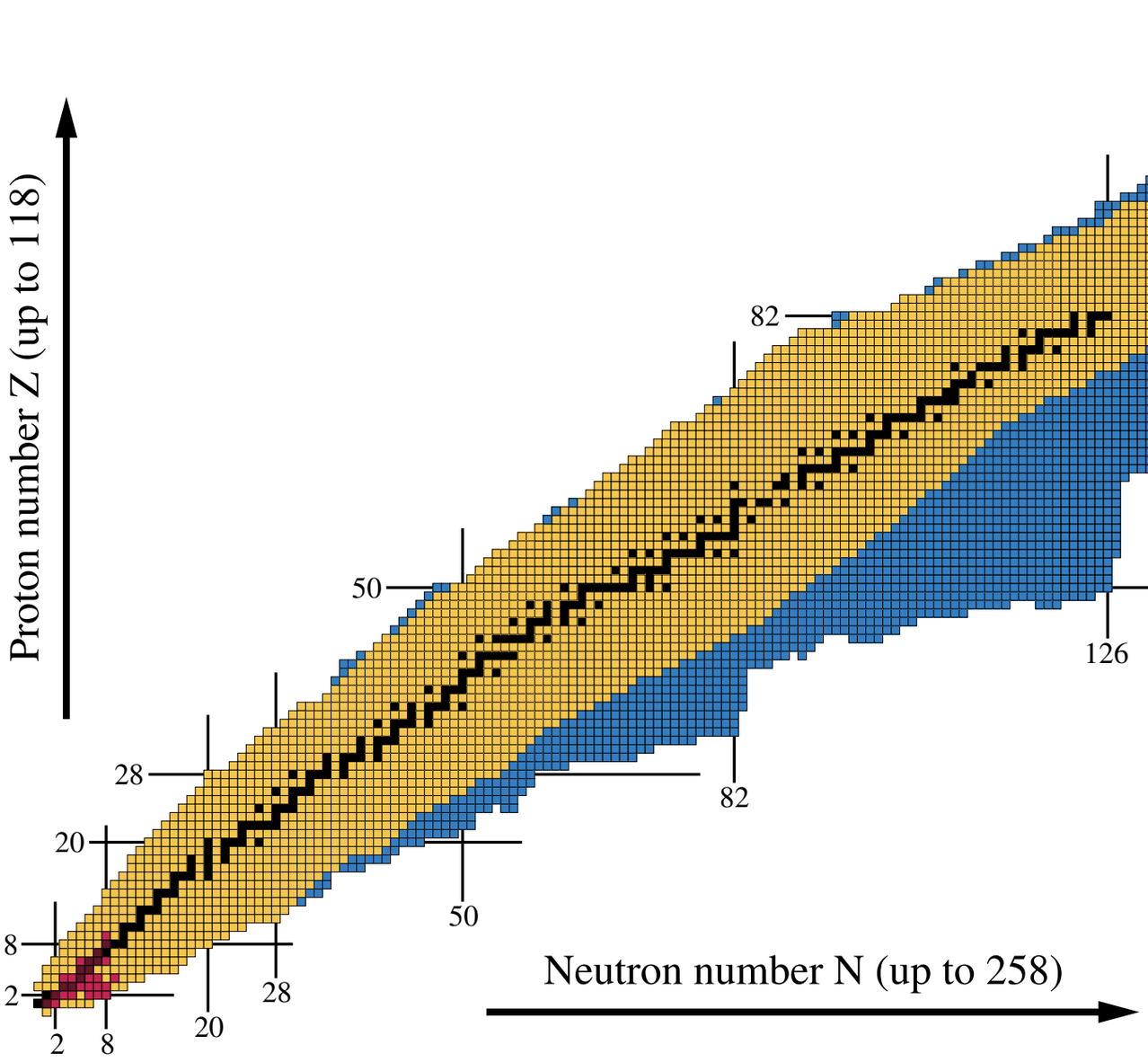
Derive ab initio effective H

Full (CI) w.f., but in **valence space**



[Stroberg *et al.* 2021]

Ab initio nuclear chart

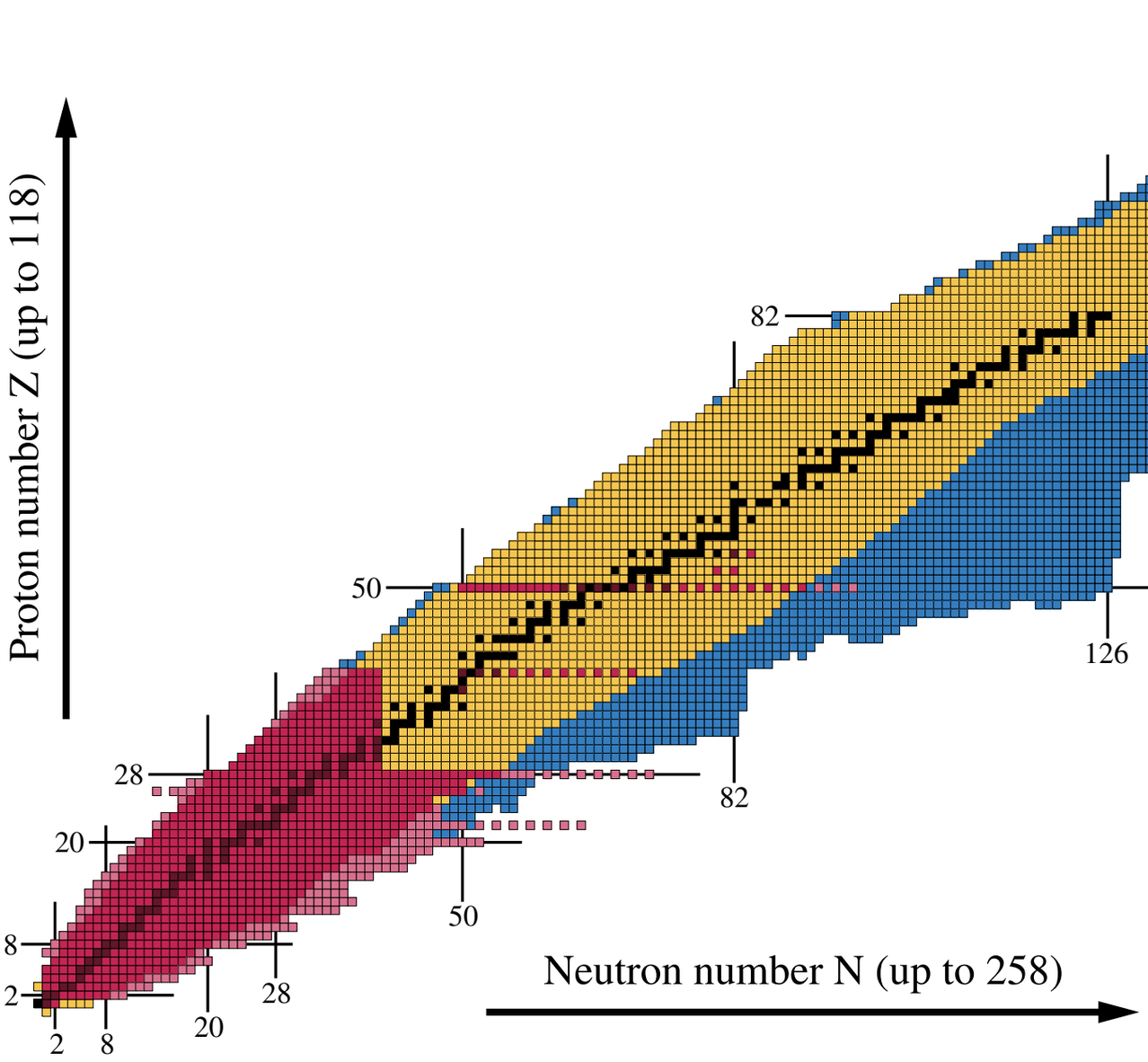


[*Figure*: B. Bally]

- 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)

Ab initio nuclear chart



[*Figure*: B. Bally]

- Stable
- Atomic mass evaluation 2020
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