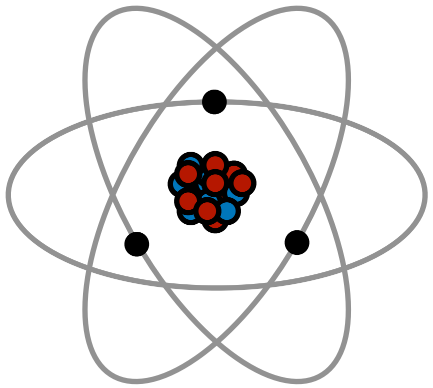
Specific computational aspects in nuclear theory

I. States, Interactions and Symmetries

GDR workshop

February 2021



Alexander Tichai

Technische Universität Darmstadt

Overview

I Basic considerations

- Single-particles states and symmetries
- Computational bases

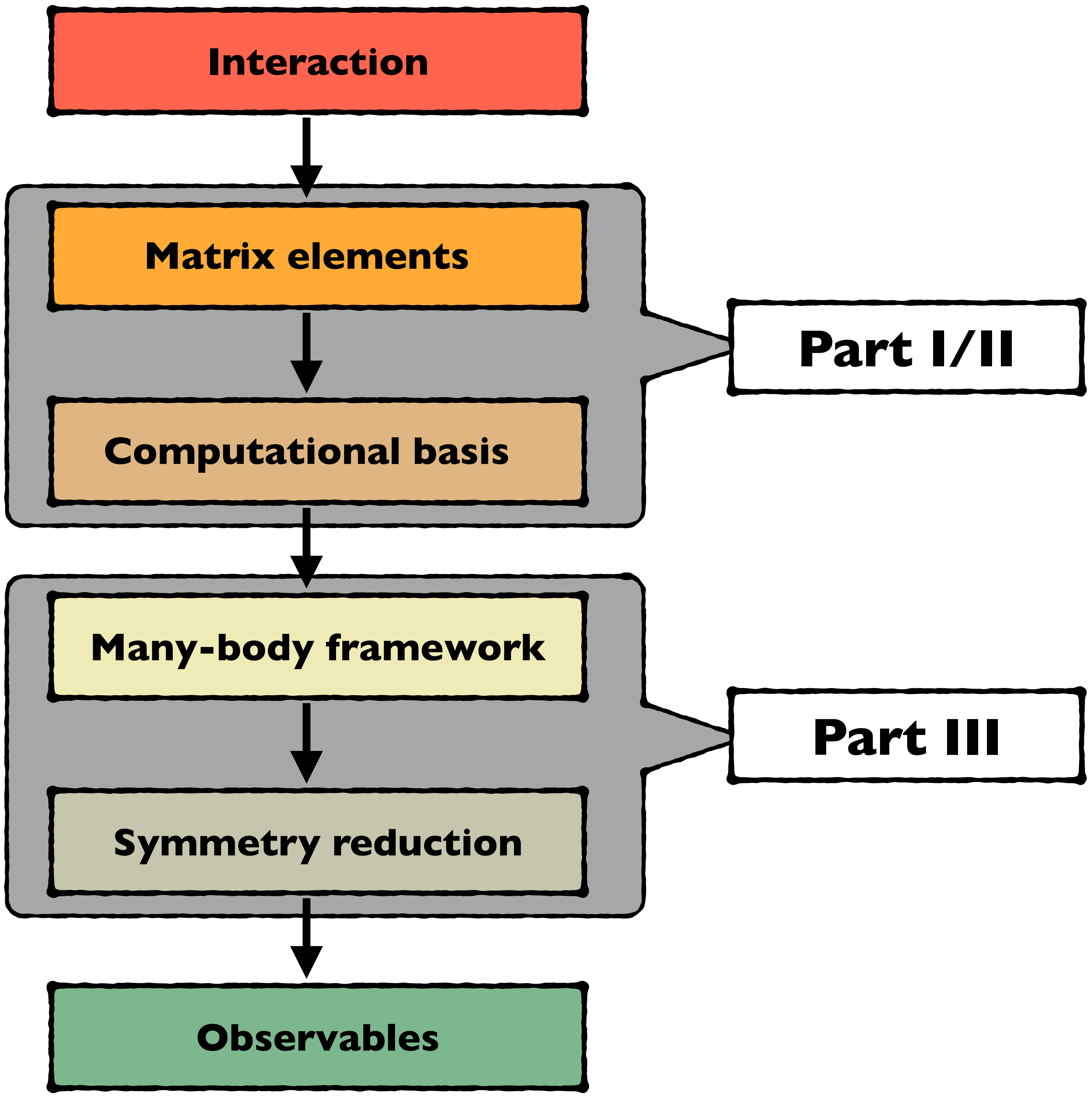
II Nuclear interaction

- Matrix elements and their origin
- Similarity renormalization group

III Symmetry adaption in nuclear physics

- Angular-momentum coupling
- Many-body examples

Guideline


Interaction
Matrix elements
Computational basis
Part I/II
Many-body framework
Symmetry reduction
Part III
Observables

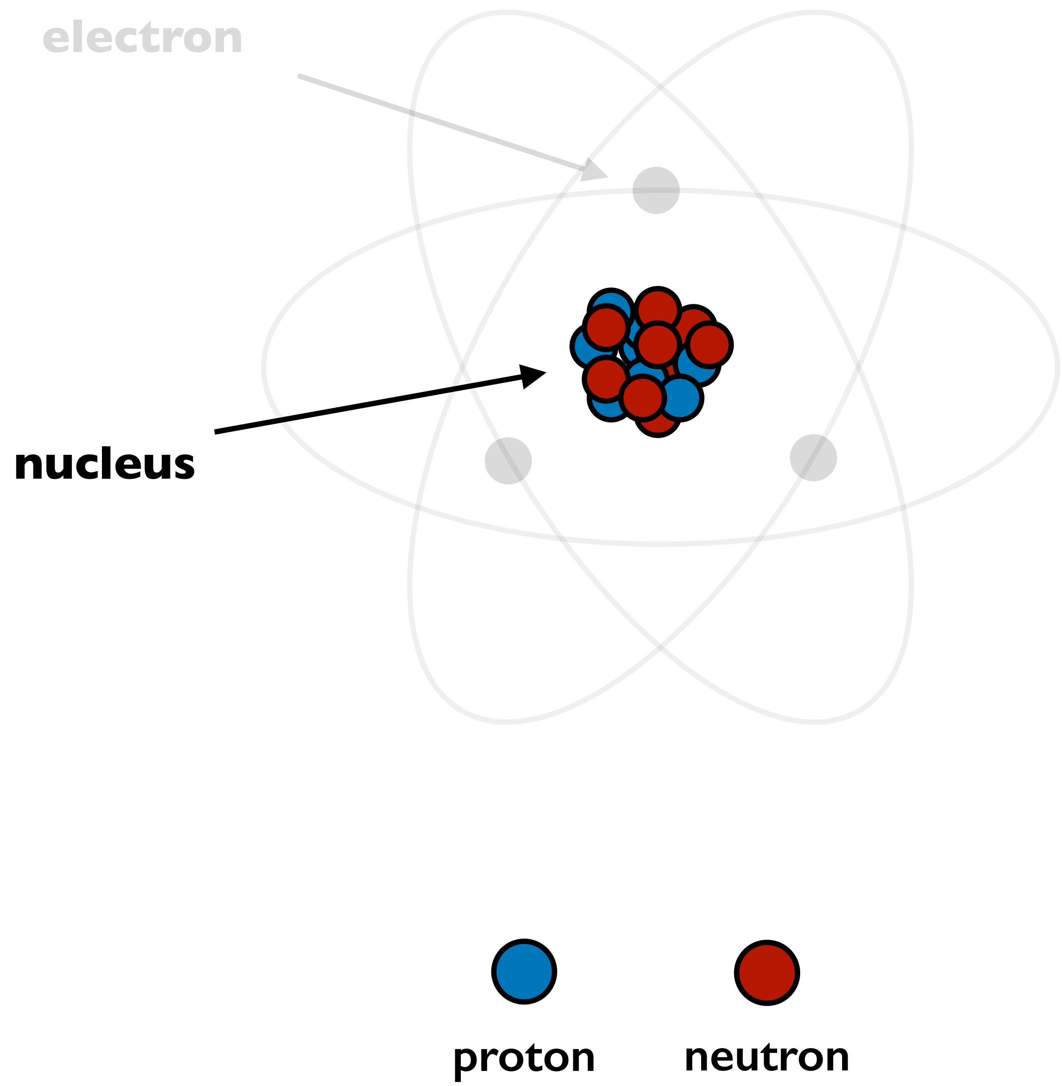
Part I

Many-body Basics

Fundamentals of nuclear systems

What is a nuclear system?

Sketch of an atom



Physical parameters

number or protons: Z

number or neutrons: N

mass number: $A = N + Z$

‘Computational parameters’

nuclear interaction model

basis set/basis size

resolution scale

treatment of three-body forces

oscillator frequency

The nuclear Hamiltonian

- General nuclear *A*-body Hamiltonian written in second quantization

(all matrix elements are anti-symmetric!)

$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{4} \sum_{pqrs} v_{pqrs} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{36} \sum_{pqrstu} w_{pqrstu} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s + \ldots$$

- Key difference: Hamiltonian comes with sizeable associated uncertainty

QCD
(quantum chromodynamics)

data
(experiment)

guidance

fitting of parameters

Hamiltonian
(input for non-rel. Schrödinger eq.)

FCI ≠ experiment

- Not to be confused with basis-size error due to finite model space!

- So far: Hamiltonian generic tensor w.r.t. generic labels *p,q,r,s,…*

Single-particle states

- Single-particle states are labelled in terms of their quantum numbers

$$|\varphi\rangle = |\varphi_{\text{spatial}}\rangle \otimes |\varphi_{\text{spin}}\rangle \otimes |\varphi_{\text{isospin}}\rangle$$

- Isospin: proton and neutron are considered two projections of quantum state

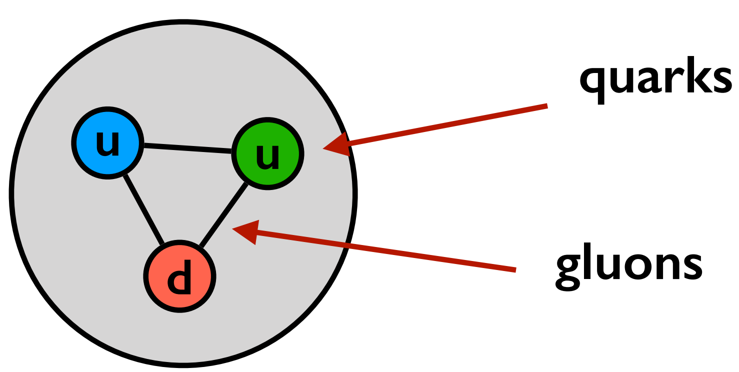
(just another spin algebra!)

$$|t m_t\rangle = |1/2 \pm 1/2\rangle \qquad m_p \approx m_n$$

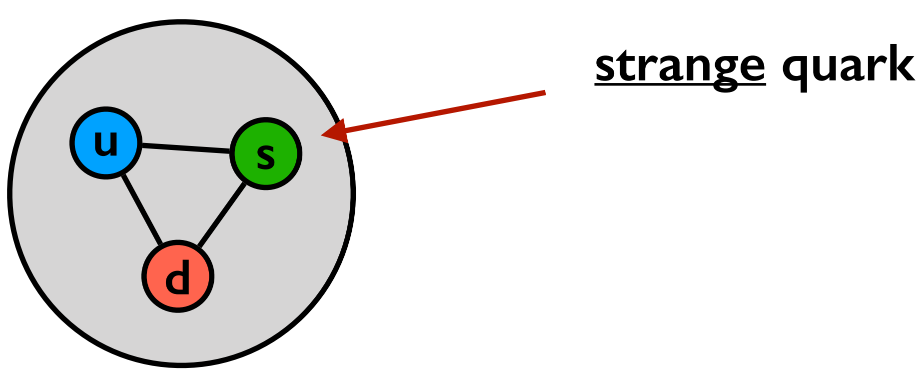
- Orbital angular momentum and spin are coupled to total angular momentum

$$j = l + s$$

- More particle species contained in Standard Model (irrelevant at low energies)



proton @ 938 MeV



Λ hyperon @ 1115 MeV

Symmetries of nuclear matrix elements

- Treatment/processing of symmetries of matrix elements crucial

$$v_{pqrs}$$

- Parity conservation linked to discrete group Z_2

$$[H, \Pi] = 0 \qquad\qquad l_p + l_q \text{ mod}2 = l_r + l_s \text{ mod}2$$

- Isospin conservation: no conversion of protons/neutrons (only strong interaction!)

$$[H, T_z] = 0 \qquad\qquad m_{t_p} + m_{t_q} = m_{t_r} + m_{t_s}$$

- Angular-momentum projection conservation linked to abelian U(1)

$$[H, J_z] = 0 \qquad\qquad m_{j_p} + m_{j_q} = m_{j_r} + m_{j_s}$$

- Rotational invariance linked to non-abelian SU(2) (more details in part 3)

$$[H, J^2] = 0$$

Computational bases

- Single-particle states typically given as eigenstates of one-body Hamiltonian

$$H_{\mathrm{sHO}} = \frac{p^2}{2m} + \frac{1}{2} m\Omega^2 r^2$$

- Characterization via quantum numbers

$$|k\rangle = |n_k\, l_k\, j_k\, m_{j_k}\, m_{t_k}\rangle$$

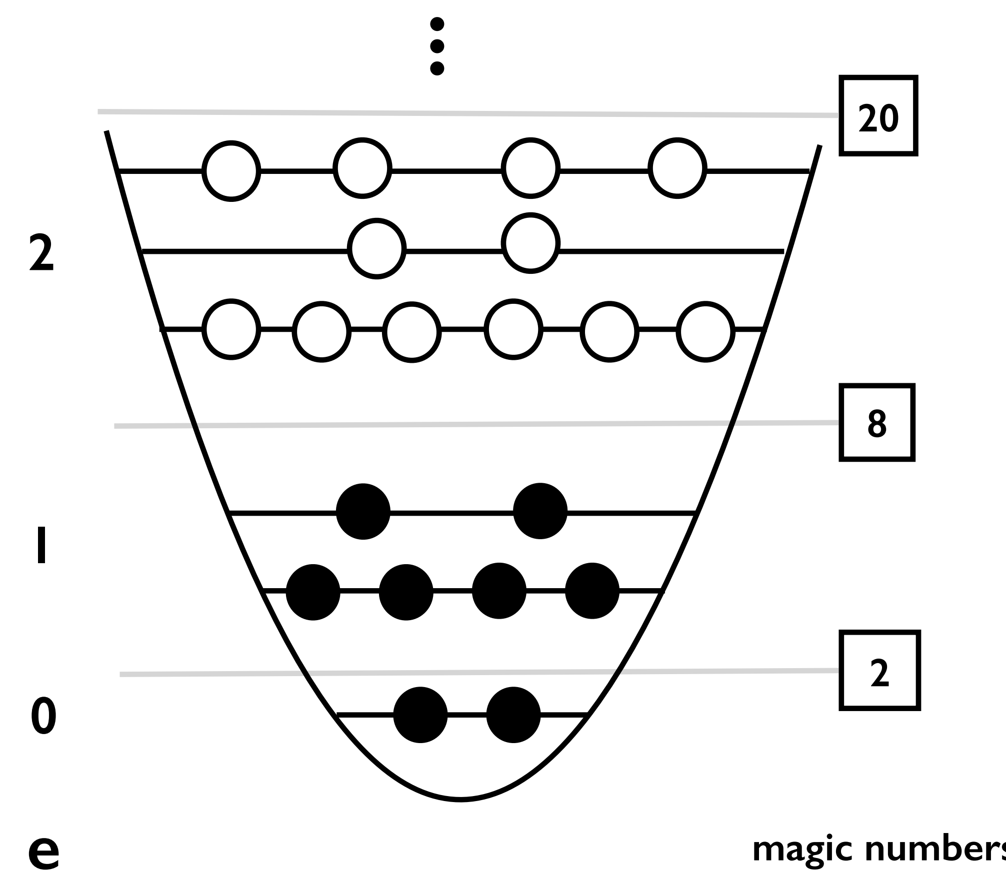
- Model space defined in terms of maximum principal quantum number:

$$e = 2n + l$$

- Introduction of computational parameter

oscillator frequency

(implicitly present in ALL calculations)



harmonic oscillator potential

Common basis sets

- **Harmonic-oscillator basis**
  - first essential step for computation of matrix elements
  - analytic separation of intrinsic and center-of-mass states
  - basis states do not depend on isospin (same for proton/neutron)
  - … but wrong asymptotic fall-off (Gaussian)

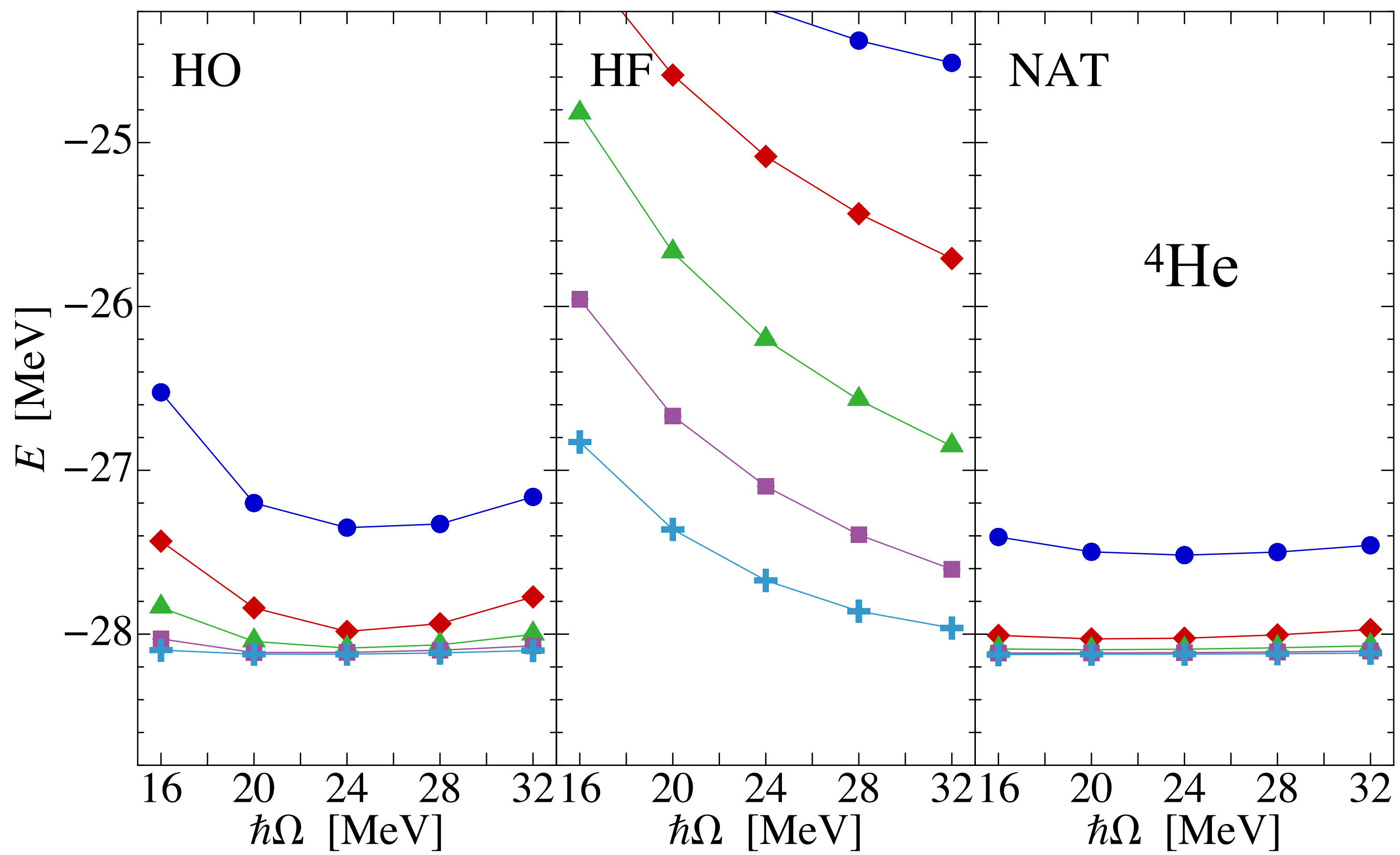
- **Hartree-Fock basis**
  - variational solution grasps typical size of atomic nucleus
  - correct exponential fall-off of single-particle wave functions
  - … but unoccupied states only fixed by normalisation constraint

- **Natural-orbital basis** (since 2018)
  - in practice obtained by diagonalization of perturbative one-body density
  - fast model-space convergence and low frequency dependence
  - optimization of unoccupied orbitals

Basis sets in practice

Tichai, Müller, Vobig, Roth
PRC 99, 034321 *"Editors' suggestion"*

NCSM calculation using various single-particle bases



- **Low frequency dependence/fast convergence for natural orbital calculations**
- **Natural orbital may enable working in much smaller single-particle bases**

Natural orbitals for many-body expansions
Hoppe, Tichai, Heinz, Hebeler, Schwenk, PRC 103, 014321

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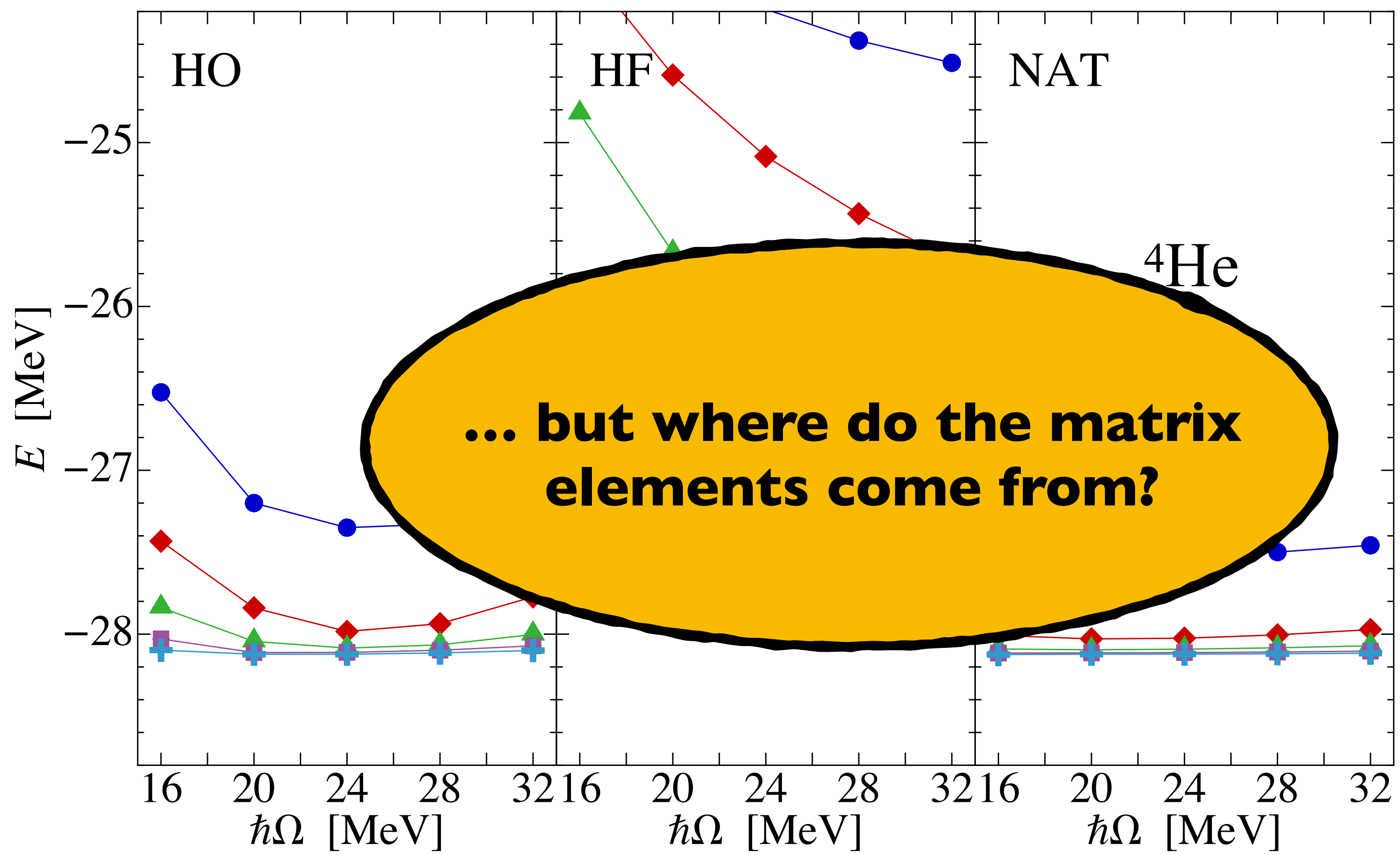

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Part II
Nuclear interaction

Representations and pre-processing tools

The nuclear potential

Machleidt, Entem, Phys. Rept. 503 (2011) 1-75

- **Nuclear interaction consists of complicated operator structure**

$$\frac{3}{\vec{r}^2}(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

angular momentum
***L* not conserved!**

$$V_{\text{nucl.}} = V_{\text{central}} + V_{\text{spin-orbit}} + V_{\text{tensor}} + \ldots$$

$$\propto \vec{L} \cdot \vec{S}$$

- **Example: simple central component from long-range pion exchange**

$$V_{\text{Yukawa}}(r) = \frac{e^{-mr}}{r}$$

- **Incorporate all operator structures consistent with symmetry principles**

$$\{(\vec{\sigma}_1 \cdot \vec{\sigma}_2), (\vec{\tau}_1 \cdot \vec{\tau}_2), \ldots\}$$

- **Matrix elements in terms of momentum and angular-momentum eigenstates**

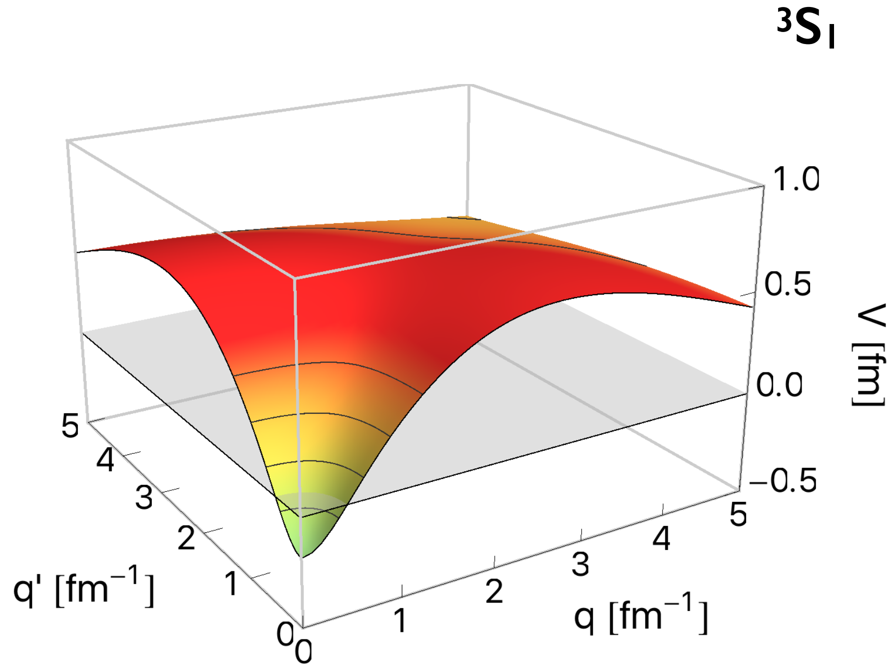
(partial-wave decomposition)

$$\langle q'(L'S)J; TM_T | V_{\text{NN}} | q(LS)J; TM_T \rangle$$

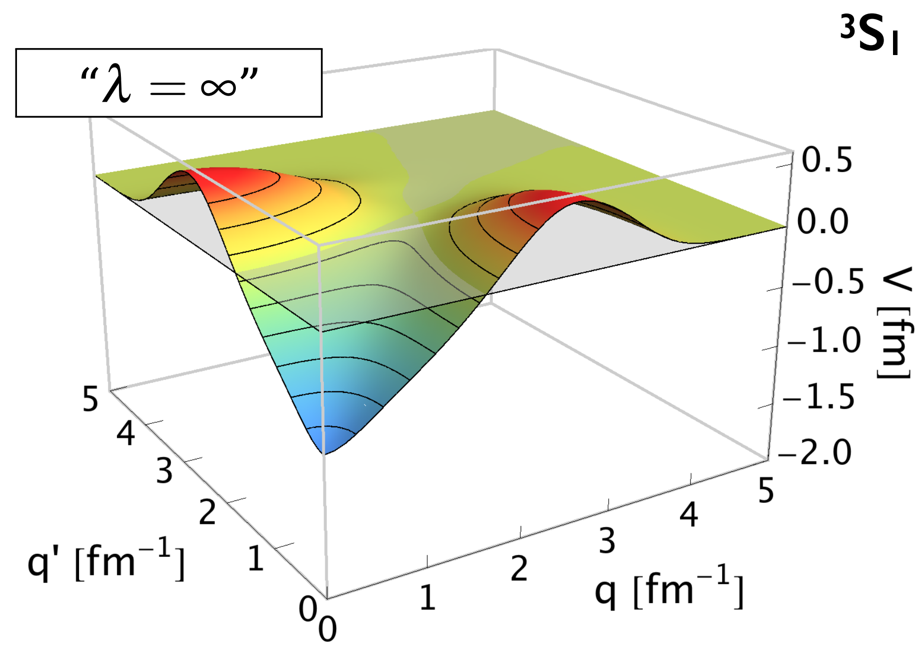
Matrix elements

phenomenological potential
(Argonne AV18)

S=1
L=0
L'=0
J=1
T=0
M_T=0



modern EFT potential
(chiral effective field theory, EM500)



Hergert *et al.*, arXiv: 1612.08315

- before 2000's: *ad hoc* postulation of operator structure based on symmetries

high-precision potentials but
uncertainty quantification complicated

- since 2000's: emergence of operator structure from low-energy EFT expansion

Matrix element toolchain

$|k\rangle = |nljtm_j\rangle$
$|\tilde{k}\rangle = |nljt\rangle$
$|\breve{k}\rangle = |nlj\rangle$

Format

Momentum space
(system independent)

$\longrightarrow$ $\langle q'(L'S)J; TM_T | V_{\mathrm{NN}} | q(LS)J; TM_T \rangle$

Talmi-Moshinsky +
HO transformation

Harmonic oscillator
(system independent)

$\longrightarrow$ $\langle \breve{k}_1 \breve{k}_2 JT | V_{\mathrm{NN}} | \breve{k}_3 \breve{k}_4 JT \rangle$

input to all
many-body calculations

V_{NN} : < 2 GB

V_{3N} : 20 - 100 GB

isospin decoupling +
s.p. basis transformation

Hartree-Fock
(system dependent)

s.p. basis transformation

Natural orbitals
(system dependent)

$\langle \tilde{k}_1 \tilde{k}_2 J | V_{\mathrm{NN}} | \tilde{k}_3 \tilde{k}_4 J \rangle$

size of 3N matrix elements
currently limiting factor

$\longrightarrow$ **see talk on Friday!**

Pre-processing

$$H\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

nuclear observable

$$\tilde{H}\,|\tilde{\Psi}_n\rangle = E_n\,|\tilde{\Psi}_n\rangle$$

nuclear observable

- unbound mean field
- MBPT divergent
- slow model-space convergence

'Direct approach'

unitary transformation

$$\tilde{H} = UHU^\dagger$$

- observables preserved
- faster convergence
- MBPT can converge

strong short-range correlations in interaction

$$H = T + V_{\mathrm{NN}} + V_{\mathrm{3N}}$$

Similarity renormalization group

- **Transformation induces decoupling of high- and low-momentum states via ODE**

$$H(\lambda) = U(\lambda) H U^\dagger(\lambda) \quad \longleftrightarrow \quad \frac{\mathrm{d}}{\mathrm{d}\lambda} H(\lambda) = [\eta(\lambda), H(\lambda)]$$

- **Standard choice for anti-Hermitian dynamic generator of the flow**

$$\eta(\lambda) = (2\mu)^2 [T_{\text{int}}, H(\lambda)]$$

- **Pre-diagonalization: vanishing generator gives fix point of the SRG flow equation**

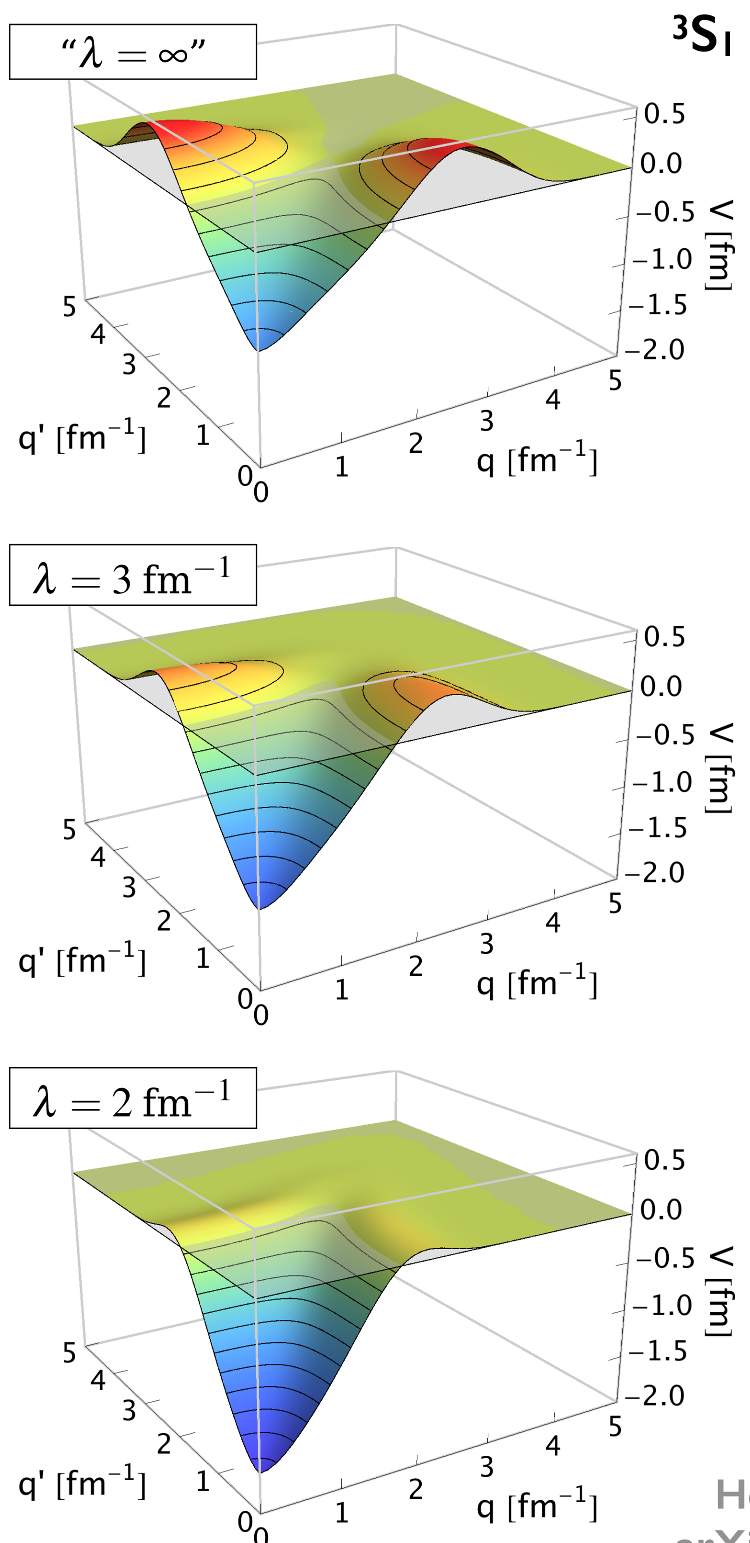
$$[T_{\text{int}}, H(\lambda)] = 0$$

- **Cluster expansion: SRG induces higher-body operators in Fock space**

$$H(\lambda) = H^{(2B)} + H^{(3B)} + H^{(4B)} + \ldots + H^{(NB)}$$

Truncation required!

Similarity renormalization group

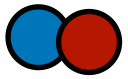


Hergert *et al.*, arXiv: 1612.08315

- Rapid **suppression of off-diagonal couplings** in momentum space
- Potential driven to band-diagonal form
- **Unitary character** preserves nuclear observables throughout flow

Unitarity test

Diagonalization of two-body system



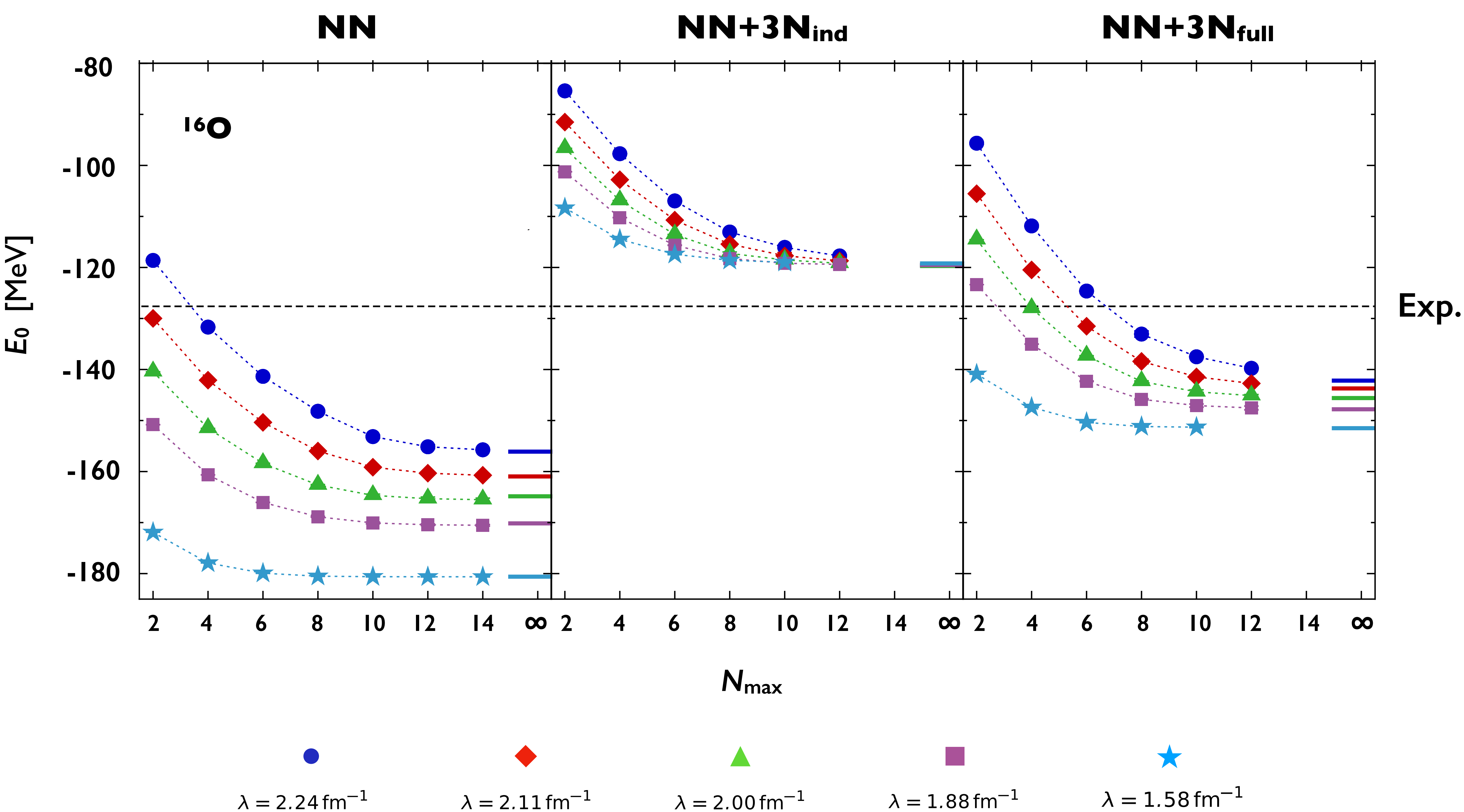
deuteron

(Z=1, N=1, A=2)

SRG in action

adapted from Roth *et al.*, PRL 107, 072501 (2011)

No-core shell model calculations using SRG-evolved interactions



Part III
Symmetry adaption

Additional ingredients for nuclear many-body codes

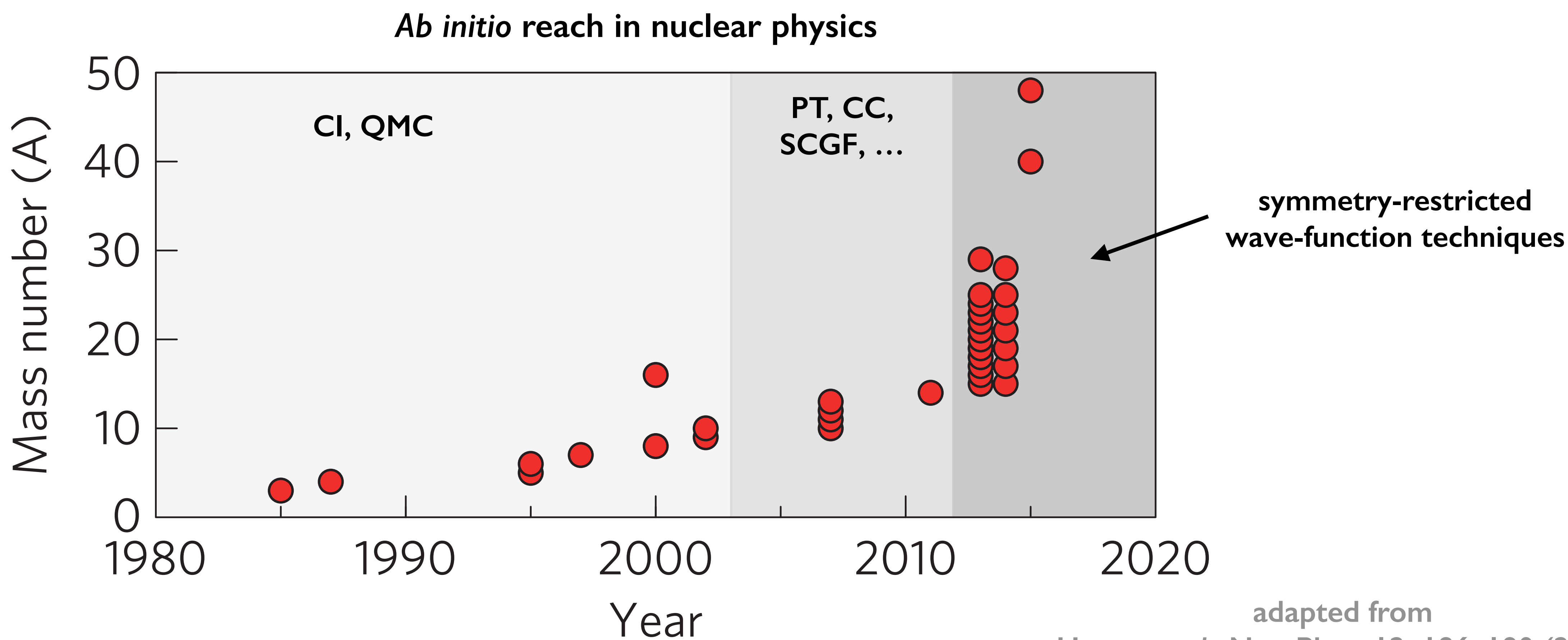
Scaling and symmetries

- Scaling arguments only give a very crude estimate of the complexity

"Coupled cluster is much more complicated than a mean-field calculation"

- This is only true if the same set of symmetries is employed in both calculations!

- Symbolic integration of quantum numbers yields scalable codes



adapted from
Hagen *et al.*, Nat. Phys. 12, 186–190 (2016)

Rotational symmetry

'Nuclear spin integration'

- *SU(2)* symmetry encodes rotational invariance of quantum objects

$$|k\rangle = |n_k l_k j_k t_k m_k\rangle = |\tilde{k} m_k\rangle$$

- Definition of angular-momentum-coupled states from symmetry transformation

$$|k_1\rangle \otimes |k_2\rangle \xrightarrow{f_{SU(2)}} |\tilde{k}_1 \tilde{k}_2 (J)\rangle \equiv \sum_{m_{k_1} m_{k_2}} \left(\begin{array}{cc|c} j_{k_1} & j_{k_2} & J \\ m_{k_1} & m_{k_2} & M \end{array} \right) |k_1 k_2\rangle$$

- Symmetry-restricted tensors: angular-momentum-coupled matrix elements

$$\tilde{O}^J_{\tilde{k}_1 \tilde{k}_2 \tilde{k}_3 \tilde{k}_4} = \sum_{m_{k_1} \dots m_{k_4}} \bar{o}_{k_1 k_2 k_3 k_4} \left(\begin{array}{cc|c} j_{k_1} & j_{k_2} & J \\ m_{k_1} & m_{k_2} & M \end{array} \right) \left(\begin{array}{cc|c} j_{k_3} & j_{k_4} & J \\ m_{k_3} & m_{k_4} & M \end{array} \right)$$

- *SU(2)*-irreducible tensor operators can be processed via Wigner-Eckart theorem

$$\langle \xi_1 j_1 m_1 | T^J_M | \xi_2 j_2 m_2 \rangle = (-1)^{2J} \frac{1}{\hat{j}_1} \left(\begin{array}{cc|c} j_2 & J & j_1 \\ m_2 & M & m_1 \end{array} \right) (\xi_1 j_1 | \mathbf{T}^J | \xi_2 j_2)$$

'geometry' 'physics'

Perturbation theory ...

m-scheme MP2 correction

$$E_{\text{MP2}} = -\frac{1}{4}\sum_{abij}\frac{H_{abij}H_{ijab}}{\epsilon_a+\epsilon_b-\epsilon_i-\epsilon_j}$$

Scaling

$$S_m^{\text{MP2}} = N_p^2 N_h^2$$

J-scheme MP2 correction

$$E_{\text{MP2}} = -\frac{1}{4}\sum_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}\sum_J (2J+1)\frac{H^J_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}H^J_{\tilde{i}\tilde{j}\tilde{a}\tilde{b}}}{\epsilon_{\tilde{a}}+\epsilon_{\tilde{b}}-\epsilon_{\tilde{i}}-\epsilon_{\tilde{j}}}$$

Scaling

$$S_J^{\text{MP2}} = \tilde{N}_p^2 \tilde{N}_h^2 J_{\max}$$

^{40}Ca using 12 oscillator shells

$N_h = 40$

$N_p = 1780$

1820 basis functions (k)

182 spherical states $(\tilde{k})$

<u>estimated speedup</u>

$S_m^{\text{MP2}}/S_J^{\text{MP2}} \approx 50$

$\tilde{N}_h = 12$

$\tilde{N}_p = 170$

$J_{\max} = 25$

Scaling advantage greatly improves at higher orders

$$S_m^{\text{MP3}}/S_J^{\text{MP3}} > 5000$$

… and beyond

- Angular-momentum coupling leverages use of non-perturbative frameworks

  (Green's functions, coupled cluster, IMSRG, …)

- Formal expression for coupled-cluster amplitude equations look like this …

$$D_{abij} \equiv \sum_{kl} \sum_{cd} H_{klcd} t_{dj} t_{ak} t_{cbil}$$

- … but what is contained in large-scale codes looks like this!

multiplicity labels

$$D^{J}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}} = \sum_{J_1 J_2 K} \frac{\hat{J}_1^2 \hat{J}_2^2 \hat{K}^2}{\hat{j}_a \hat{j}_j} \sum_{\tilde{k}\tilde{l}\tilde{c}\tilde{d}} \delta_{j_d j_j} \delta_{j_k j_a} H^{J_1}_{\tilde{k}\tilde{l}\tilde{c}\tilde{d}} (\tilde{d}|\mathbf{T_1}|\tilde{j})(\tilde{a}|\mathbf{T_1}|\tilde{k})\, t^{J_2}_{\tilde{c}\tilde{b}\tilde{i}\tilde{l}} \begin{Bmatrix} j_i & j_b & K \\ j_a & j_j & J \end{Bmatrix} \begin{Bmatrix} j_c & j_l & K \\ j_a & j_j & J_1 \end{Bmatrix} \begin{Bmatrix} j_l & j_i & J_2 \\ j_b & j_c & K \end{Bmatrix}$$

reduced matrix elements
(Wigner-Eckart theorem)

Wigner 6j-symbols

- Nuclear applications involve time-consuming symmetry adaption of equations

Automated tools

- Symbolic evaluation can be **automated** using graph-theory tools

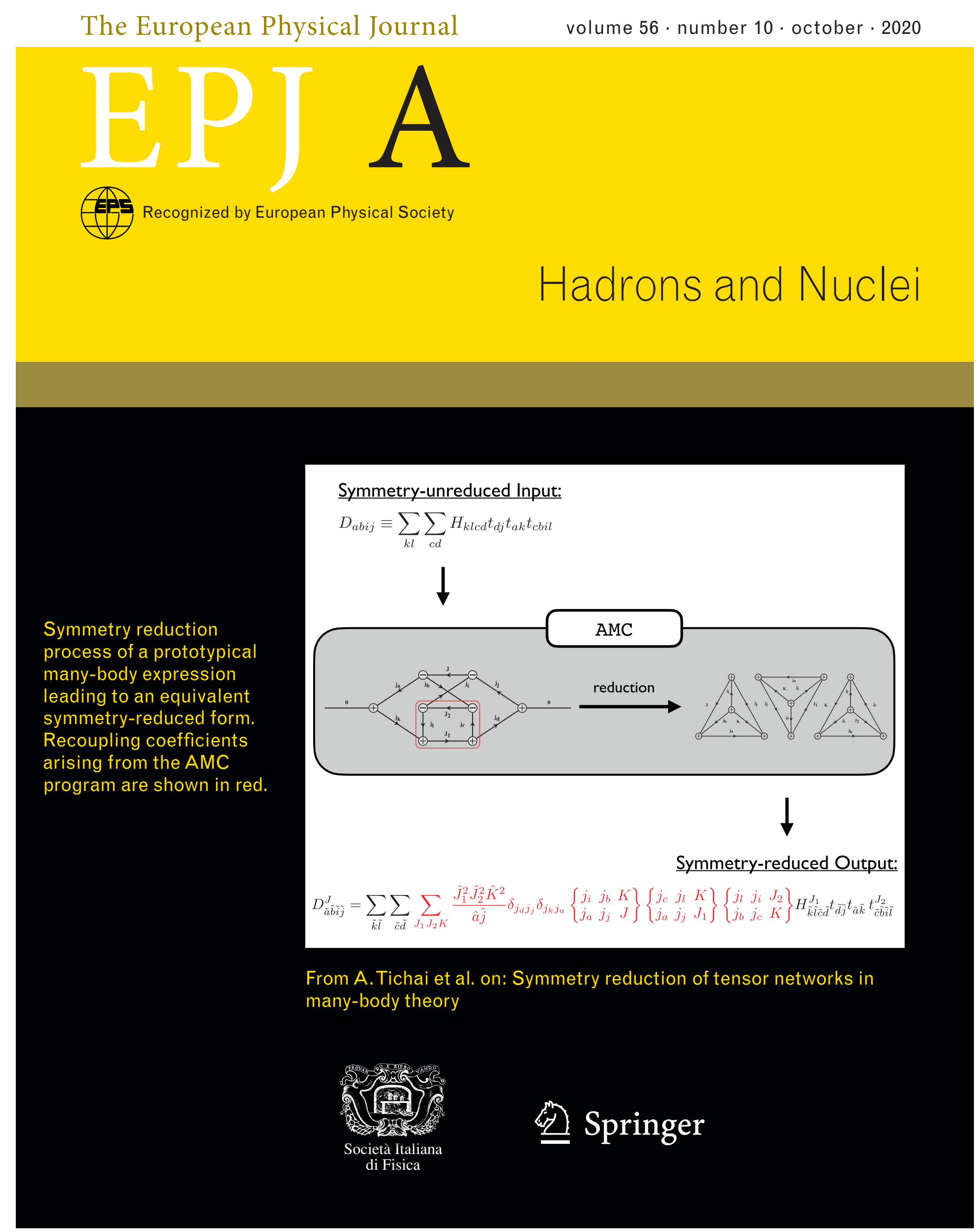
- Integral step for advancing many-body theory to **higher precision** by relaxing the many-body truncation

- Saves practitioners **months of work**

  50 pages of CC diagrams
  in 2 seconds!

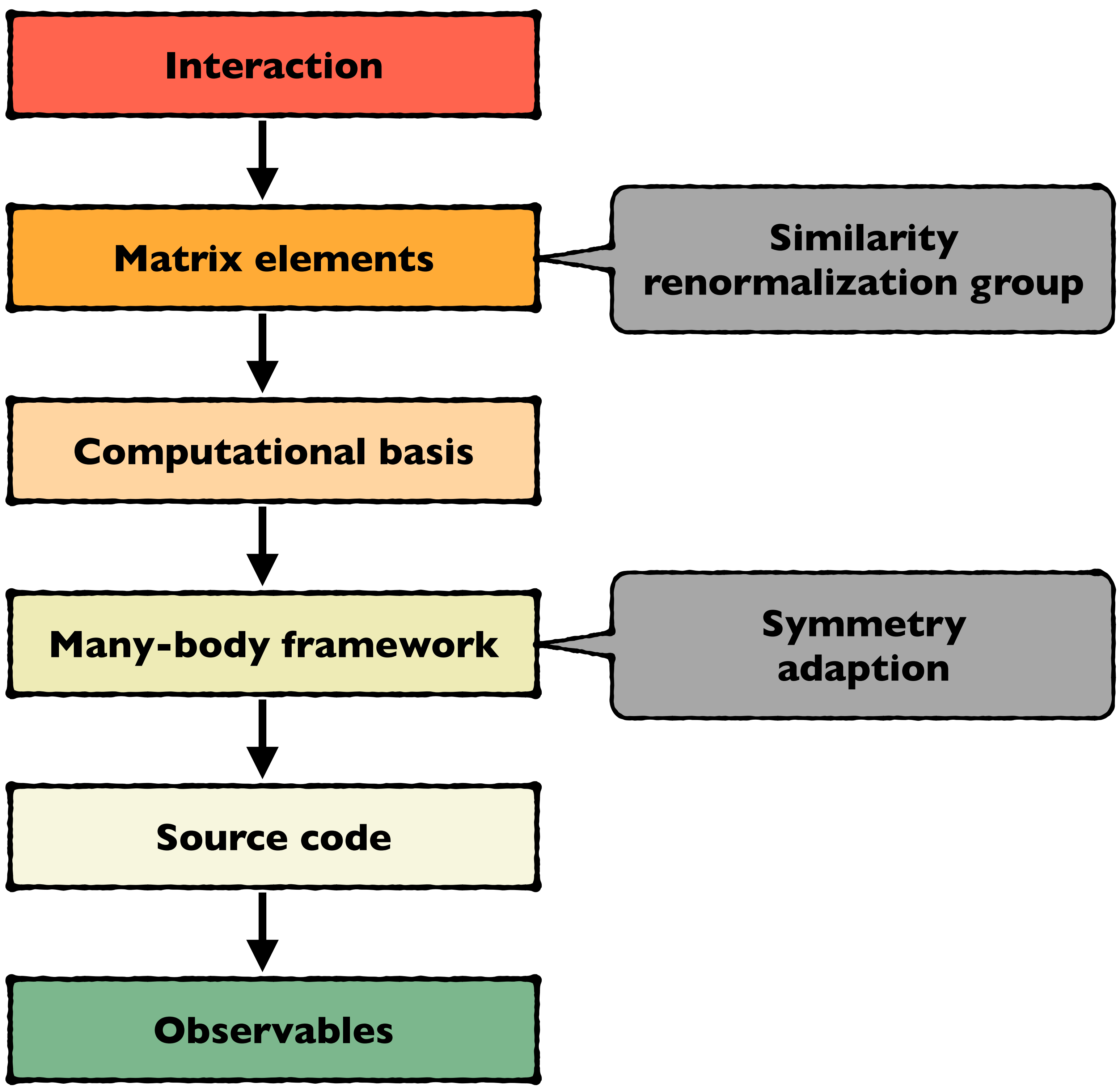
- Try it: **python code** freely available

```
pip3 install amc
```



Tichai, Wirth, Ripoche, Duguet, Eur. Phys. J. A (2020) **56**: 272

Wrap-up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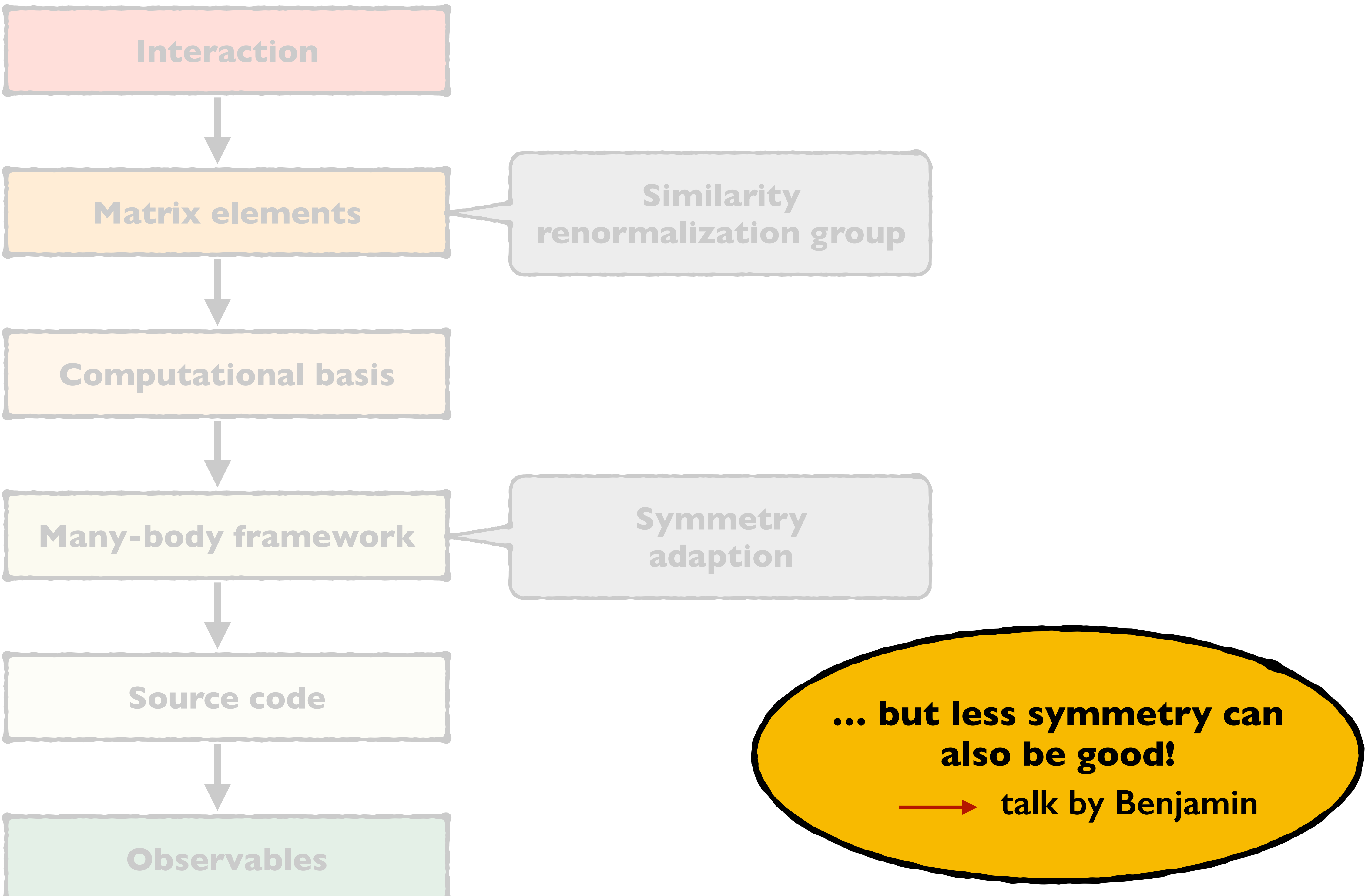
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... but less symmetry can
also be good!
talk by Benjamin