Recent Advances in *Ab Initio* Nuclear Theory

Farewell Seminar, CEA Saclay

31 October 2019

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Tichai, Arthuis, Duguet, Hergert, Somà, Roth, Phys. Lett. B 786 (2018)
Arthuis, Duguet, Tichai, Lasseri, Ebran, CPC 240C (2019)
Tichai, Ripoche, Duguet, EPJ A 55:90, (2019)

Outline

Introduction

Part I : Symmetry-broken correlation expansions

- Symmetries in (nuclear) many-body theory
- Mid-mass systems from Bogoliubov many-body perturbation theory

Intermezzo: „The curse of dimensionality“

Part II : Pre-processing the many-body problem

- Reduction principles for ‘effective problems’
- Size of Hilbert space and nuclear observables

Outlook

Introduction

What is ab initio many-body theory and what are its (current) limits?

Nuclear structure from first principles

Ab initio

"The approximate solution must be systematically improvable and approach the exact solution in a well-defined limit."

$$H\,|\Psi_k^{JA\Pi}\rangle = E_k^{JA\Pi}\,|\Psi_k^{JA\Pi}\rangle$$

Input Hamiltonian (derived from EFT)

Many-body expansion

Nuclear structure from first principles

<u>This talk:</u>
Take the Hamiltonian as given and investigate the many-body expansion scheme for the wave function.
(Expansion of Hamiltonian and many-body solution are kept independent)

<u>Next step:</u>
Combined treatment of EFT and many-body approximations.

'Renormalization of pionless effective field theory in the A-body sector'
Drissi, Duguet, Somà, arXiv:1908.07578 (2019)

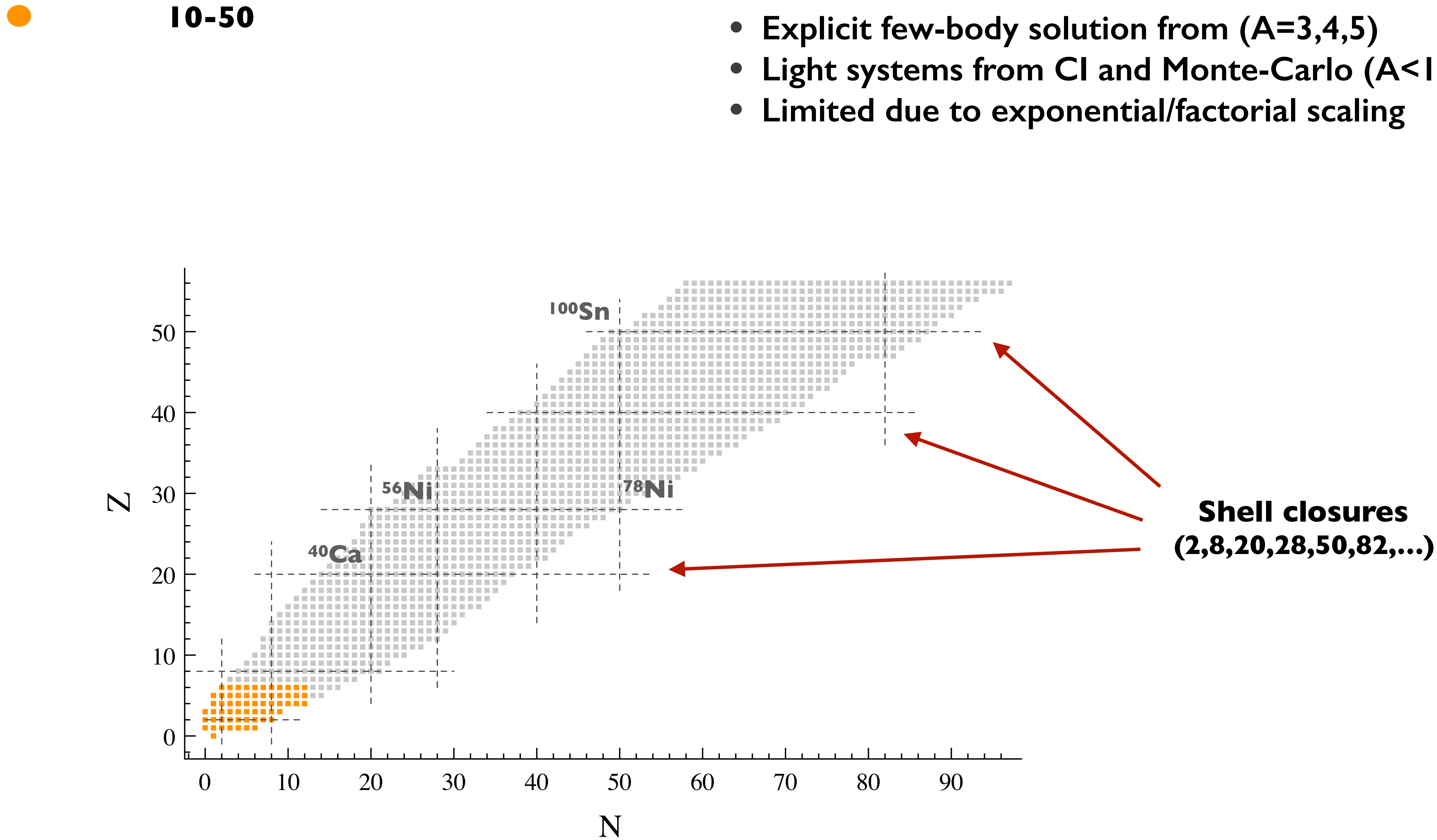
Ab initio nuclear structure

Number of nuclei

10-50

'Exact' solution (early 2000's)

- Explicit few-body solution from (A=3,4,5)
- Light systems from CI and Monte-Carlo (A<12)
- Limited due to exponential/factorial scaling



Ab initio nuclear structure

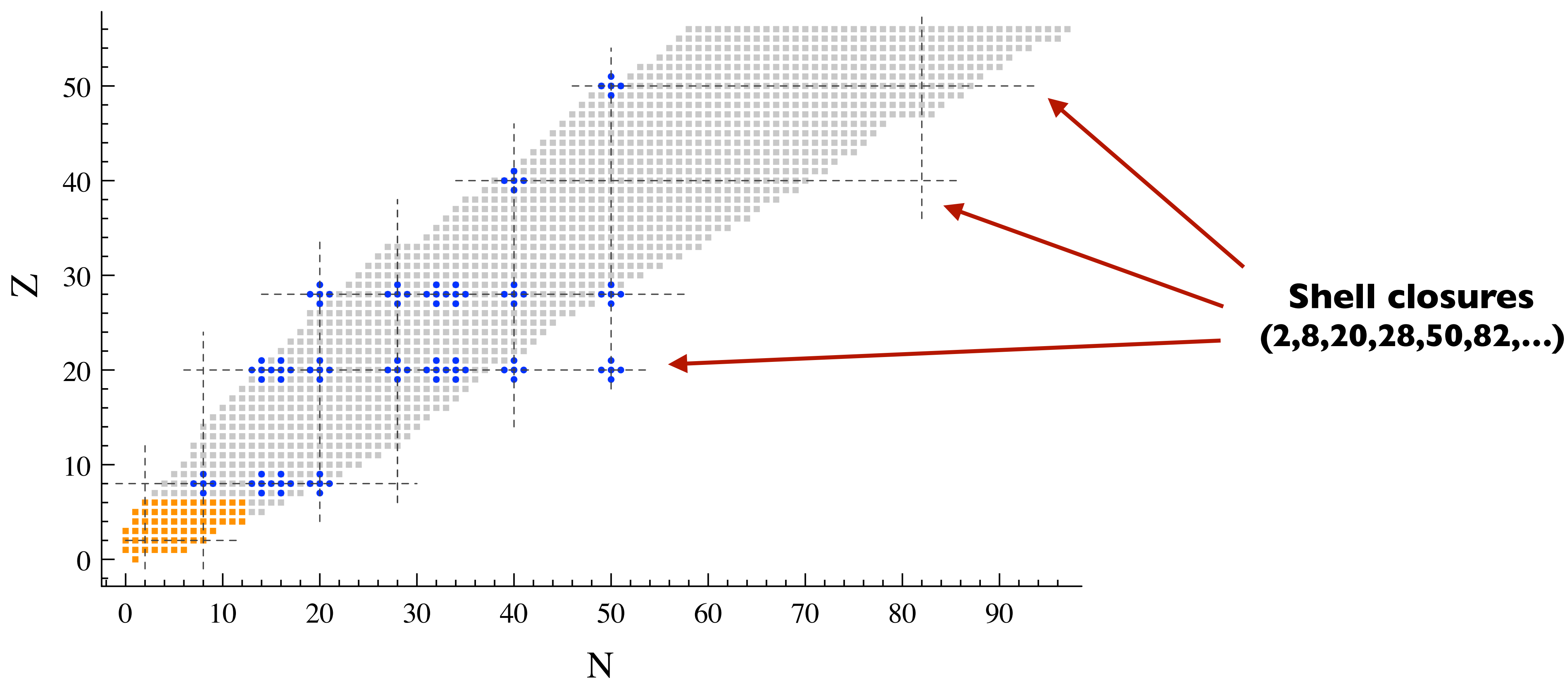
Number of nuclei

- **10-50** (orange)
- **50-100** (blue)

<u>Closed-shell systems (2005-now)</u>

- Ground-state expansion from mean-field determinant

  MBPT, CC, SCGF, IMSRG, …
- EOM-methods for systems near closed shells and spectra
- Low polynomial scaling enables for large basis size



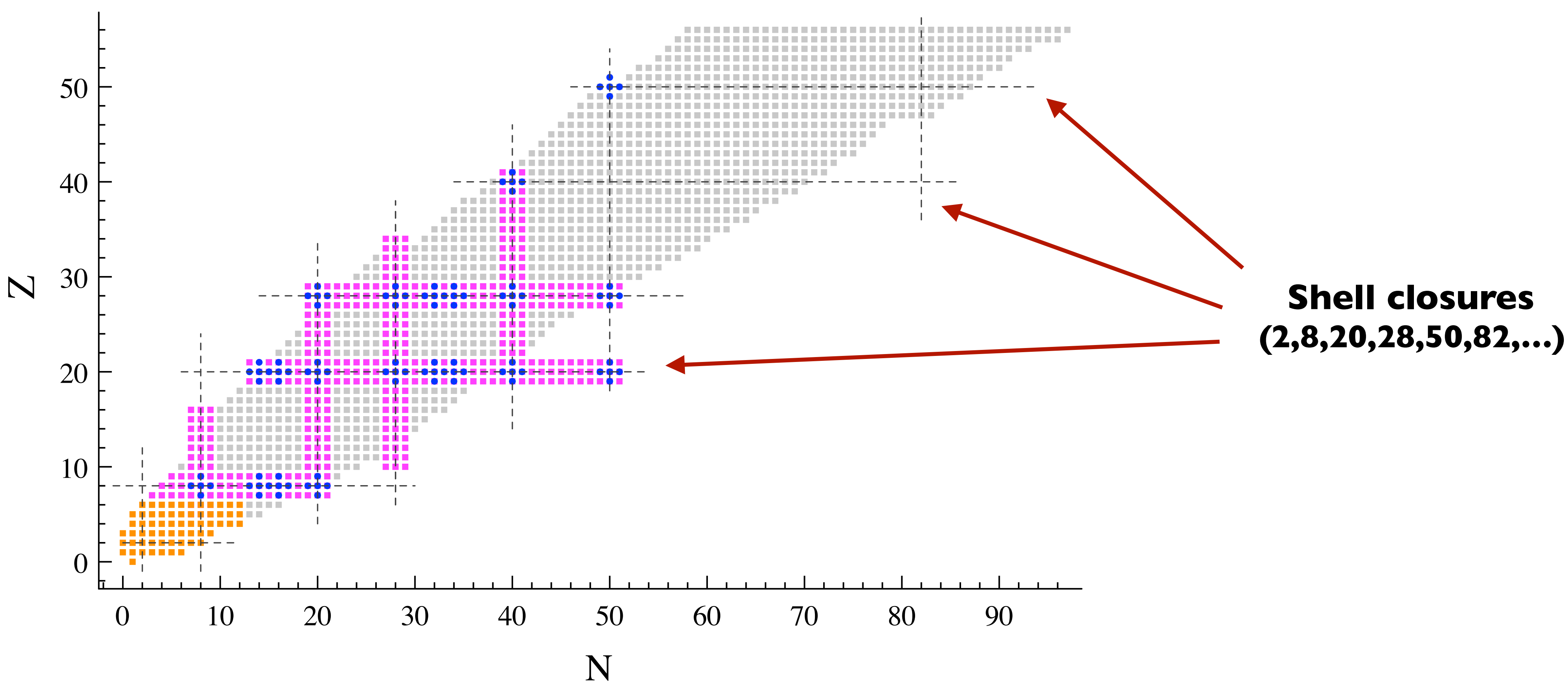
Ab initio nuclear structure

Number of nuclei

- 10-50
- 50-100
- 200-300

Open-shell systems (2011-now)

- Ground-state expansion from correlated reference state
- Accurate description of semi-magic nuclei (A<80)
- Full access to medium-mass isotopic/isotonic chains
- Still polynomial scaling with respect to basis size



Ab initio nuclear structure

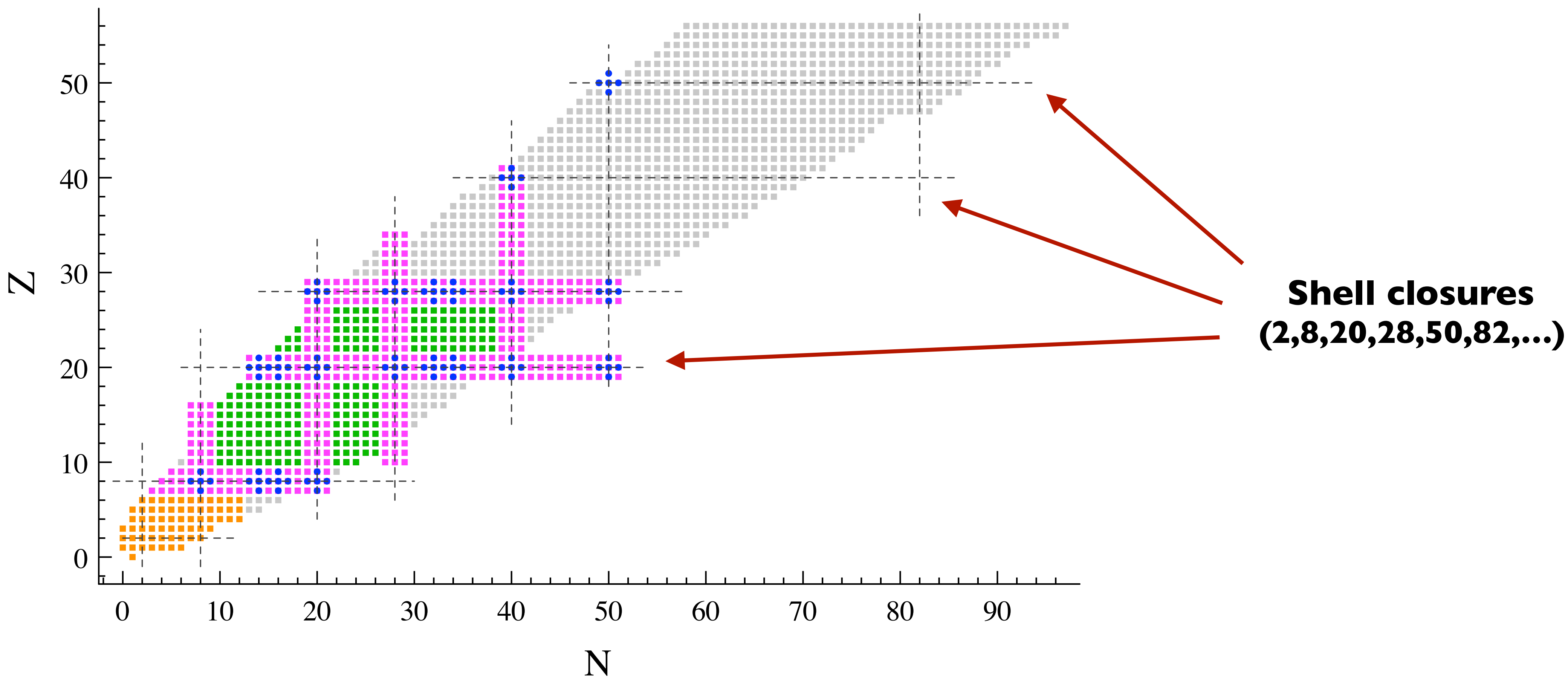
Number of nuclei

- 10-50
- 50-100
- 200-300
- >500

<u>Hybrid methods (2014-now)</u>

- Construction of dressed Hamiltonian in limited valence space
- Access to arbitrary open-shell nuclei in medium-mass regime
- Dressing of operator involves polynomial computational cost

… but diagonalization scales factorially



Ab initio nuclear structure

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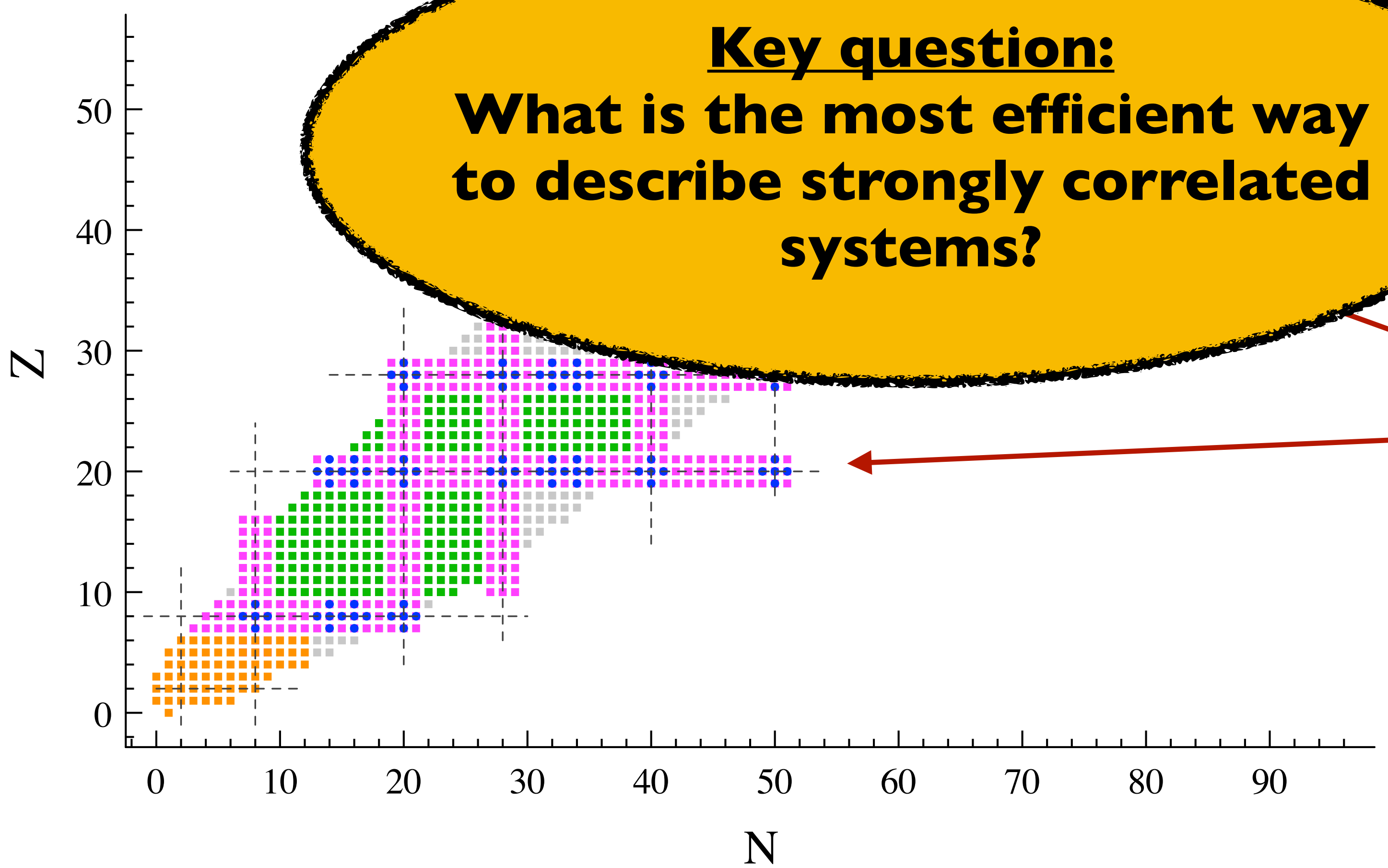


<u>Key question:</u>
What is the most efficient way to describe strongly correlated systems?

Shell closures (2,8,20,28,50,82,…)

Part I
Symmetry-broken correlation expansions

Exploiting symmetry breaking for strongly correlated systems

Many-body expansions

Horizontal expansion

- Authorize breaking of symmetry group G

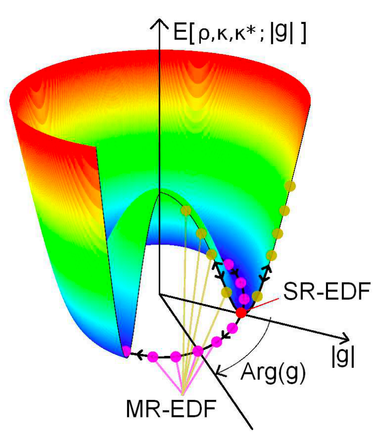
  $U(1)$: pairing correlations

  $SU(2)$: quadrupolar correlations

- Mixing of vacua within manifold of rotated states

$$|\Psi\rangle = \int_G dg\, f(g) R(g) |\Phi\rangle$$

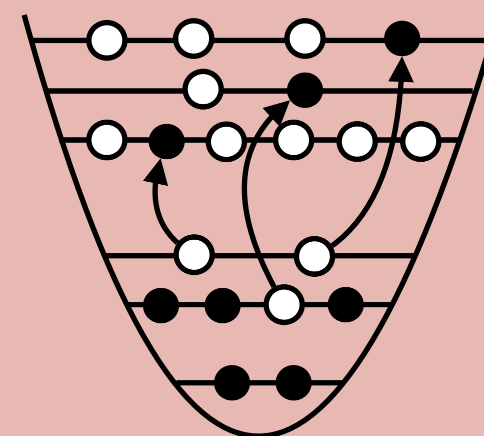
- Rot. states are related in non-perturbative way



- Historically preferred strategy in EDF theory

Vertical expansion

- Account of dynamic correlation effects
- Expansion in terms of particle-hole excitations



- Goal: determine wave-function coefficients

$$|\Psi\rangle = |\Phi\rangle + \sum_{ai} c_i^a |\Phi_i^a\rangle + \sum_{\substack{a<b \\ i<j}} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots$$

- Large variety of different expansion schemes
- Collectivity is complicated to account for!
- Historically preferred strategy in *ab initio* theory

Combined expansions

Nuclear Hamiltonian

↓

Deformed mean-field

↓

Normal ordering

↓

Correlation expansion

↓

Symmetry restoration

↓

Observables

- Generation of symmetry-broken vacuum
- Account of non-dynamical correlation effects
- Grants access to genuine open-shell nuclei

Combined expansions

Nuclear Hamiltonian

↓

Deformed mean-field

↓

Normal ordering

↓

Correlation expansion

↓

Symmetry restoration

↓

Observables

- **Operator basis w.r.t. *A*-body reference state**
- **Enables for approximating three-body effects**

$$O^{(\mathrm{eff})}_{pqrs} \equiv \sum_{tu} w_{pqtrsu}\,\rho_{tu}$$

- **Partially circumvents curse of dimensionality**

Combined expansions

Nuclear Hamiltonian

↓

Deformed mean-field

↓

Normal ordering

↓

Correlation expansion

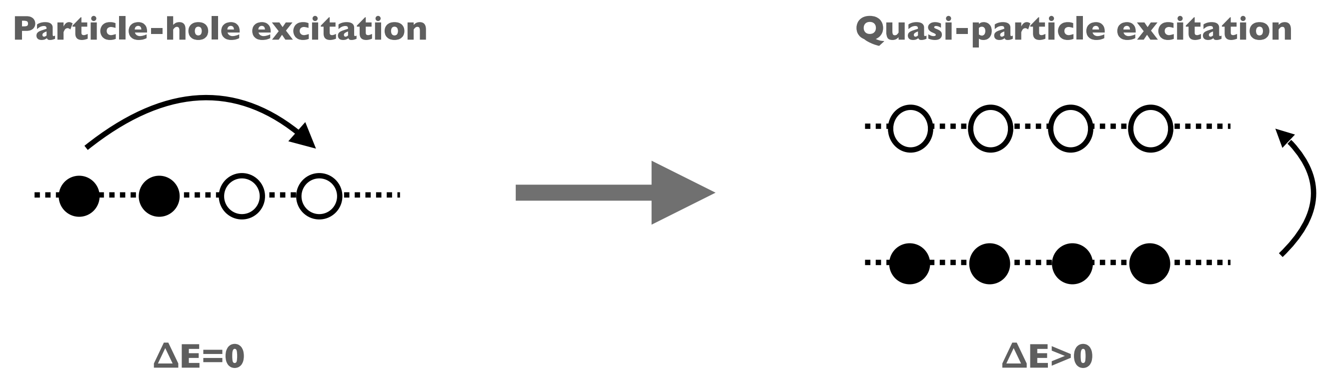
↓

Symmetry restoration

↓

Observables

Lifting the degeneracy



- **Systematic account of dynamic correlation**
- **Vertical expansion in elementary excitations**
- **Finite truncation yields polynomial scaling**

Combined expansions

Nuclear Hamiltonian

↓

Deformed mean-field

↓

Normal ordering

↓

Correlation expansion

↓

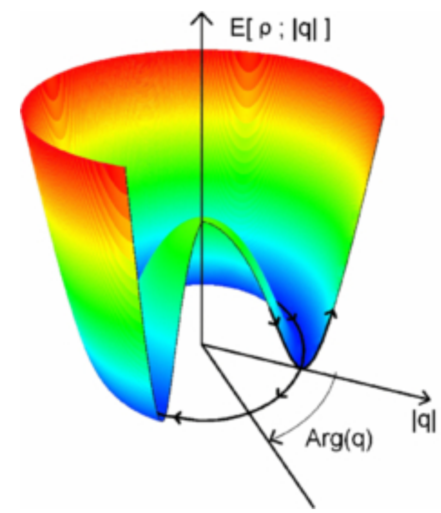
Symmetry restoration

↓

Observables

Work in progress!

Mexican-hat potential for gauge integration



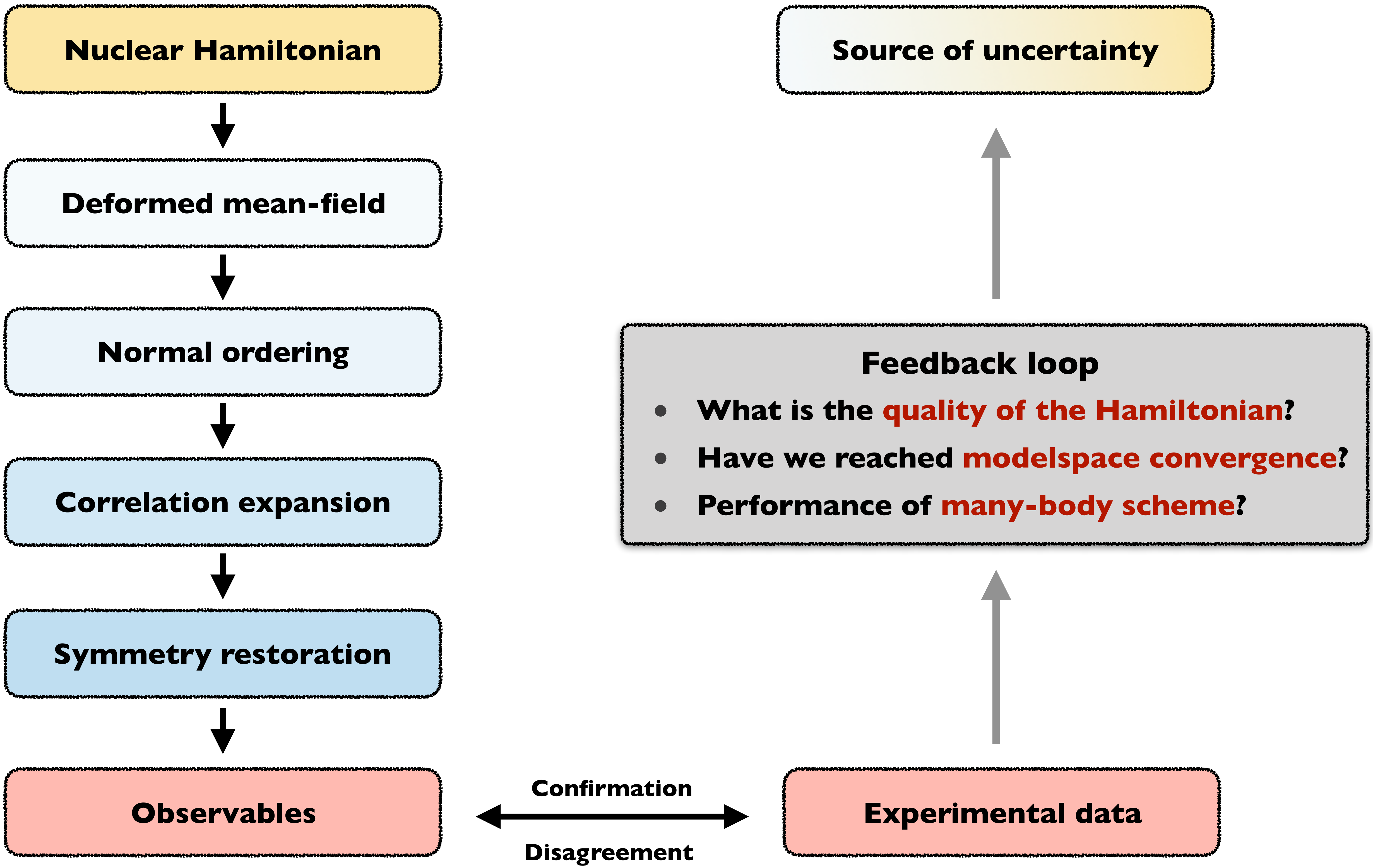
- Integration over **broken symmetry group**
- **Non-perturbative physics** from rotated states
- **Good quantum numbers** in finite systems

'Symmetry-broken and restored coupled-cluster theory'
Duguet, Signoracci, J. Phys. G: Nucl. Part. Phys. 44 015103 (2017)

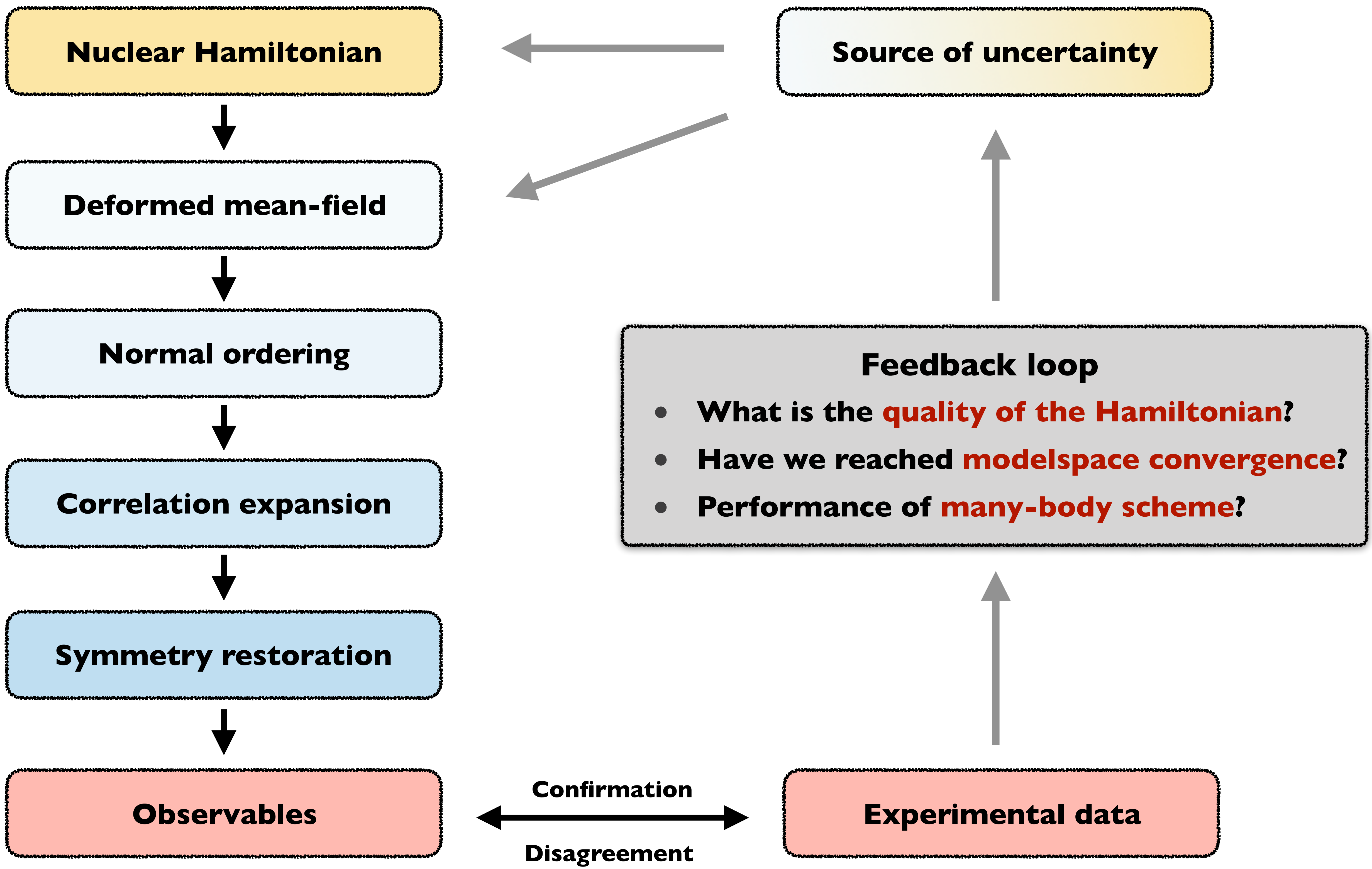
'Projected coupled cluster theory'
Qiu, Henderson, Zhao, Scuseria, J. Chem. Phys. **147**, 064111 (2017)

'Particle-number projected Bogoliubov-coupled-cluster theory'
Qiu, Henderson, Duguet, Scuseria, Phys. Rev C **99**, 044301 (2019)

Combined expansions



Combined expansions



Combined expansions

Nuclear Hamiltonian → **Chiral effective field theory**

↓

Deformed mean-field → **Hartree-Fock-Bogoliubov (particle-number breaking)**

↓

Normal ordering → **Quasiparticle normal ordering**

↓

Correlation expansion → **Bogoliubov many-body perturbation theory**

↓

Symmetry restoration

↓

Observables

Quasiparticle representation

- **Breaking of particle-number conservation linked to (abelian) global *U(1)* gauge symmetry**

$$U(1) = \left\{ S(\varphi) \equiv e^{iA\varphi} \, , \, \varphi \in [0, 2\pi] \right\}$$

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- **Hamiltonian is replaced by grand potential operator involving Lagrange multiplier**

$$\Omega = H - \lambda A$$

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- **Correlated reference state is of product type in quasi-particle space (change of algebra!)**

$$|\Phi\rangle = \mathcal{C} \prod_k \beta_k |0\rangle \qquad \beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \qquad \beta_k = \sum_p U_{pk}^\star c_p + V_{pk}^\star c_p^\dagger$$

Bogoliubov transformation

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Bogoliubov transformation

- While the operators commute with particle number the reference state is not an eigenstate of *A*

$$[H, S(\varphi)] = [A, S(\varphi)] = [\Omega, S(\varphi)] = 0 \qquad A|\Phi\rangle \neq A_0 |\Phi\rangle$$

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- **Final task: design of a correlation expansion for vacuum obeying Bogoliubov algebra**

Perturbative expansion

- **Partitioning: definition of a splitting into unperturbed part and perturbation**

$$\Omega = \Omega_0 + \Omega_1 \quad with \quad [\Omega_0, S(\varphi)] \neq 0 \quad and \quad [\Omega_1, S(\varphi)] \neq 0$$

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- Correlation energy obtained from extension of Goldstone's formula to symmetry-broken phase

$$\Delta\Omega_0^{A_0} = \langle\Phi|\Omega_1 \sum_{k=1}^{\infty} \Big(\frac{1}{\Omega^{00} - \Omega_0}\Omega_1\Big)^{k-1} |\Phi\rangle_c$$

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- Low-order expressions are obtained from using generalized Wick's theorem

$$E^{(2)} = \frac{1}{4}\sum_{abij} \frac{H_{abij}H_{ijab}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

Hartree-Fock matrix elements

grand potential matrix elements

$$E^{(2)} = -\frac{1}{24}\sum_{k_1k_2k_3k_4} \frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$

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Hartree-Fock single-particle energies

Hartree-Fock-Bogoliubov quasiparticle energies

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Sum run over particle/hole subspaces
Computational scaling:
$N_p^2 N_h^2$

Sum run over full space
Computational scaling:
N^4

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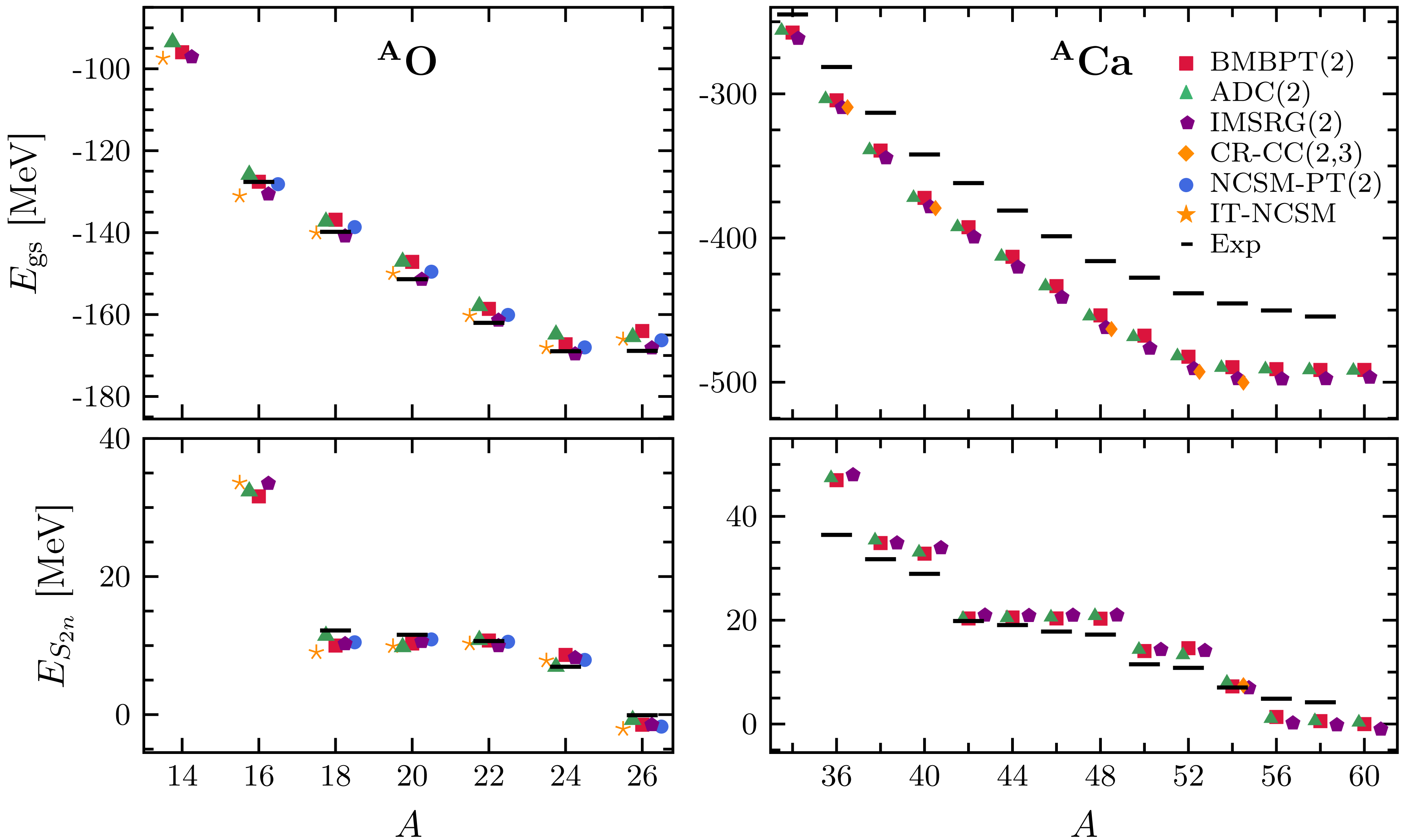
- **When applied to closed-shell systems BMBPT(p) reduces to HFMBPT(p)**

Medium-mass results



Calculation details

Chiral NN+3N Hamiltonian
NO2B approximation
SRG: α = 0.08 fm⁴
13 major shells (1820 s.p. states)
canonical HFB reference

Runtime

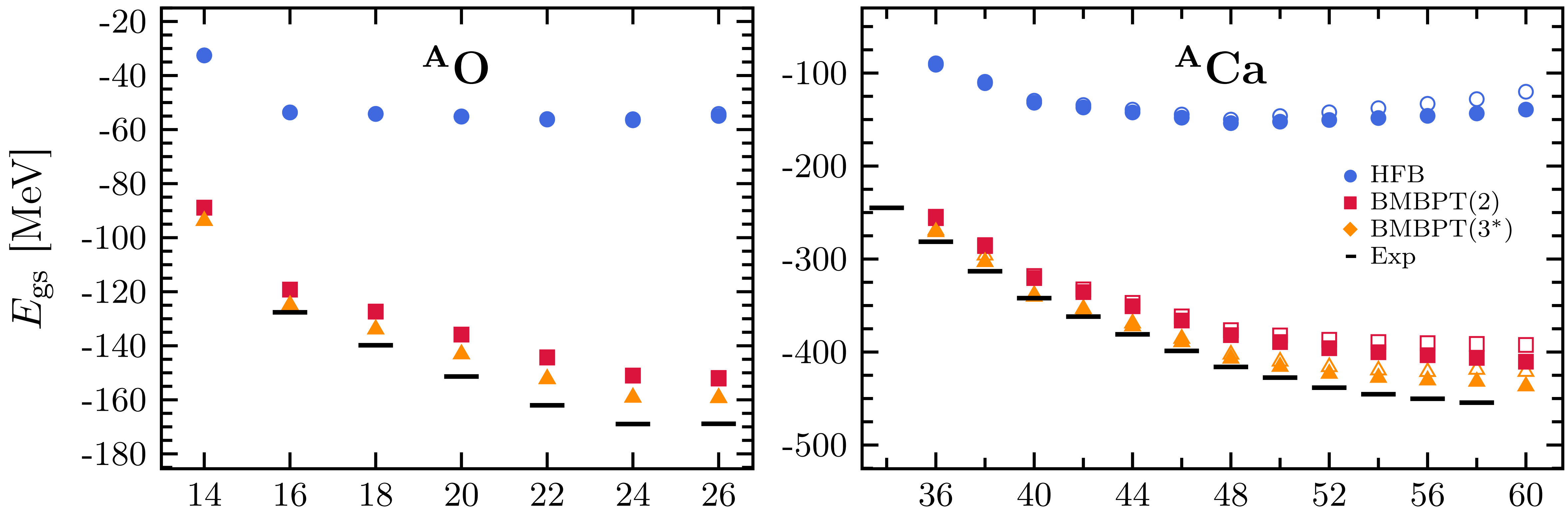
NCSM:	20.000 hours
MCPT:	2.000 hours
IMSRG:	1.500 hours
ADC:	400 hours
BMBPT:	**< 1min !**

Tichai *et al.*, PLB **786** 195 (2018)

- Excellent agreement of all methods with 'exact' results (IT-NCSM)
- Different truncation schemes yield consistent description of open-shell nuclei
- BMBPT is optimal for cheap survey calculations of next-generation chiral Hamiltonians

Next-generation Hamiltonians

Interaction: Hüther, Roth, *et al.*, in preparation (2019)



Chiral NN+3N interaction at N3LO, SRG α=0.04 fm^4, e_{max}=14, open/bold: E_{3max} = 14/16

Tichai, Roth, Duguet, in preparation (2019)

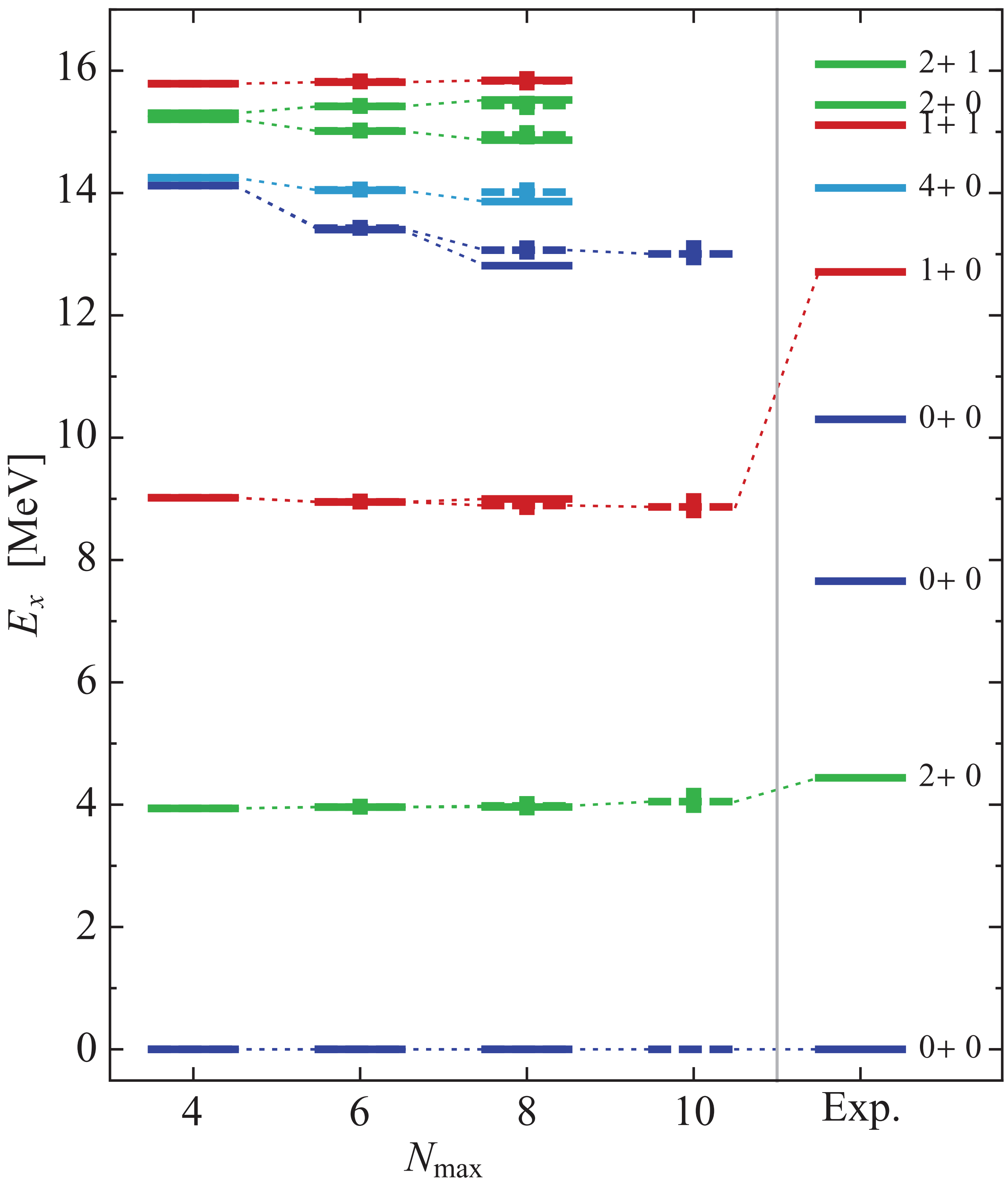
- **New families of nuclear Hamiltonians available with highly improved medium-mass accuracy**
- **Third-order *a posteriori* correction BMBPT(3*) provides systematic improvement**
- **Neutron-rich calcium isotopes not fully converged w.r.t. size of modelspace**
- **Reference state accounts for 30 % of overall binding: 70 % is due to dynamic correlations**

Intermezzo
The curse of dimensionality

Practical challenges for a famous problem

Intermezzo - The infamous 'Hoyle state'

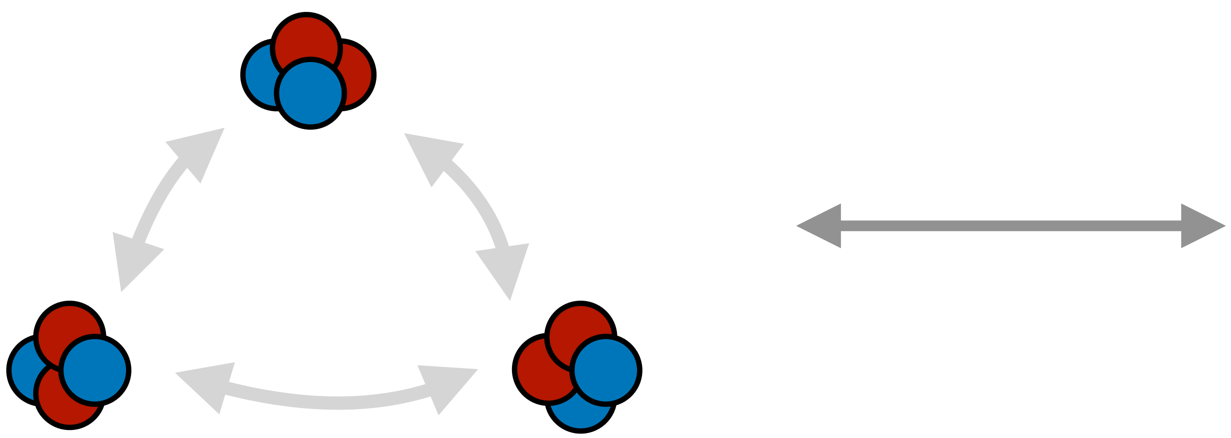
Maris et al., Phys. Rev. C **90**, 014314 (2014)

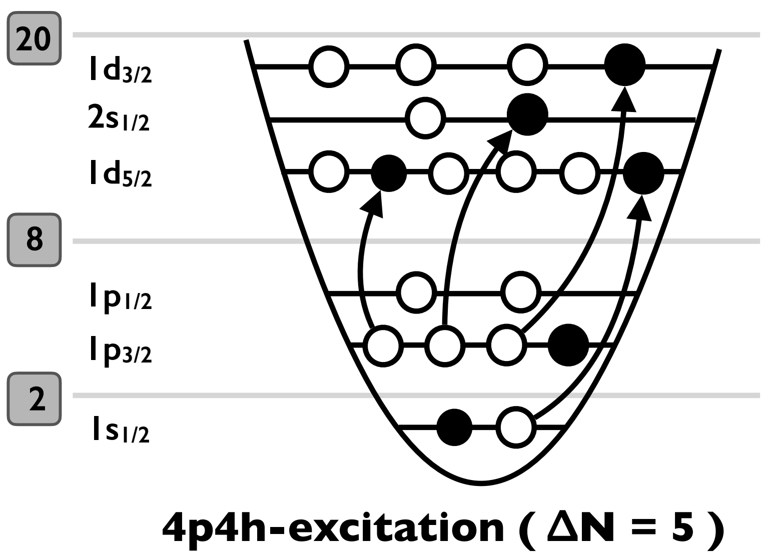


- First excited 0^+-state in C^{12} exhibits notorious slow model-space convergence
- Independent of input Hamiltonian, resolution scale (SRG) or basis parameters
- Finite oscillator basis cannot account for collective structure of the excitation
- Lattice EFT simulations reveal localisation of three α-particles

Intermezzo - Clustering

Spectroscopy of C^{12} emerges from interplay between α-particles





<u>Note</u>:
No-core shell model includes 4p4h-excitations
... but only the ones close to the Fermi surface
(N_{max} truncation)

Full configuration space required!
(Single-particle truncation)

Intermezzo - A quick estimate

Naive expectation: 4p4h-excitations are important for clustering

$$|\Psi\rangle = |\Phi\rangle + \sum_{ai} c_i^a |\Phi_i^a\rangle + \sum_{abij} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \sum_{abcijk} c_{ijk}^{abc} |\Phi_{ijk}^{abc}\rangle + \sum_{abcdijkl} c_{ijkl}^{abcd} |\Phi_{ijkl}^{abcd}\rangle$$

Storage	$N_p N_h$	$N_p^2 N_h^2$	$N_p^3 N_h^3$	$N_p^4 N_h^4$

Converged results in C^{12}: 12 occupied states and 2000 virtual states

1p1h-excitations	**100 kb**
2p2h-excitations	**4 Gb**
3p3h-excitations	**100 Tb**
4p4h-excitations	**>10^6 Tb**

Explosion of required resources

Intermezzo - A quick estimate

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Storage $N_p N_h$ $N^2 N^2$ $N_p^4 N_h^4$

Converged resu ... **0 virtual states**

Take away-message:
Brute force does not resolve this...
New technology required!

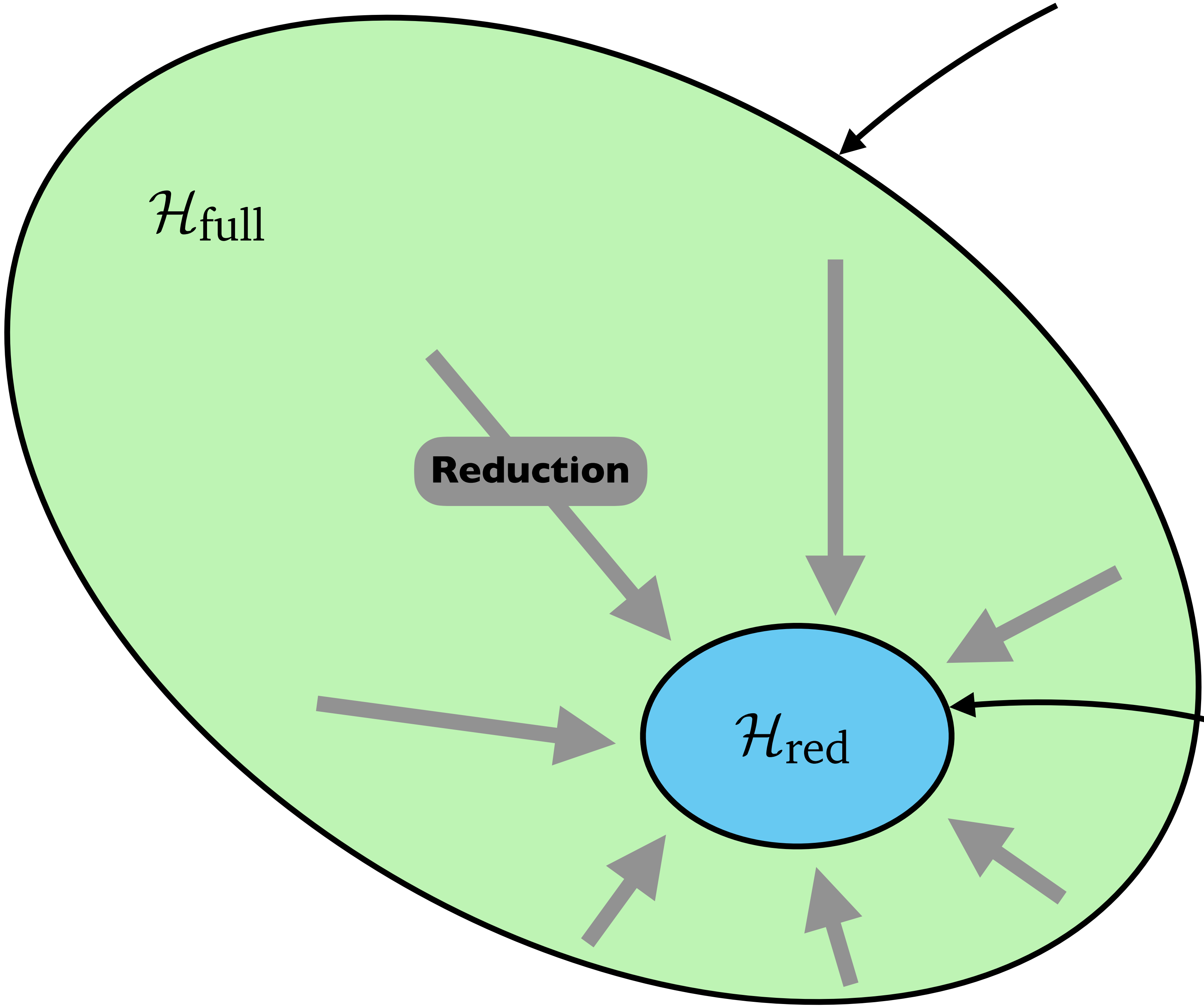
1p1h-excitations	**100 kb**
2p2h-excitations	**4 Gb**
3p3h-excitations	**100 Tb**
4p4h-excitations	**>10^6 Tb**

Part II
Pre-processing
the many-body problem

Why is quantum mechanics so hard?

‘Effective’ problems

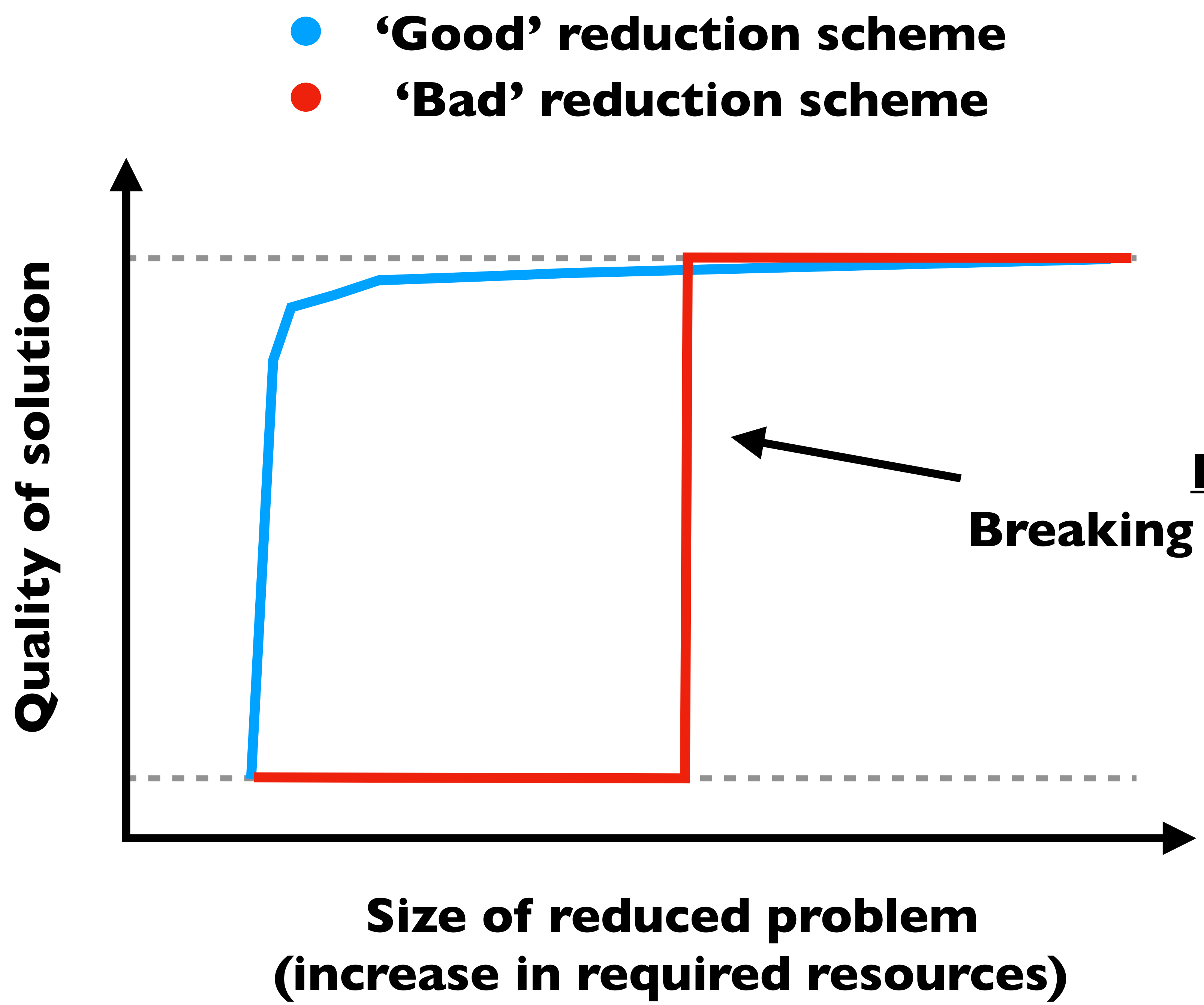
parameter space of full problem



$\mathcal{H}_{\text{red}} \subset \mathcal{H}_{\text{full}}$

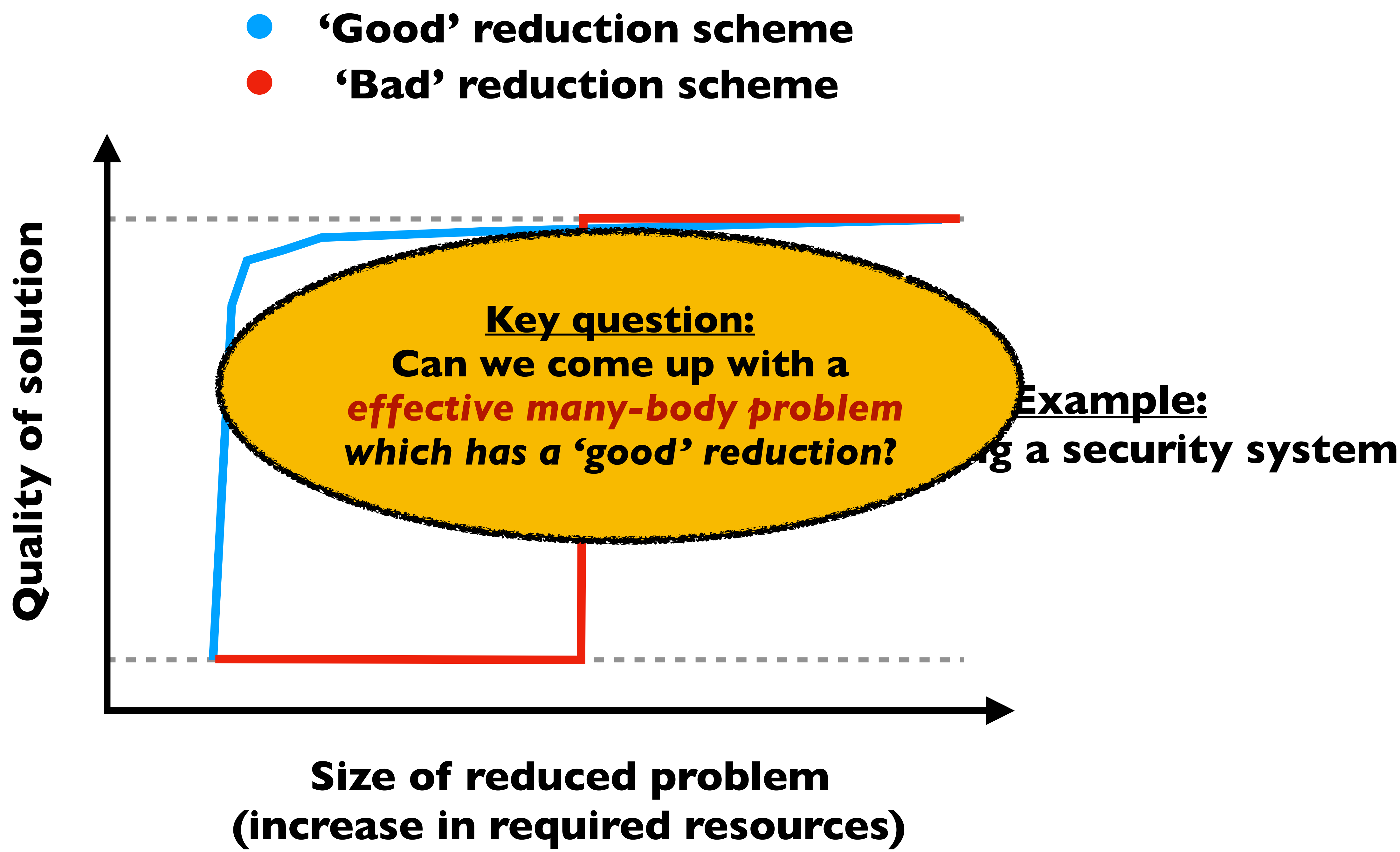
parameter space of reduced problem

Quality of reduced solution



Example:
Breaking a security system

Quality of reduced solution



Importance truncation

(NCSM: Roth, Navrátil, Barret, …; QMC: Abe, Otsuka, …; CC: Deustua, Shen, Piecuch)

- Challenge in wave-function theory is the growth of basis dimension of *A*-body Hilbert space

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- Challenge in wave-function theory is the growth of basis dimension of *A*-body Hilbert space
- Often the largest part of Hilbert space is (almost) irrelevant for nuclear observable
- Idea of importance truncation (IT): pre-selection of relevant Hilbert-space elements

$$\mathcal{T}_n(\kappa^{(p)}_{\min}) \equiv \{ t^{2n0}_{k_1 \ldots k_{2n}} \text{ such that } \kappa^{(p)}(t^{2n0(p)}_{k_1 \ldots k_{2n}}) \geq \kappa^{(p)}_{\min} \}$$

Wave-function amplitudes

A priori importance measure
(e.g. based on MBPT arguments)

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- Idea of importance truncation (IT): pre-selection of relevant Hilbert-space elements

$$\mathcal{T}_n(\kappa^{(p)}_{\text{min}}) \equiv \{t^{2n0}_{k_1\dots k_{2n}} \text{ such that } \kappa^{(p)}(t^{2n0(p)}_{k_1\dots k_{2n}}) \geq \kappa^{(p)}_{\text{min}}\}$$

Wave-function amplitudes

A priori importance measure (e.g. based on MBPT arguments)

- Sum over important states only, i.e. states of the parameter space of the effective problem

$$E^{(2)} = -\frac{1}{24} \sum_{k_1k_2k_3k_4} t^{40(1)}_{k_1k_2k_3k_4} \Omega^{04}_{k_1k_2k_3k_4} \qquad t^{40(1)}_{k_1k_2k_3k_4} = \frac{\Omega^{40}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

Importance truncation

(NCSM: Roth, Navrátil, Barret, …; QMC: Abe, Otsuka, …; CC: Deustua, Shen, Piecuch)

- Challenge in wave-function theory is the growth of basis dimension of *A*-body Hilbert space
- Often the largest part of Hilbert space is (almost) irrelevant for nuclear observable
- Idea of importance truncation (IT): pre-selection of relevant Hilbert-space elements

$$\mathcal{T}_n(\kappa^{(p)}_{\text{min}}) \equiv \{ t^{2n0}_{k_1 \dots k_{2n}} \text{ such that } \kappa^{(p)}(t^{2n0(p)}_{k_1 \dots k_{2n}}) \geq \kappa^{(p)}_{\text{min}} \}$$

Wave-function amplitudes

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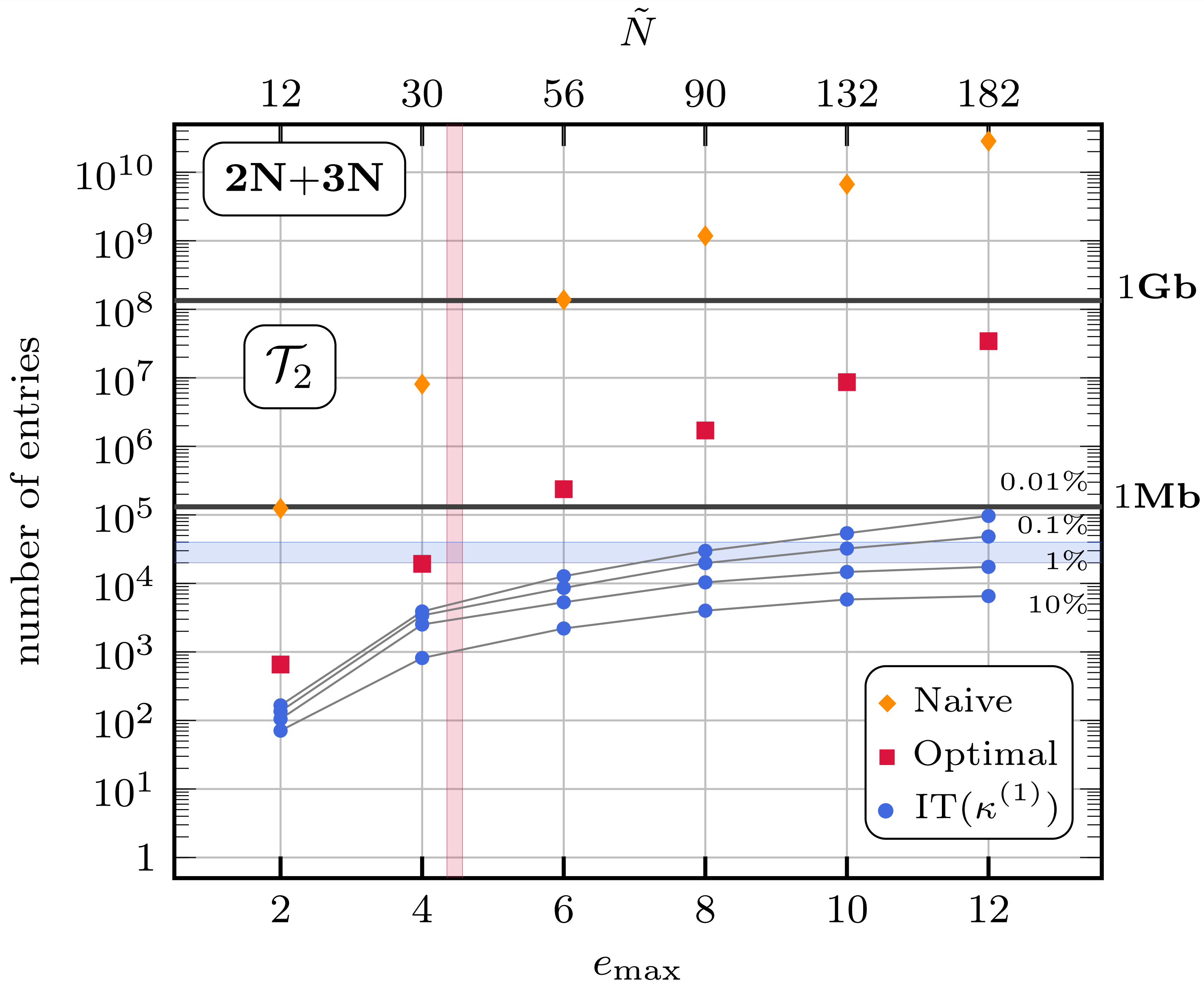
- Systematically improvable: Full value of observable is obtained in the limit of zero threshold

This is very much in the *ab initio* spirit!

Analysis of double amplitudes



Calculation details

Chiral NN+3N Hamiltonian
α = 0.08 fm⁴
13 major shells (1820 s.p. states)
canonical HFB reference
4-quasi-particle excitations
^{18}O

1st pre-processing paradigm:
'Make hard calculations routine'

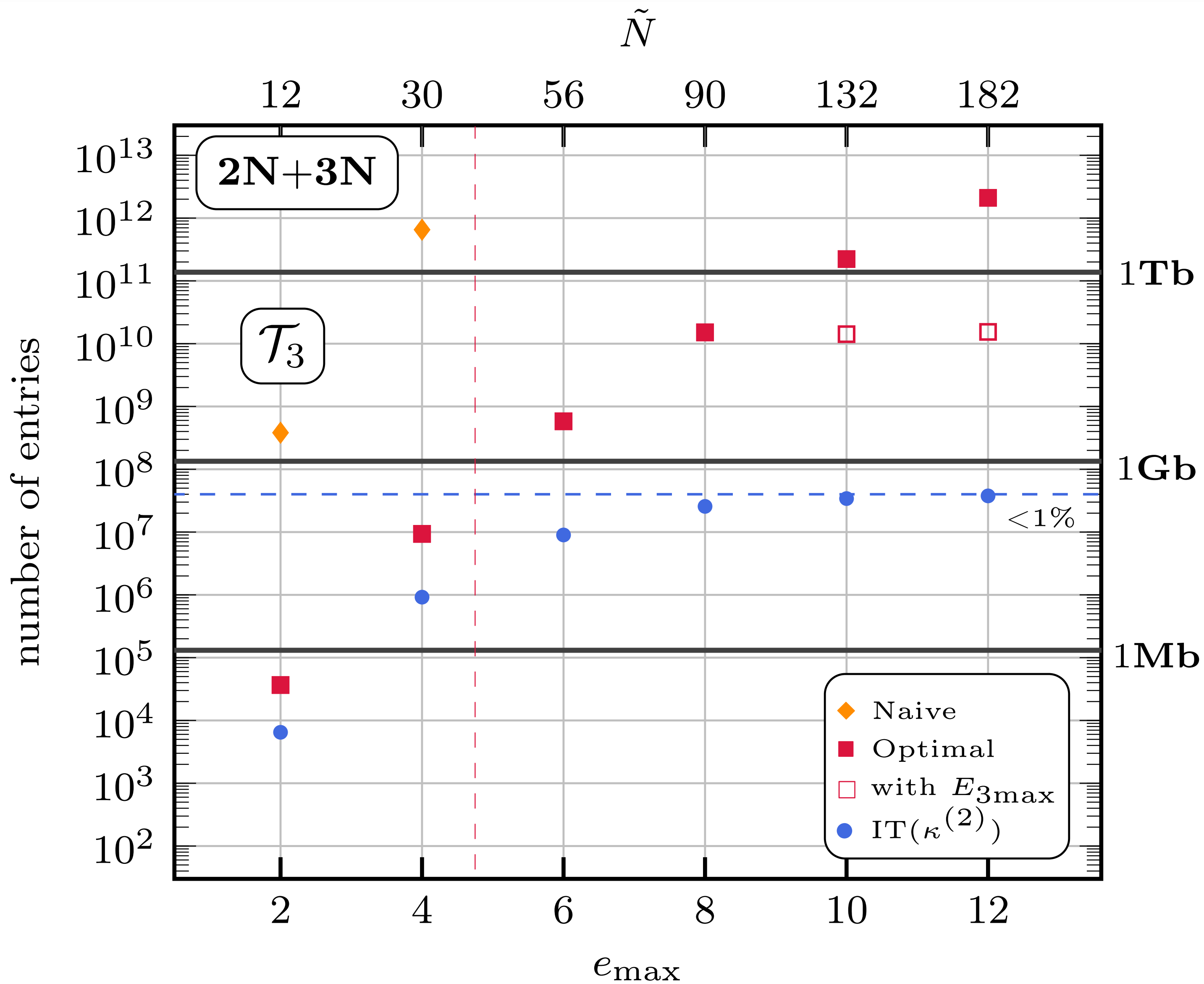
Tichai, Ripoche, Duguet, EPJ A 55:90, (2019)

$$E^{(2)} = -\frac{1}{24} \sum_{k_1 k_2 k_3 k_4} t^{40(1)}_{k_1 k_2 k_3 k_4} \Omega^{04}_{k_1 k_2 k_3 k_4}$$

- Estimate quality of IT based on 2nd-order energy correction in CC-like form
- Storage requirements of IT wave function reduced by several orders of magnitude

99.9 % accuracy with 0.1% of configurations!

Analysis of triple amplitudes



Calculation details

Chiral NN+3N Hamiltonian
α = 0.08 fm⁴
13 major shells (1820 s.p. states)
canonical HFB reference
6-quasi-particle excitations
^{18}O

2nd pre-processing paradigm:
'Make impossible calculations feasible'

Tichai, Ripoche, Duguet, EPJ A 55:90, (2019)

- Explosion of storage requirements without data compression (> 10 Tb)
- Estimate error on observables via BCCSD[T] correction (fourth-order complete!)

$$\Delta\Omega_0^{[4_T]} = \sum_{k_1k_2k_3k_4k_5k_6} |t^{60(2)}_{k_1k_2k_3k_4k_5k_6}|^2 E_{k_1k_2k_3k_4k_5k_6}$$

- Storage of pre-processed amplitudes possible: full IT-BCCSDT in reach!

Perspectives

Ab initio nuclear structure

- Improved chiral EFT interactions for medium-mass applications
- Novel computational tools to deal with size of many-body tensors in heavy systems
- Doubly open-shell nuclei from simultaneously breaking $U(1)$ and $SU(2)$ symmetry

Correlation expansions

- Systematic understanding of convergence properties of BMBPT expansion
- Extension to other nuclear observables and low-lying excited states
- Implementation of HFB-based symmetry-broken coupled-cluster theory

Pre-processing tools

- Application of importance truncation to non-perturbative many-body frameworks
- Further investigation of rank-reduction schemes using tensor-factorization tools
- Exceed boundaries of conventional computational strategies in many-body theory

Epilogue

- **CEA group**
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- **Collaborators**
  - P. Arthuis, C. Barbieri
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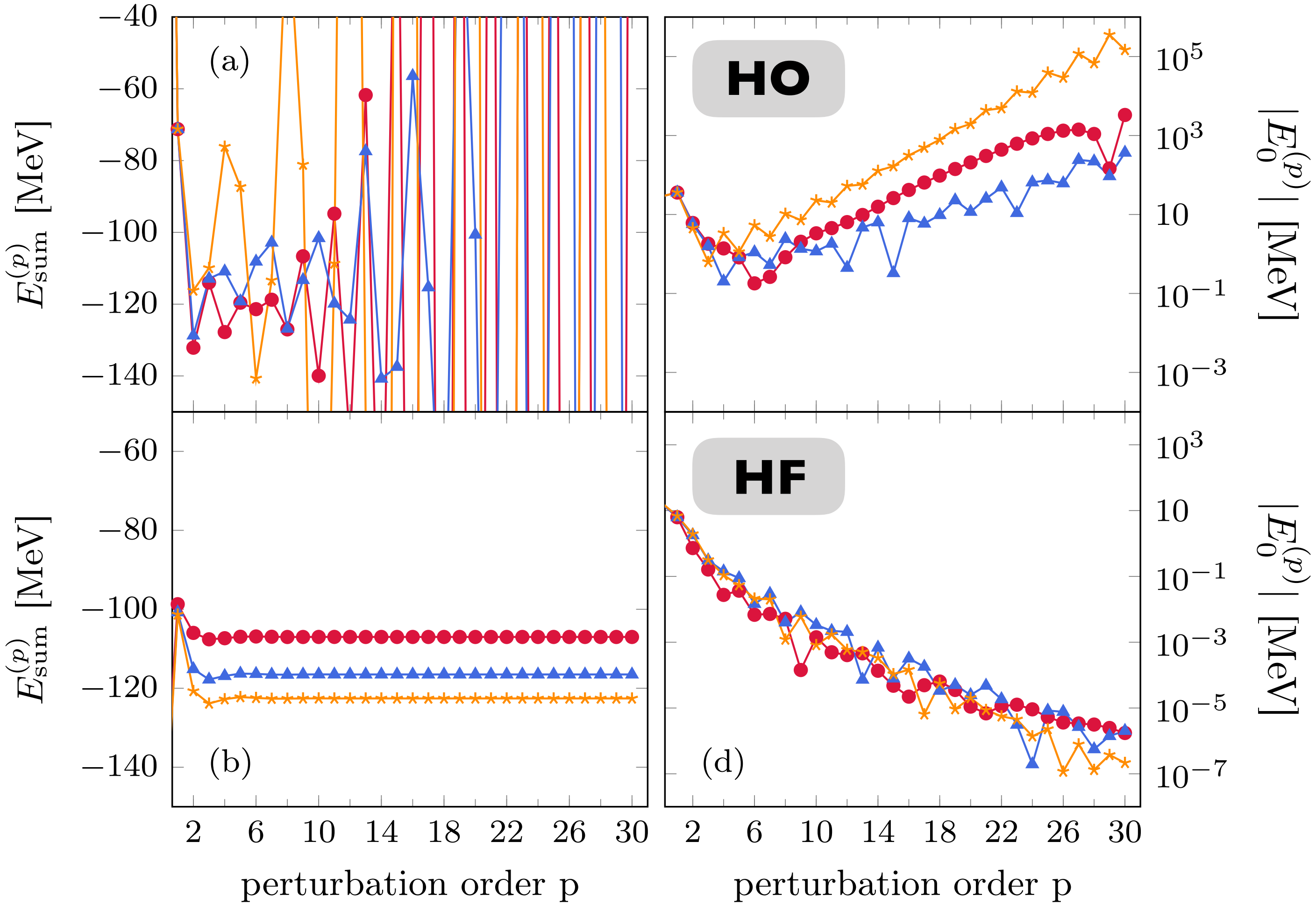
    KU Leuven, Belgium
  - J. Müller, R. Roth, K. Vobig
    Technische Universität Darmstadt, Germany
  - G. Scuseria, J. Zhao
    Rice University, USA
  - R. Schutski
    Skoltech, Russia

Ab initio?

The renaissance of MBPT after the ‘great depression’ of the 80's

MBPT - Partitioning

Tichai, Langhammer, Binder, Roth, PLB 756 283, (2016)



Calculation details

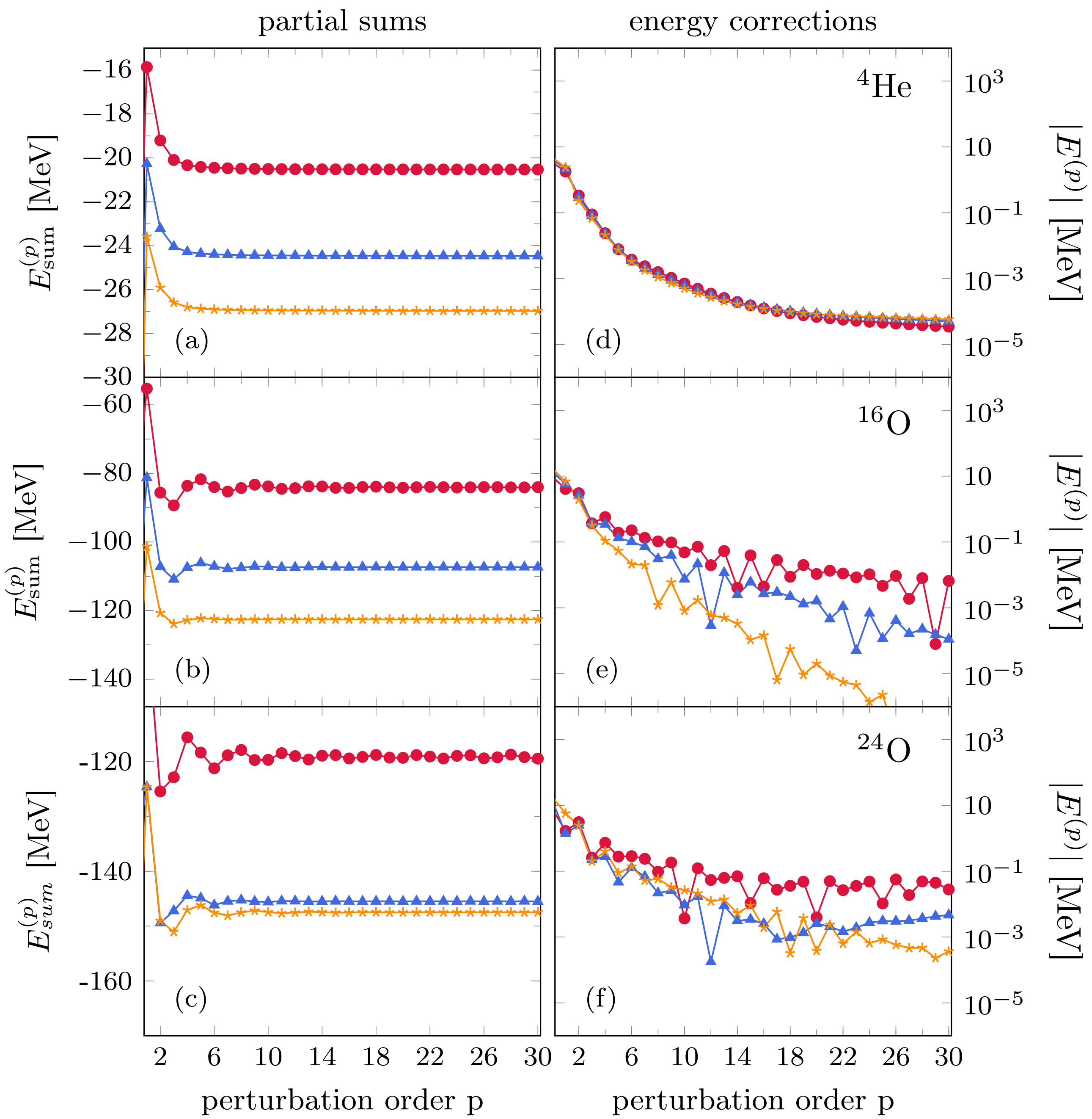
Chiral NN+3N Hamiltonian
4 major shells (140 s.p. states)
N_{max} = 4
SRG parameter α = 0.08 fm⁴
Møller-Plesset partitioning

Account of IR-divergence:
'You must have a good leading order'

- Variation of partitioning (reference states) changes qualitative behaviour of MBPT expansion
- Optimized Hartree-Fock state captures the bulk part of the binding energy
- HO determinant does not account for correct asymptotics of single-particle wave functions

MBPT - Hamiltonian

Tichai, Langhammer, Binder, Roth, PLB 756 283, (2016)



SRG parameter

- 0.02 fm^4
- 0.04 fm^4
- 0.08 fm^4

Calculation details

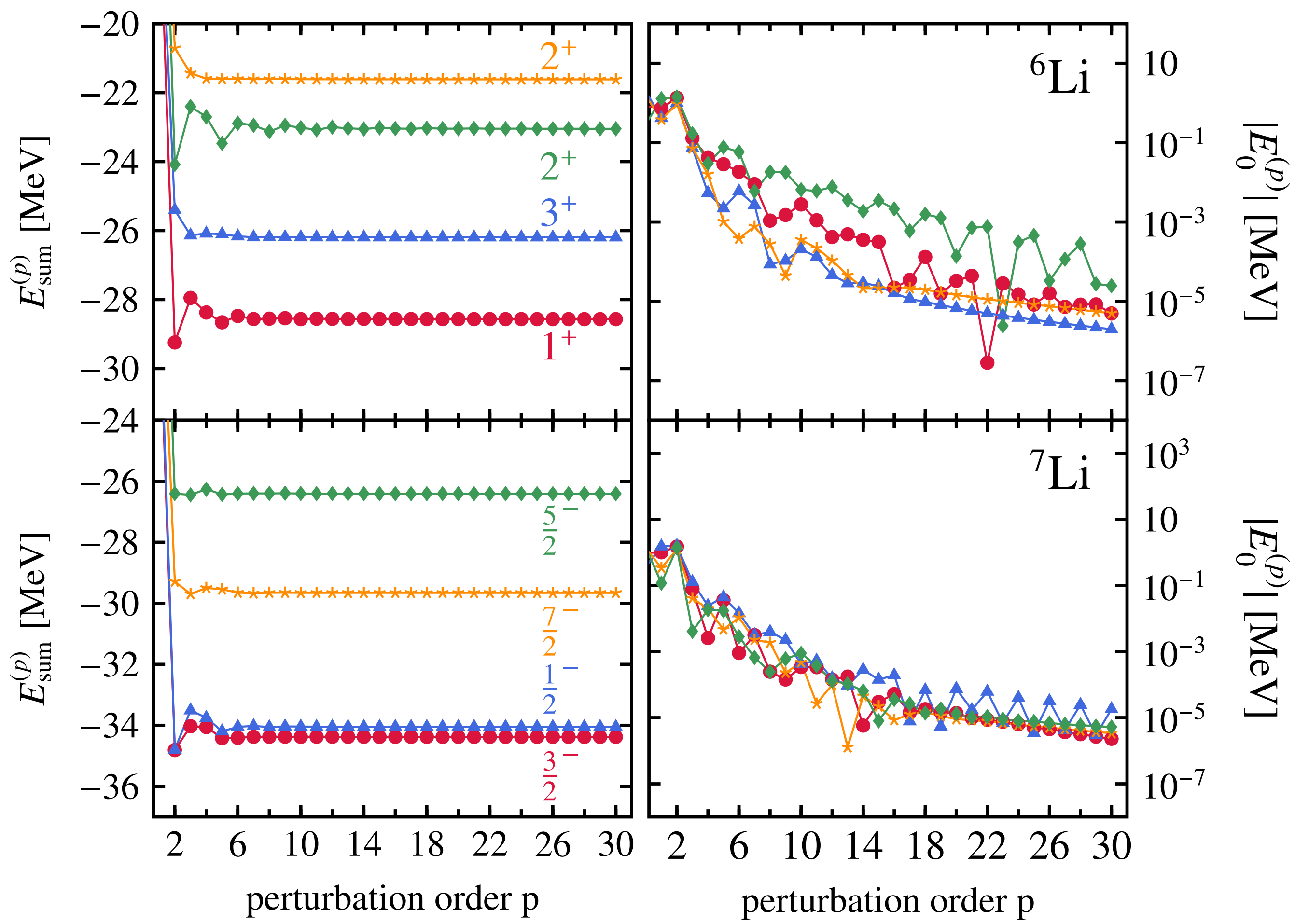
Chiral NN+3N Hamiltonian
4 major shells (140 s.p. states)
N_{max} = 4
canonical HF reference state

Account of UV-divergence:

'You must have a soft Hamiltonian'

- **Softness of interaction** has strong impact on convergence characteristics
- **Strong suppression** of high-order corrections via SRG-evolved Hamiltonians

MBPT - open-shell nuclei



Calculation details

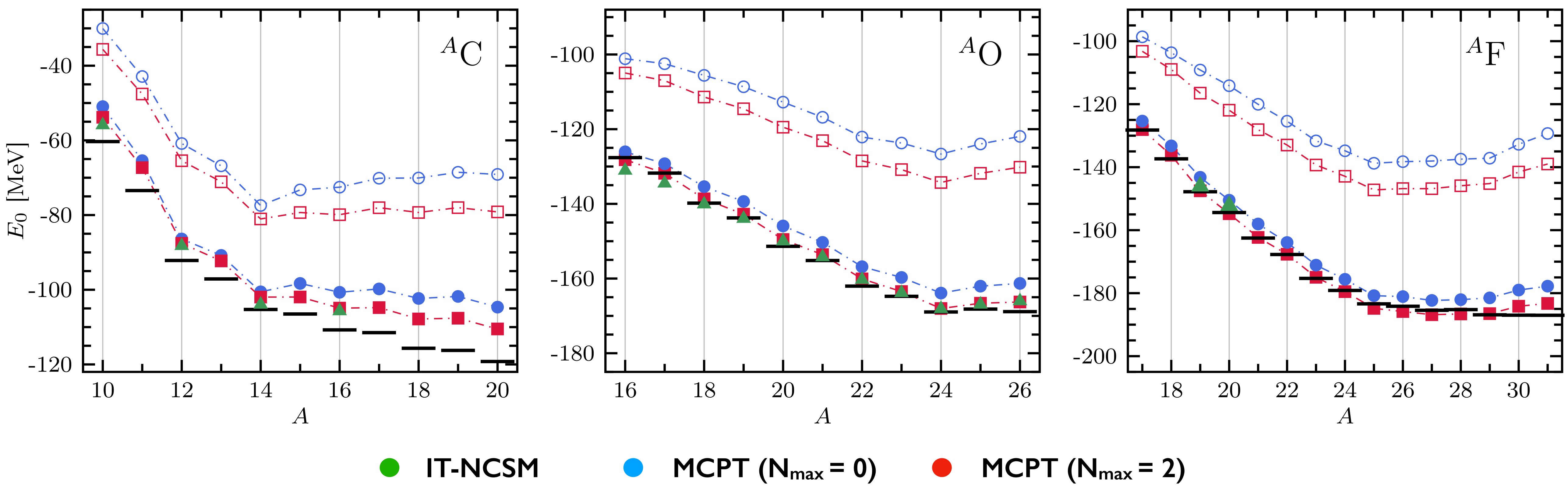
Chiral NN+3N Hamiltonian
4 major shells (140 s.p. states)
N_{max} = 4
SRG parameter α = 0.08 fm⁴
Møller-Plesset partitioning
NCSM reference state with N_{max}=0

MBPT for NCSM states:
'PT expansion with respect to multi-determinantal reference state'

- Exponential convergence of MCPT expansion for various nuclei and targeting states
- Converged results agrees up to numerical accuracy with exact no-core-shell model limit
- NCSM reference state capture static correlations in open-shell nuclei (and lift the degeneracy)

Frontiers in MBPT

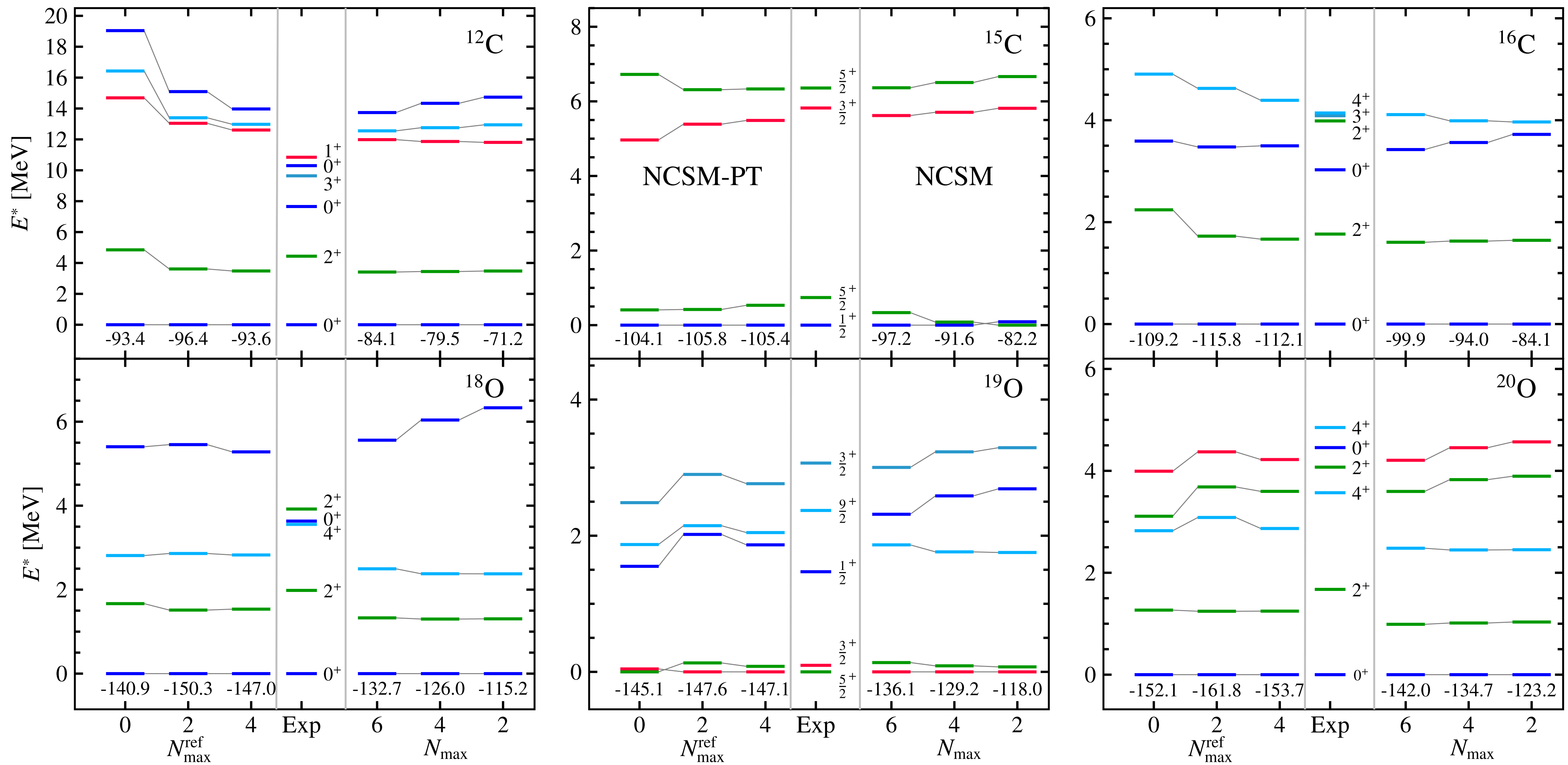
Tichai, Gebrerufael, Vobig, Roth, PLB 786 448-452 (2018)



- Excellent reproduction of ground-state energies obtained from large-scale IT-NCSM
- MCPT enables for description of even and odd systems due to working within *m*-scheme
- Better agreement when enlarging the variational space for the construction of reference states
- MCPT calculations require two orders of magnitude less computational resources

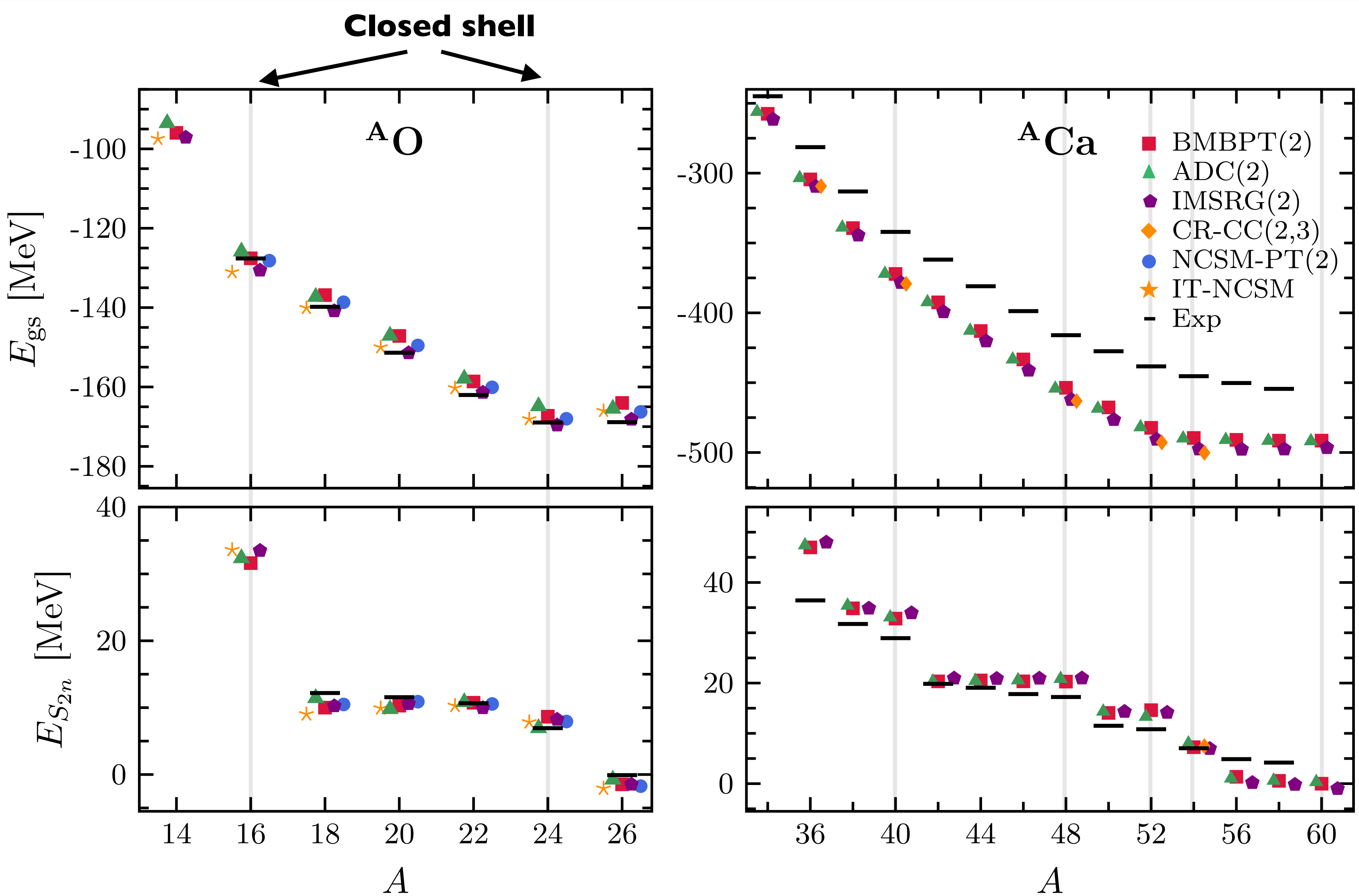
Frontiers in MBPT

Tichai, Gebrerufael, Vobig, Roth, PLB 786 448-452 (2018)



- **Good agreement** of level orderings and excitation energies obtained from IT-NCSM
- Enlargement of reference space necessary to obtain correct *J* for the ground-state of ^{19}O

Frontiers in MBPT



Calculation details

Chiral NN+3N Hamiltonian
NO2B approximation
SRG: $\alpha = 0.08\ \mathrm{fm}^4$
13 major shells (1820 s.p. states)
canonical HFB reference

Runtime

NCSM:	20.000 hours
MCPT:	2.000 hours
IMSRG:	1.500 hours
ADC:	400 hours
BMBPT:	**< 1min !**

Tichai *et al.*, PLB **786** 195 (2018)

- Excellent agreement of all methods with 'exact' results (IT-NCSM)
- Different truncation schemes yield consistent description of open-shell nuclei
- BMBPT is optimal for cheap survey calculations of next-generation chiral Hamiltonians