Nuclear many-body formalisms and (classical) computation

ESNT workshop
Quantum computing and scientific research:
State of the art and potential impact in nuclear physics

Alexander Tichai

CEA Saclay

Duguet, Signoracci, (2017), Journal of Physics G 44, 015103
Tichai, Arthuis, Duguet, Hergert, Somà, Roth, Phys. Lett. B 786 (2018)
Arthuis, Duguet, Tichai, Lasseri, Ebran, CPC 240C (2019)
Tichai, Ripoche, Duguet, (2019), in preparation

Outline

Part I - Nuclear structure and computational complexity

- Theoretical uncertainties and the nuclear Hamiltonian
- Softening techniques and normal ordering
- Many-body complexity and ways around it

Part II - Symmetry breaking in *ab initio* many-body theory

- Horizontal and vertical expansion schemes
- Quasi-particle representations and Bogoliubov many-body frameworks
- Numerical results for open-shell nuclei

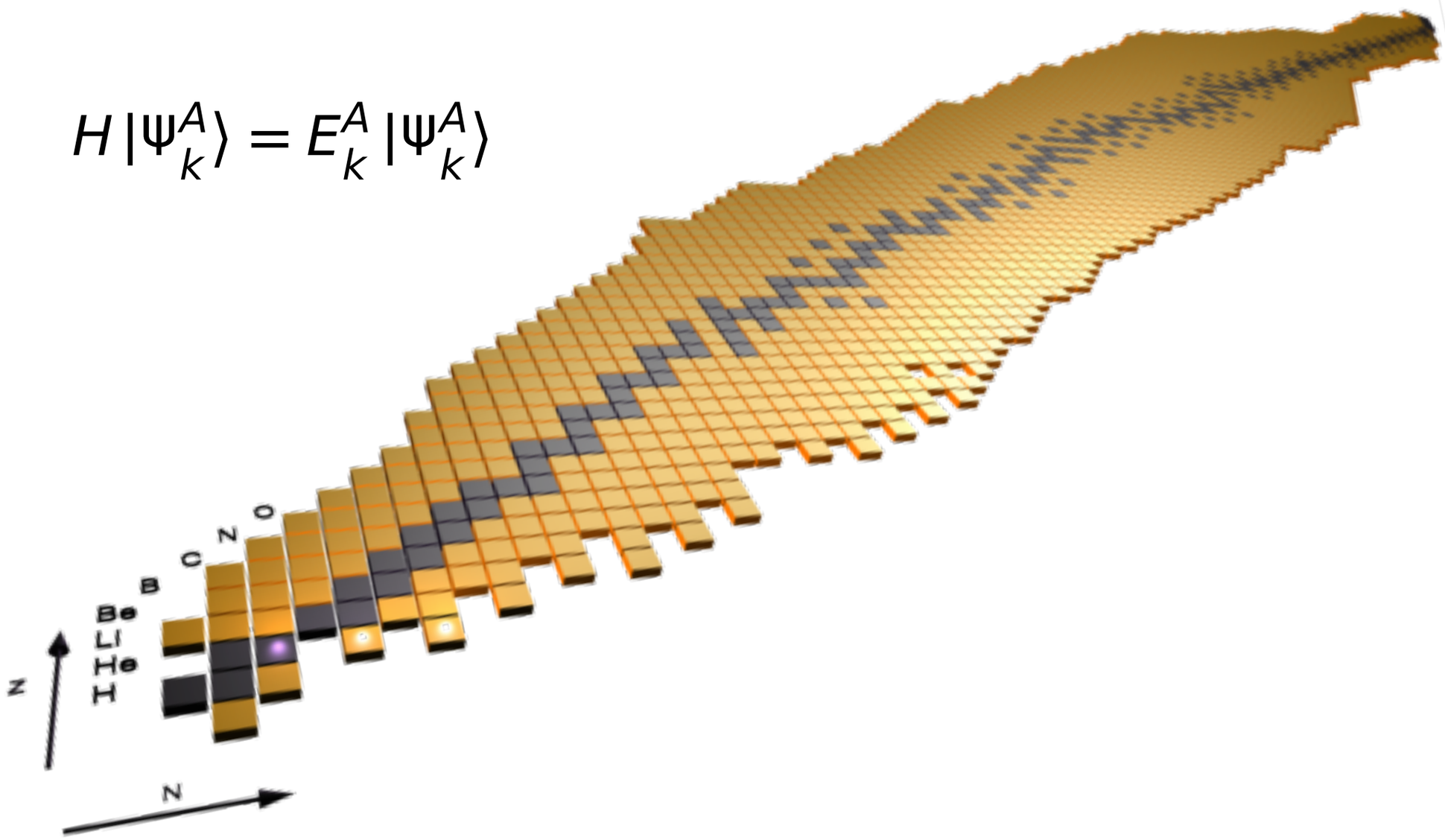
The nuclear Many-body Problem

Part I
Recent challenges in *ab initio* nuclear structure

Theoretical uncertainties

Ab Initio **('From first principles'):**
'The approximate solution must be systematically improvable and approach the exact solution in a well-defined way.'

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



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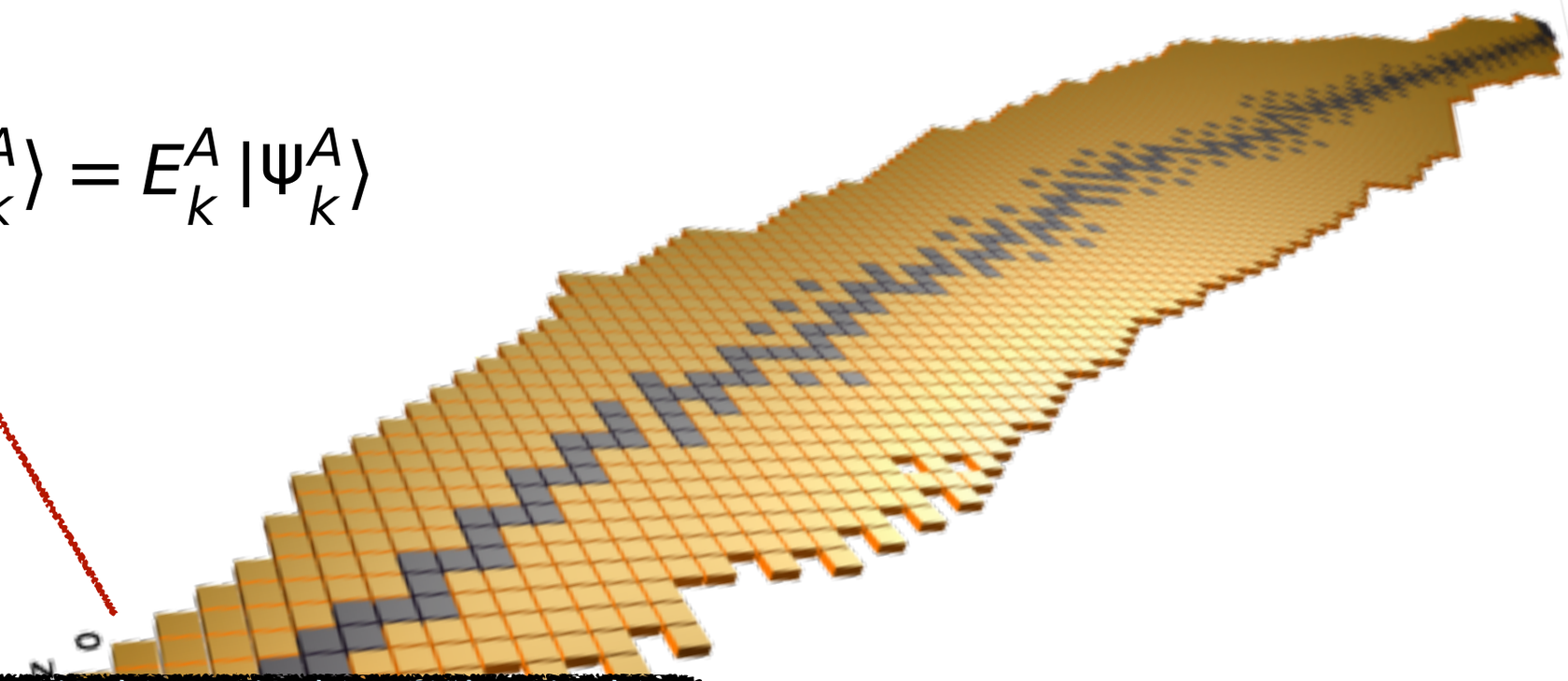

Input Hamiltonian

- What is the form of $V^{2N}, V^{3N}, \ldots$?

$$H = T + V^{2N} + V^{3N} + \ldots + V^{AN}$$

- How do they emerge from QCD?
- Uncertainties from (S)RG transformations

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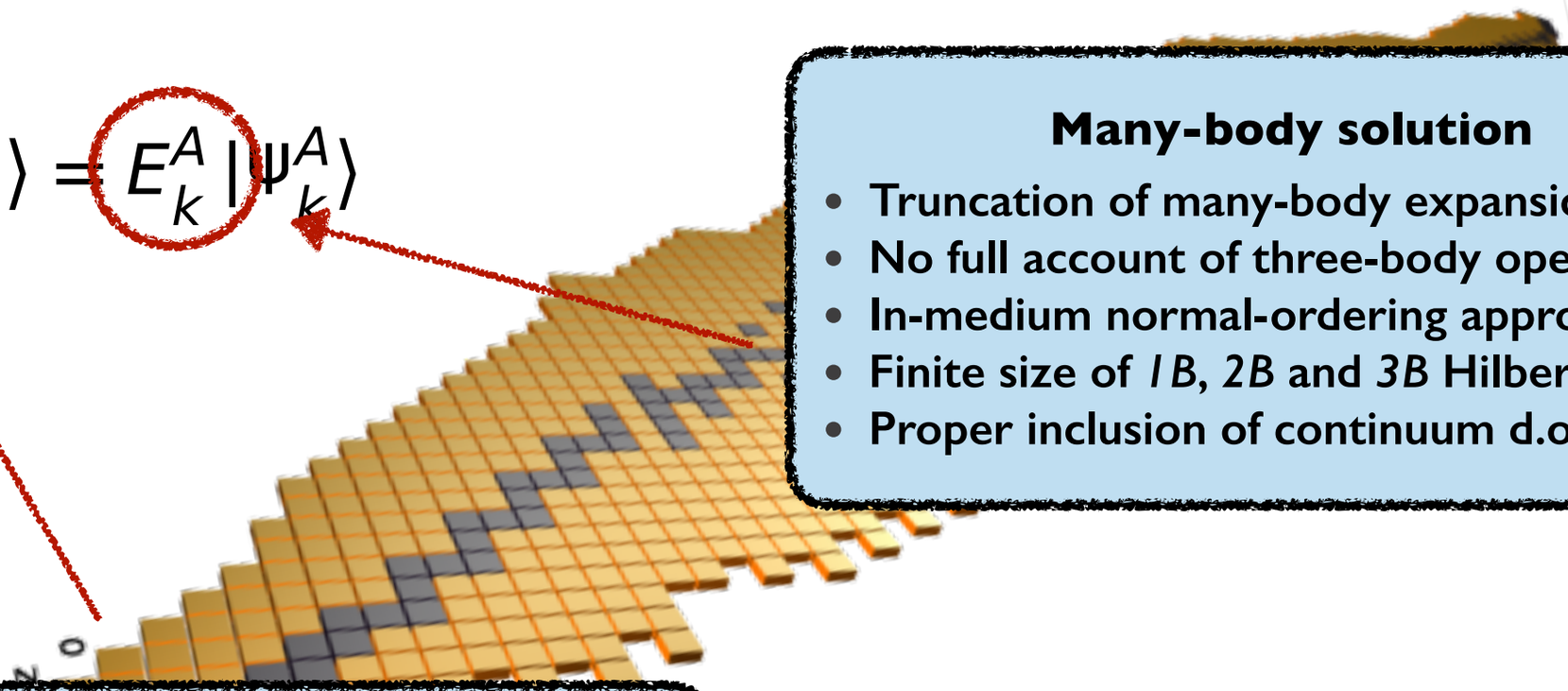

Many-body solution

- Truncation of many-body expansion
- No full account of three-body operators
- In-medium normal-ordering approximation
- Finite size of *1B*, *2B* and *3B* Hilbert space
- Proper inclusion of continuum d.o.f.

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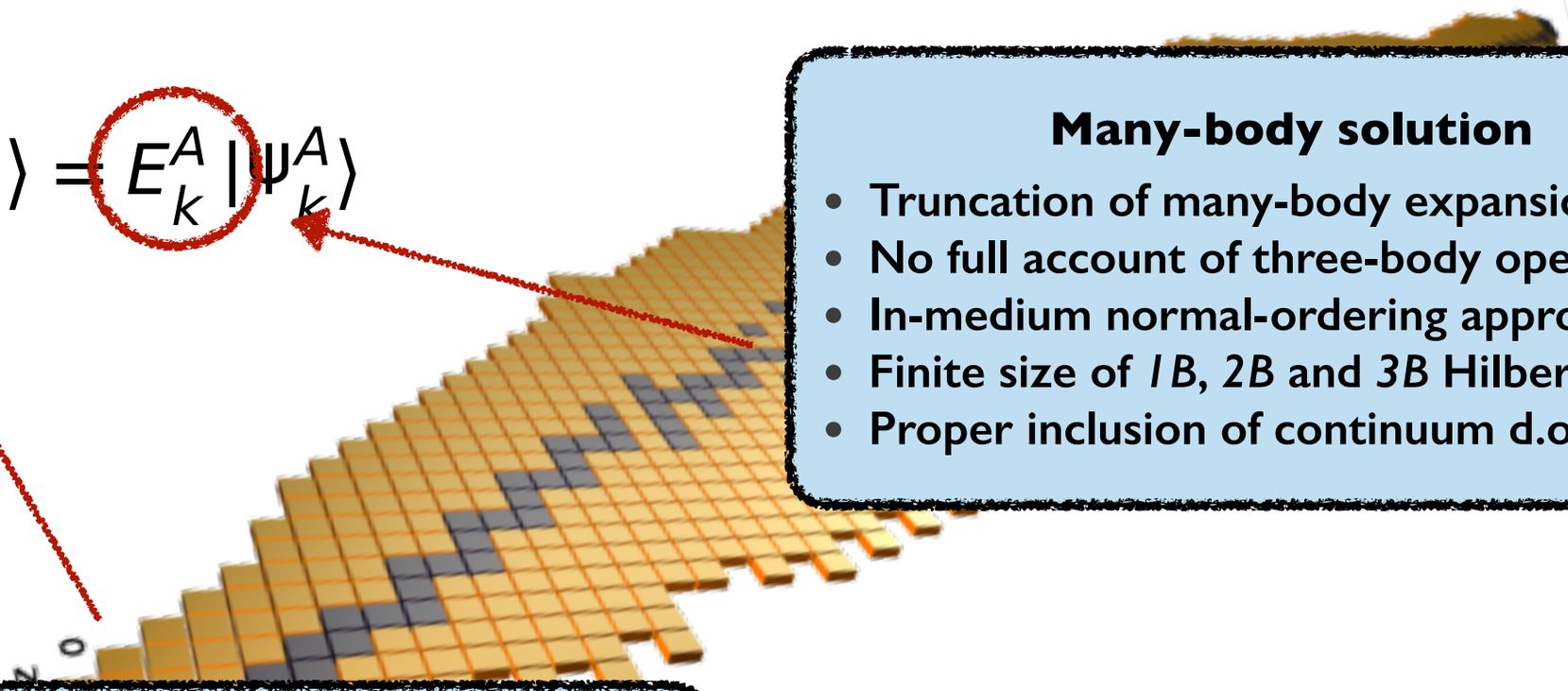

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Typical error on observables

- Hamiltonian (10 - 20 %) in mid-mass region
- Many-body truncation (3 - 5 %)
- Model-space truncation effects (1 %)

Ab initio Hamiltonians - chiral EFT

- Explicit framework to construct *A*-body forces (*A*=2,3,…) linked to QCD symmetries
- Basic idea: employ the separation of scales in low-energy nuclear structure

Typical momentum at play

$$\frac{Q}{\Lambda}$$

High-energy scale
(not included explicitly)

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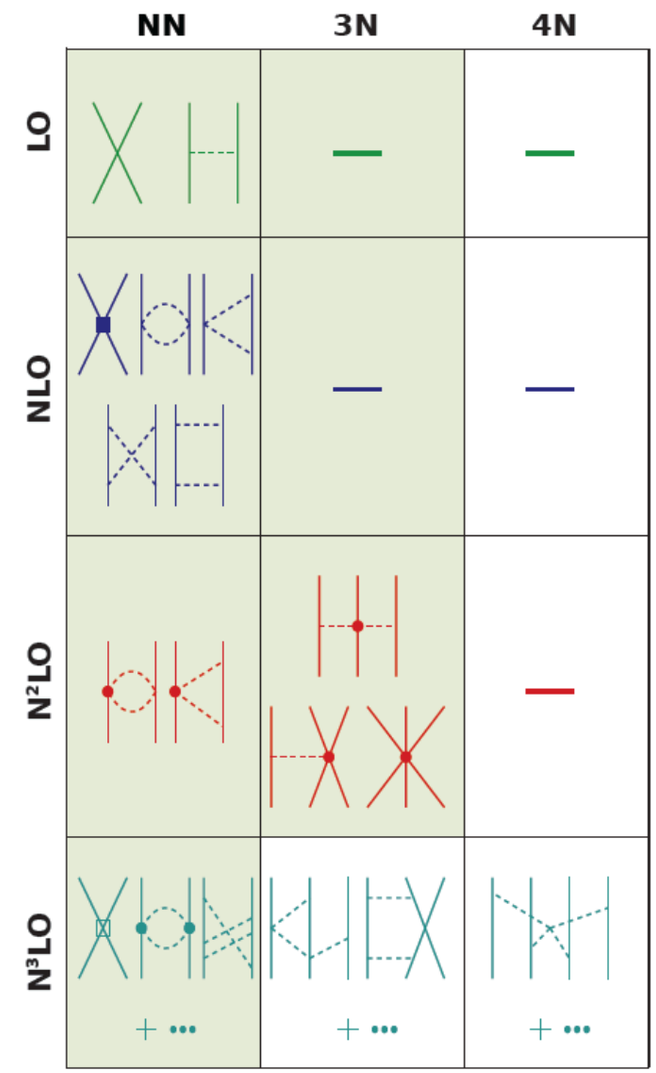
- Parametrize physics beyond Λ and write all terms allowed by symmetries of underlying theory
- Systematic expansion from ordering all possible terms according to their size ('power counting')
- Truncation at given order and adjust low-energy constants (LEC's) to data (experiment or lattice QCD)

Systematic error analysis possible (in principle)!



Weinberg, van Kolck, Machleidt, Entem, Meißner, …

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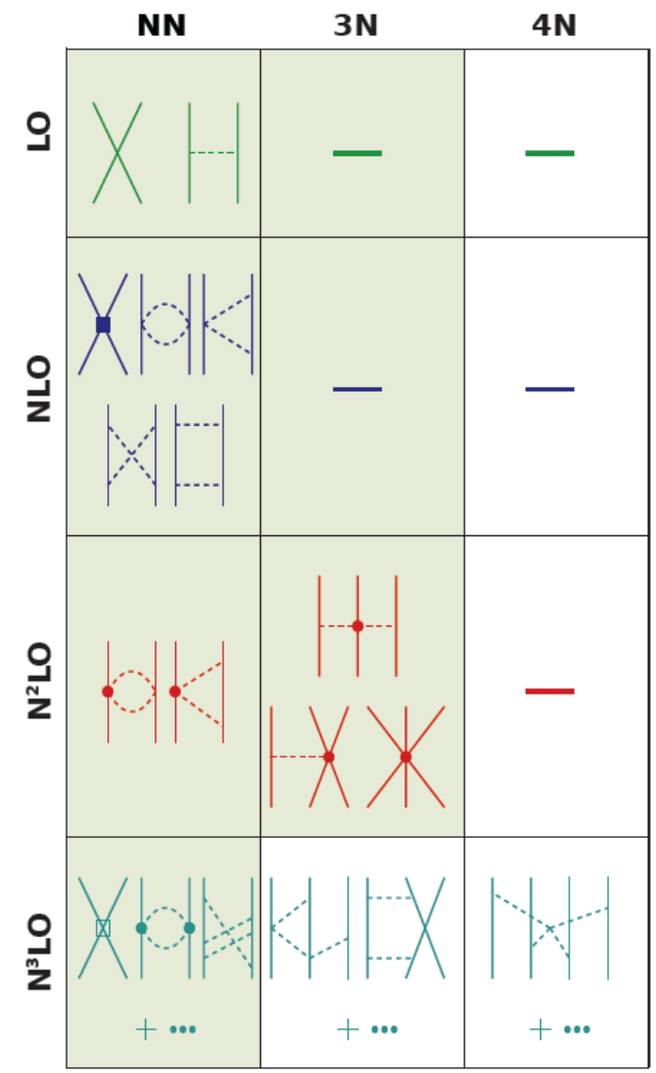
- Key differences compared to electronic structure problem
  - Basis size can be significantly larger (~2000 basis functions)
  - Irreducible three-body operators are important
  - Interaction contains non-central parts (spin-orbit, tensor, …)
  - Almost all nuclei are of open-shell character!



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Similarity renormalization group

- Perform pre-diagonalization via unitary transformation: $\hat{H}_\alpha = \hat{U}_\alpha^\dagger \hat{H} \hat{U}_\alpha$
- Recast into a set of first-order differential equations for anti-Hermitian dynamic generator

$$\frac{d}{d\alpha}\hat{H}_\alpha = \left[\hat{\eta}_\alpha, \hat{H}_\alpha\right] \qquad \hat{\eta}_\alpha = (2\mu)^2 \left[\hat{T}_{\text{int}}, \hat{H}_\alpha\right]$$

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- Tradeoff: induces many-body operators

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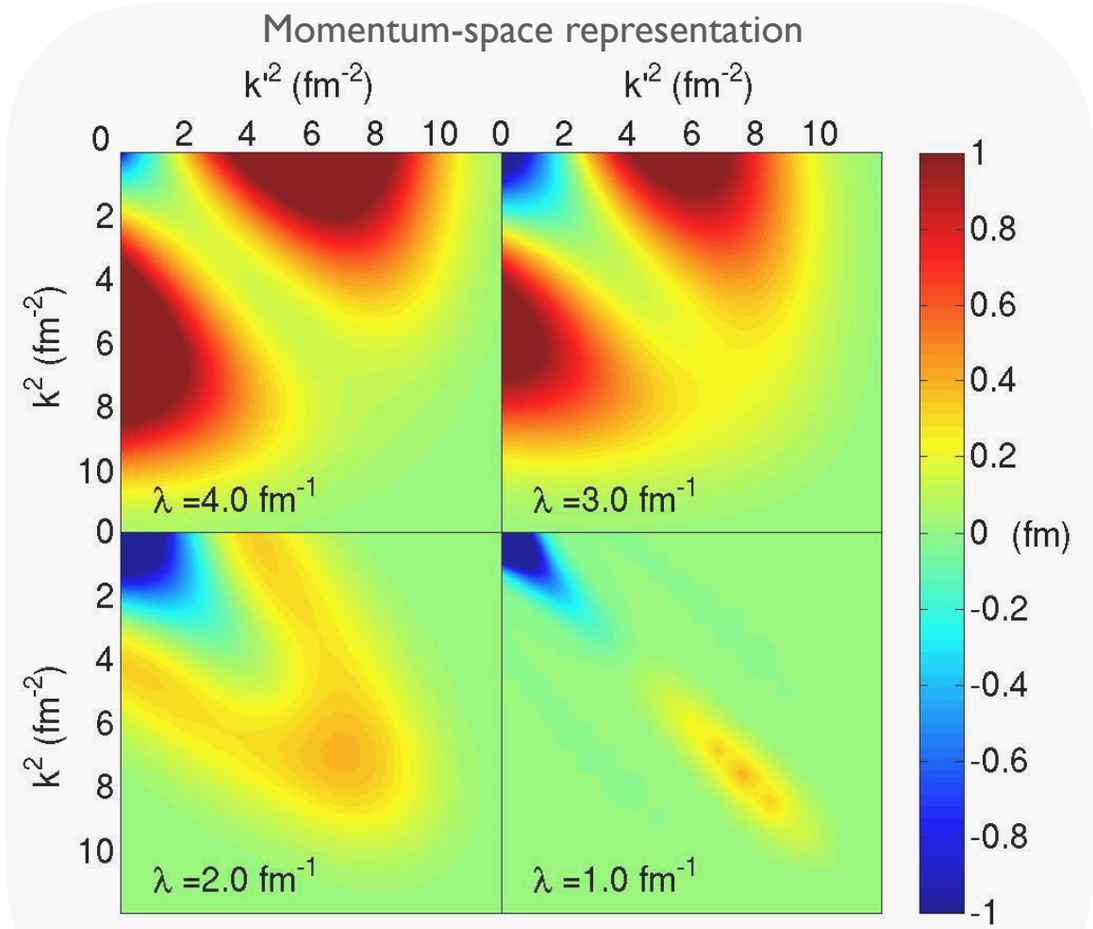

Bogner *et. al.*, **PRC** 75 (2007) 061001

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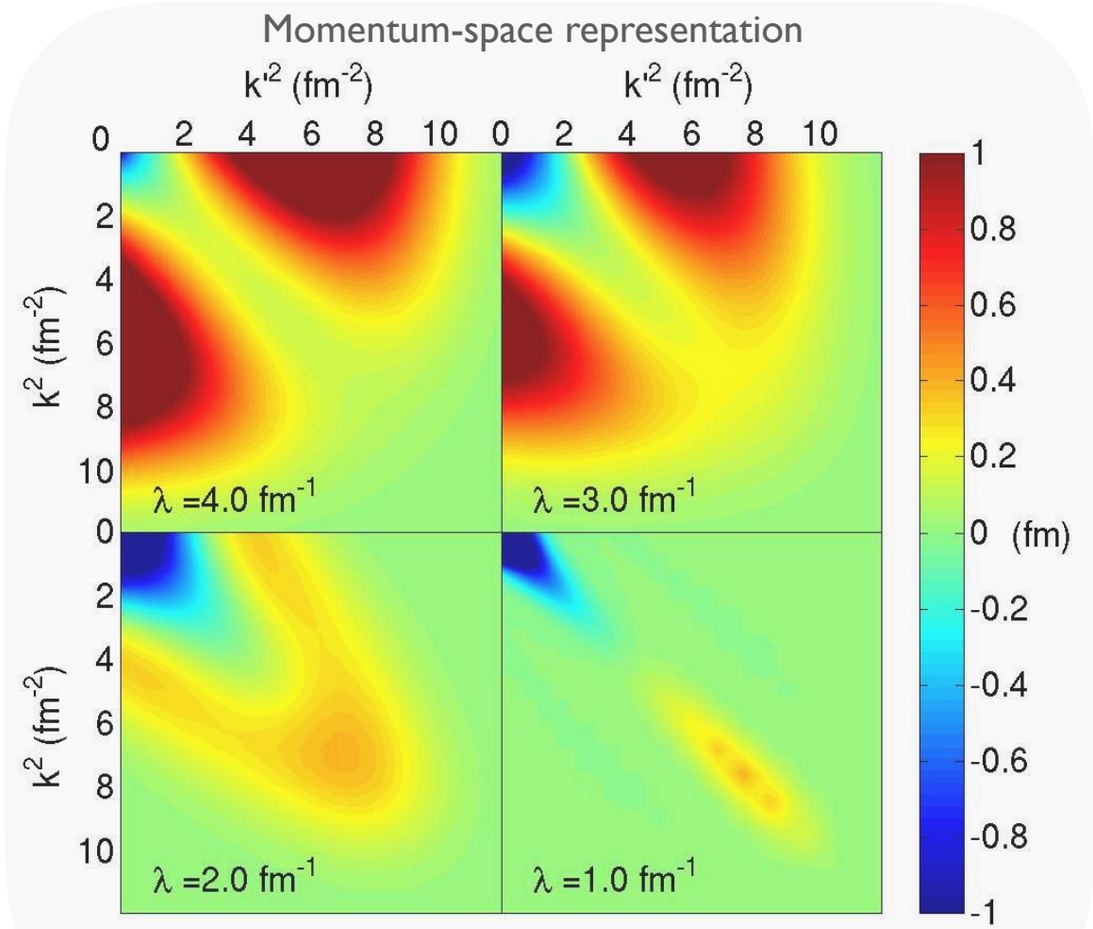
- Soft interaction: faster MBPT convergence



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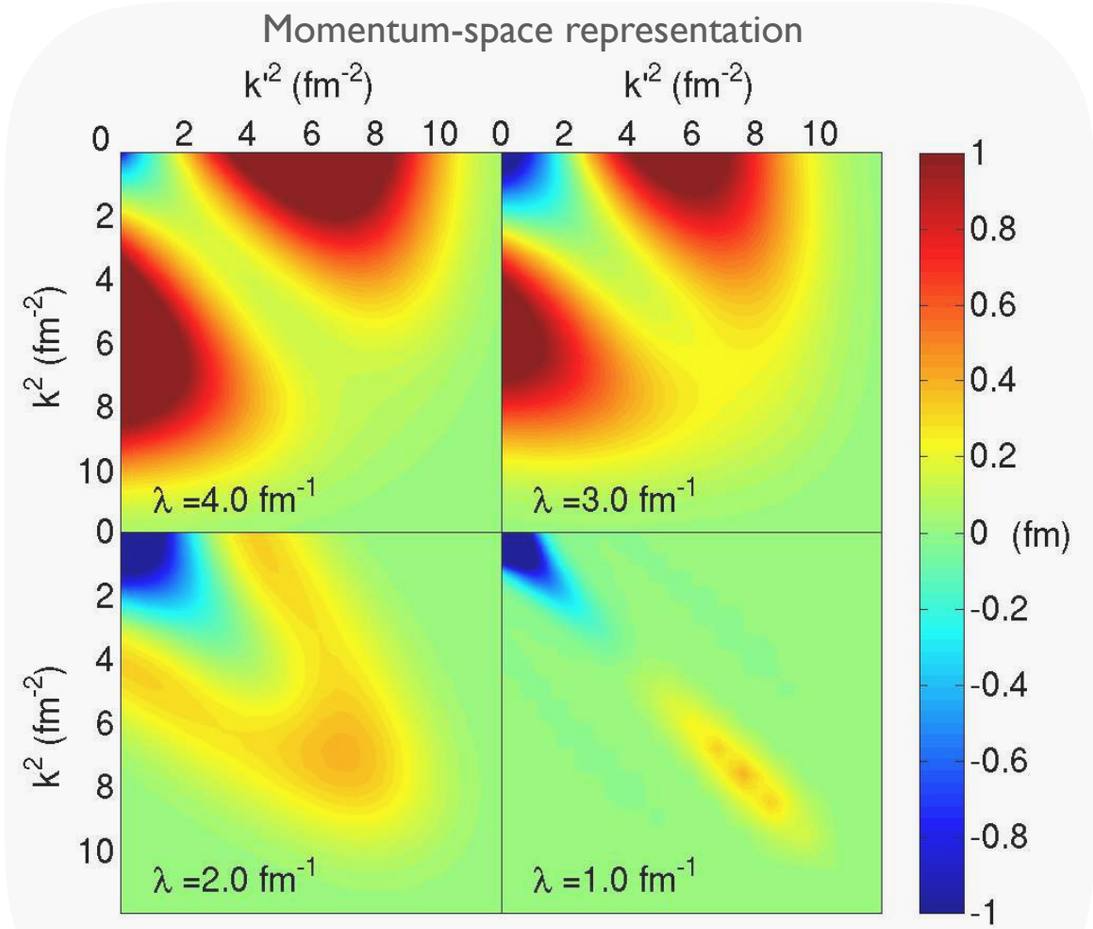
- Lift to many-body framework by in-medium decoupling of ph-excitations from vacuum

In-medium
Similarity Renormalization Group



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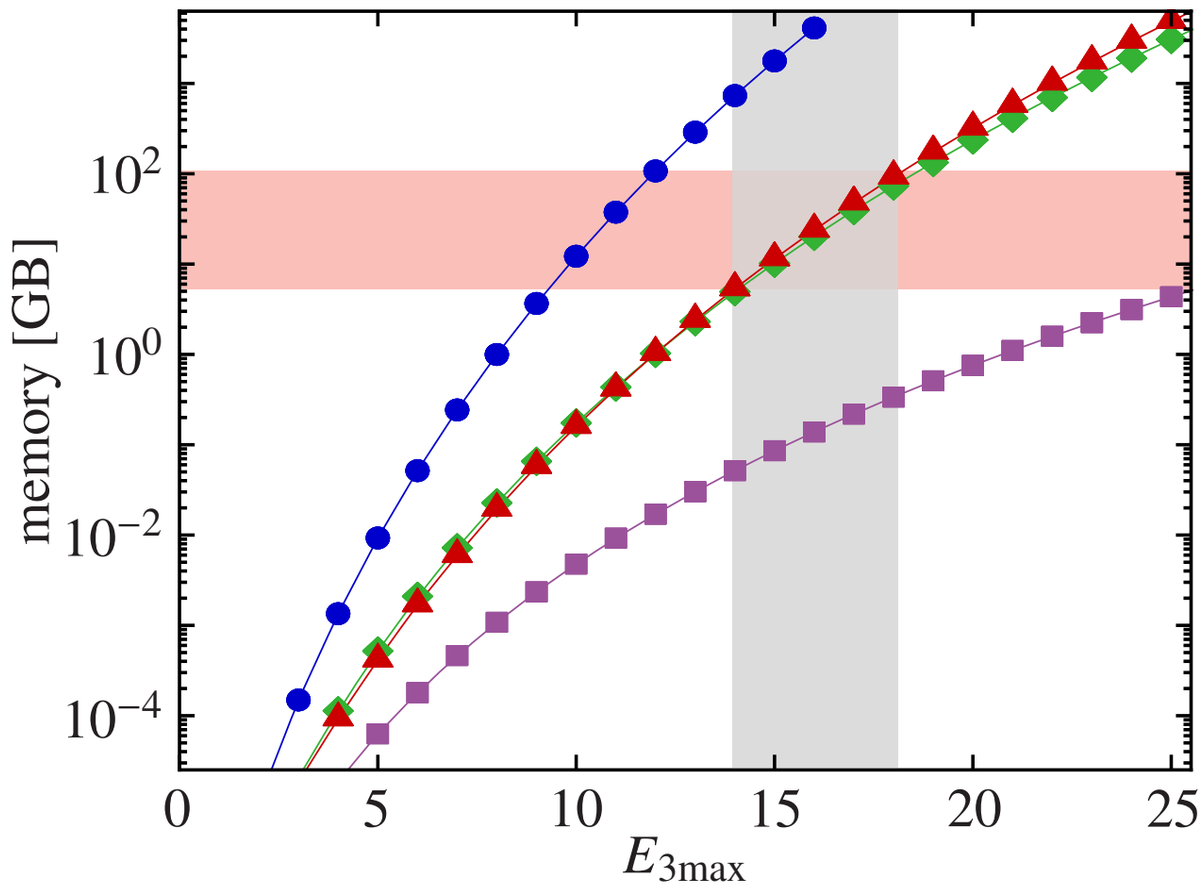
Dimensionality of many-body operators



Roth *et al.*, PRC **90** 024325

Storage schemes

- M-scheme
- J-scheme
- JT-scheme
- Jacobi basis

Truncation in 3B space

$$e_{k_1} + e_{k_2} + e_{k_3} \leq E_{3\max}$$

- Storage of full three-body basis is computationally out of reach (even in coupled form)
- Additional 3B truncation penalizes configurations with highly excited single-particle states
- In large-scale applications 3B matrix element files can be 100 Gb in size
- Benchmark from full diagonalization in light systems: 4B effects are small (≈100 keV in He^4)

We do not know the size of 4B forces in medium-mass systems!

Normal-ordering approximation

- A full inclusion of three-body operators in a correlation expansion is very expensive
- Rewriting of three-body operator in normal-ordered form w.r.t. *A*-body reference state

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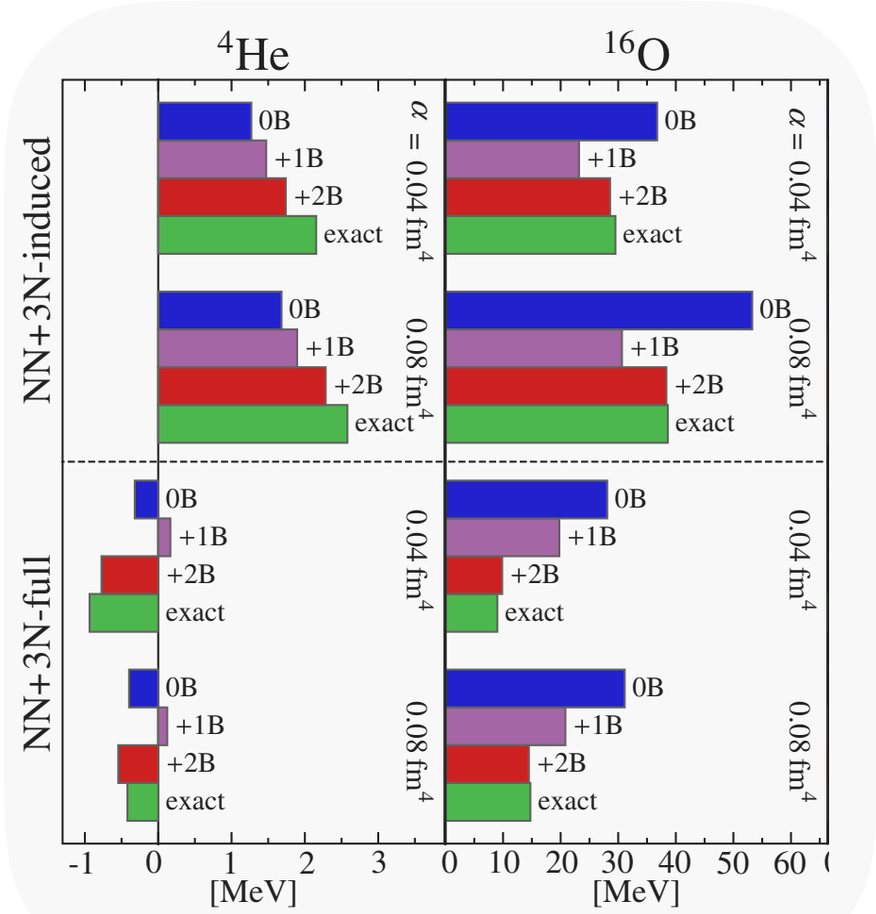

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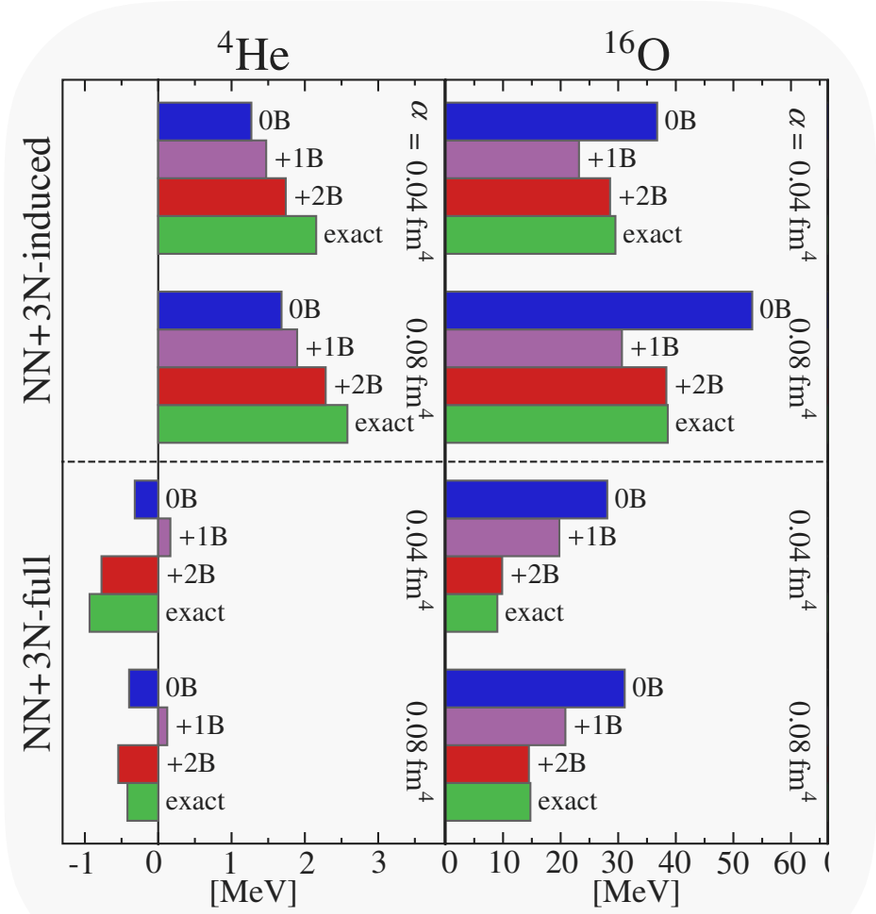

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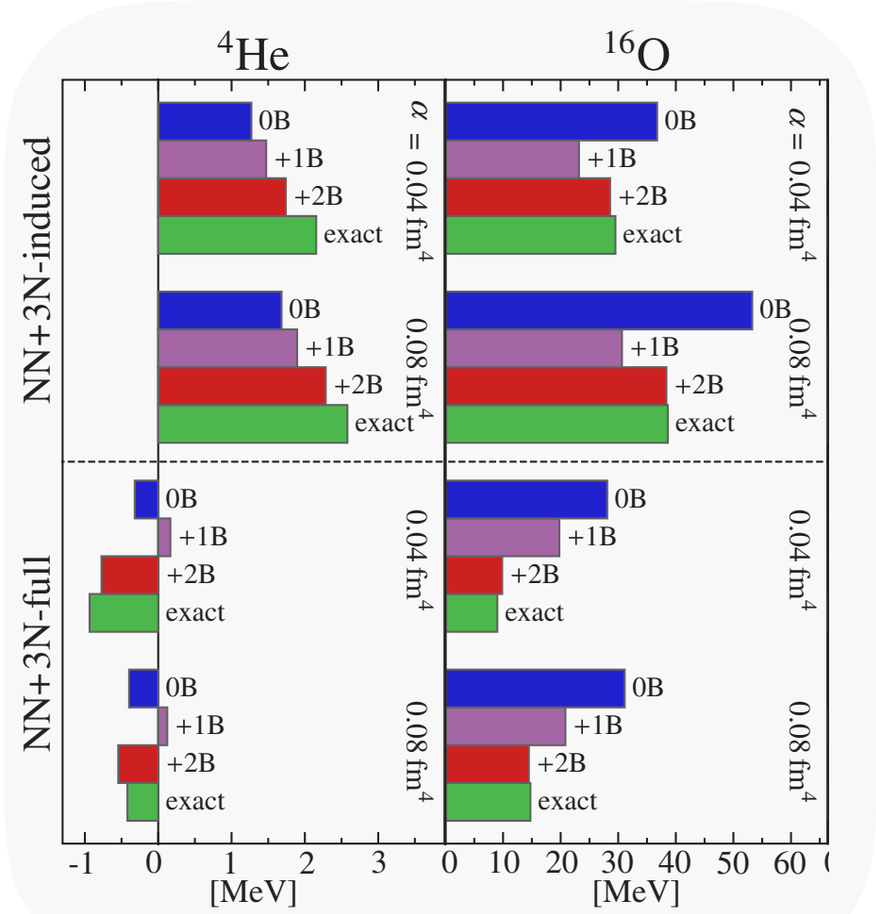
- Extended normal ordering for multi-configurational vacua

Mukherjee-Kutzelnigg formalism



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Tensors and many-body theory

- **Many-body calculations employ mode-*n* tensors and compute tensor networks (TN)**

1) Input

$$H_{\rm nucl} = \frac{1}{(1!)^2}\sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{(2!)^2}\sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2}\sum_{pqrstu} \bar{w}_{pqrstu} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

storage cost N^k (here k=2,4,6)

2) Output

CC: $$E_0 = E_0^{\rm HF} + \frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_i^b + \frac{1}{4}\sum_{ijab} \bar{v}_{ijab}\, t_{ij}^{ab}$$

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  - Going to larger model spaces for many-body operators: increase N
  - Relaxing many-body truncations yielding higher-mode tensors: increase k and p
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- **Example**: α-clustering in deformed basis from coupled cluster theory up to quadruples (CCSDTQ)

Storage of 10^{17} tensor entries: 10^6 Tb in ^{12}C

How large is Hilbert space really?

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

$$\left\{|\Phi_{i_1}^{a_1}\rangle, |\Phi_{i_1 i_2}^{a_1 a_2}\rangle, \ldots, |\Phi_{i_1 \ldots i_k}^{a_1 \ldots a_k}\rangle\right\} \longrightarrow N^2, N^4, \ldots, N^{2k}$$

Exponentially many degrees of freedom

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- Pre-selection of relevant Hilbert-space elements

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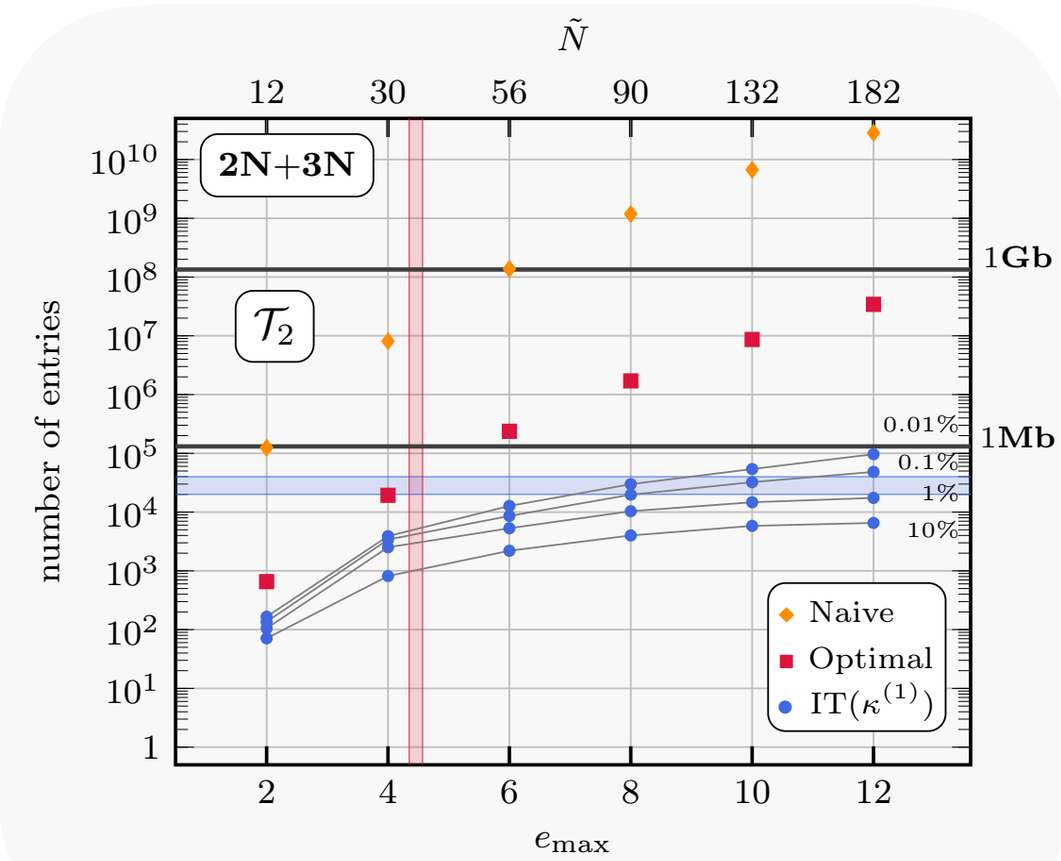
- Restrict summation in TN to important states

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

- 99.9 % accuracy with 0.1% of configurations!



Tichai, Ripoche, Duguet, EPJA 55: 90 (2019)

How large is Hilbert space really?

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

$$\left\{|\Phi^{a_1}_{i_1}\rangle, |\Phi^{a_1 a_2}_{i_1 i_2}\rangle, \ldots, |\Phi^{a_1 \ldots a_k}_{i_1 \ldots i_k}\rangle\right\} \longrightarrow N^2, N^4, \ldots, N^{2k}$$

Exponentially many degrees of freedom

- The full CI wave function can never be stored in medium-mass systems
- Often the largest part of Hilbert space is (almost) irrelevant for nuclear observable
- Pre-selection of relevant Hilbert-space elements

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

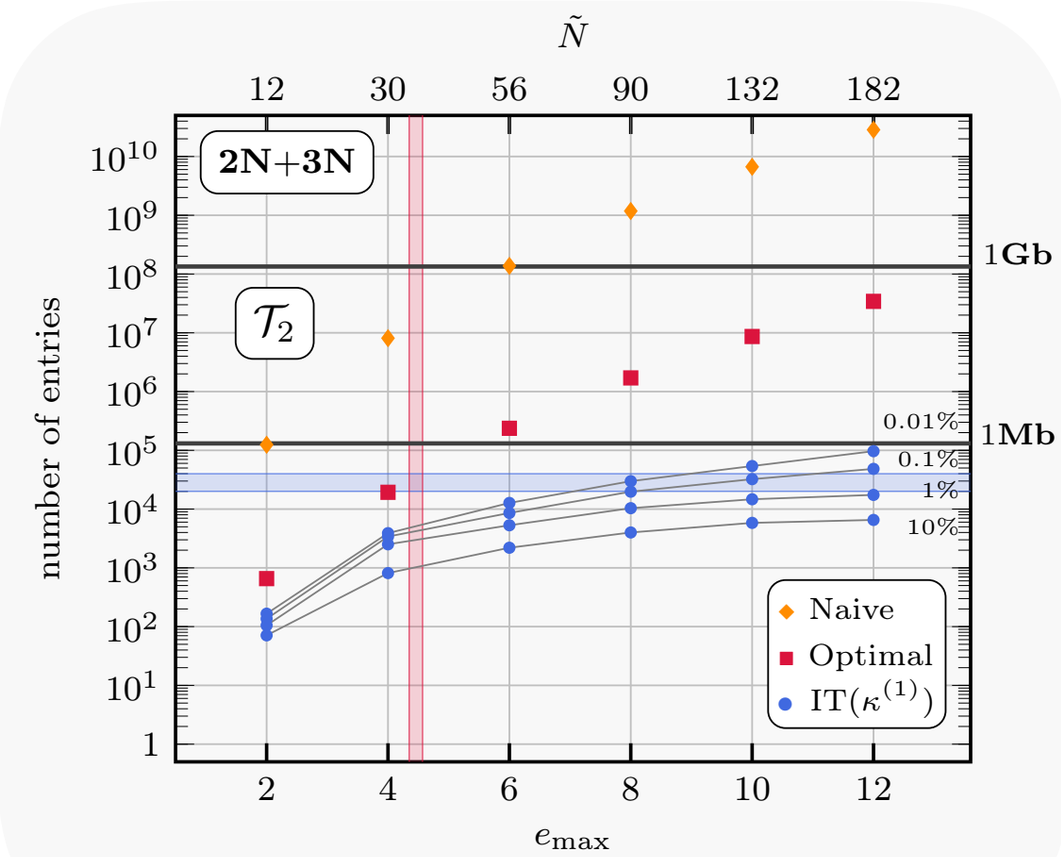
A priori importance measure
(typically based on MBPT arguments)

- Restrict summation in TN to important states

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

- 99.9 % accuracy with 0.1% of configurations!
- Refined selection in chemistry from Monte Carlo

Deustua, Shen, Piecuch, PRL **119**, 223003



Tichai, Ripoche, Duguet, EPJA 55: 90 (2019)

Symmetry breaking in *ab initio* nuclear structure

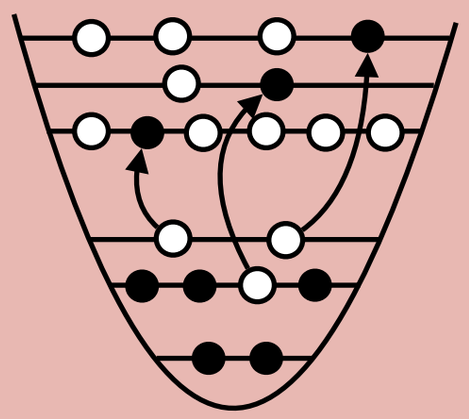
Part II
Open-shell nuclei from symmetry-broken correlation expansions

Tichai, Arthuis, Duguet, Hergert, Somà, Roth, Phys. Lett. B 786 (2018)
Arthuis, Duguet, Tichai, Lasseri, Ebran, CPC 240C (2019)
Qiu, Henderson, Duguet, Scuseria, PRC **99**, 044301 (2019)

Many-body expansions

Vertical expansion

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



- Goal: determine wave-function coefficients

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

- Intrinsic hierarchy arising from excitation rank
- Large variety of different expansion schemes

  MBPT or CC, CI, IMSRG, SCGF

- Collectivity is complicated to account for!
- Historically preferred strategy in *ab initio* theory

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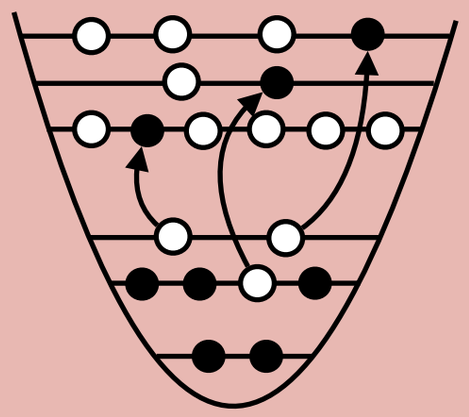

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Horizontal expansion

- Authorize breaking of symmetry group *G*

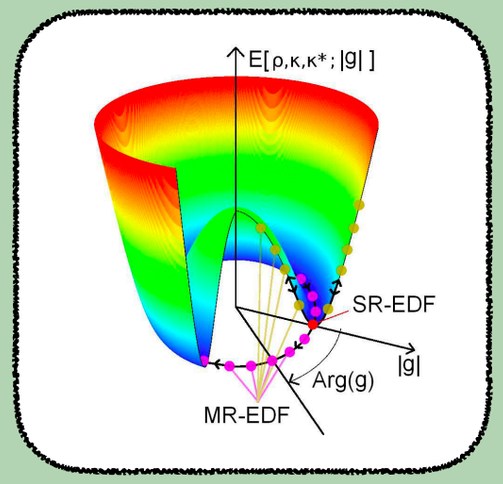
  U(1) : pairing correlations (superfluidity)

  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



- Configuration mixing within GCM framework
- Historically preferred strategy in EDF theory

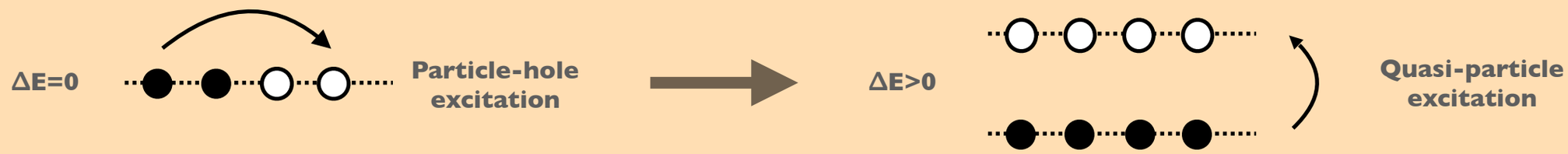
Many-body expansions

Combined expansion

- Generation of a symmetry-broken vacuum from a deformed mean-field calculation using input Hamiltonian
- Normal-ordering of the initial operators w.r.t. deformed vacuum using (generalized) Wick's theorem

$$O \longrightarrow O_{|\Phi\rangle}$$

- Identification of proper elementary excitations yields well-defined (i.e. non-singular) correlation expansion



- Final projection onto good quantum numbers provides additional inclusion of non-perturbative physics
- Advantage: Multi-step procedure allows for systematic account of static and dynamic correlation effects
- Consistent symmetry-restoration protocol must be designed beyond the mean-field level

This is specific to the <u>many-body method</u> and the <u>symmetry group</u>!

- Useful alternative to formally complicated multi-reference approaches where symmetries are conserved

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

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$$O \equiv \underbrace{O^{00}}_{O^{[0]}} + \underbrace{O^{20} + O^{11} + O^{02}}_{O^{[2]}} + \underbrace{O^{40} + O^{31} + O^{22} + O^{13} + O^{04}}_{O^{[4]}}$$

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- **Quasiparticle matrix elements inherit tensorial properties of the original operators (*J*-coupling)**

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

Bogoliubov coupled cluster

Signoracci, Duguet, Hagen, Jansen, PRC **91**, 064320 (2015)

- **Exponential wave-function parametrization enables for size-extensive many-body scheme**

$$\exp\left(\mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \ldots\right) \qquad \mathcal{T}_k \equiv \frac{1}{(2n)!} \sum_{k_1 \ldots k_{2n}} t_{k_1 \ldots k_{2n}} \beta^\dagger_{k_1} \cdots \beta^\dagger_{k_{2n}}$$

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$$\Delta E = \langle \Phi | \bar{\Omega} | \Phi \rangle \qquad 0 = \langle \Phi^{k_1 k_2 \ldots} | \bar{\Omega} | \Phi \rangle$$

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Qiu, Henderson, Duguet, Scuseria, PRC **99**, 044301 (2019)

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- **Simulation of open-shell nuclei on quantum devices from BUCC ansatz (see talk of Dallaire-Demers)**

Dallaire-Demers *et al.*, arXiv1801.01053

$$|\Psi(\theta)\rangle \equiv \exp\left(i\left(\mathcal{T}(\theta) + \mathcal{T}^\dagger(\theta)\right)\right)|\Phi\rangle$$

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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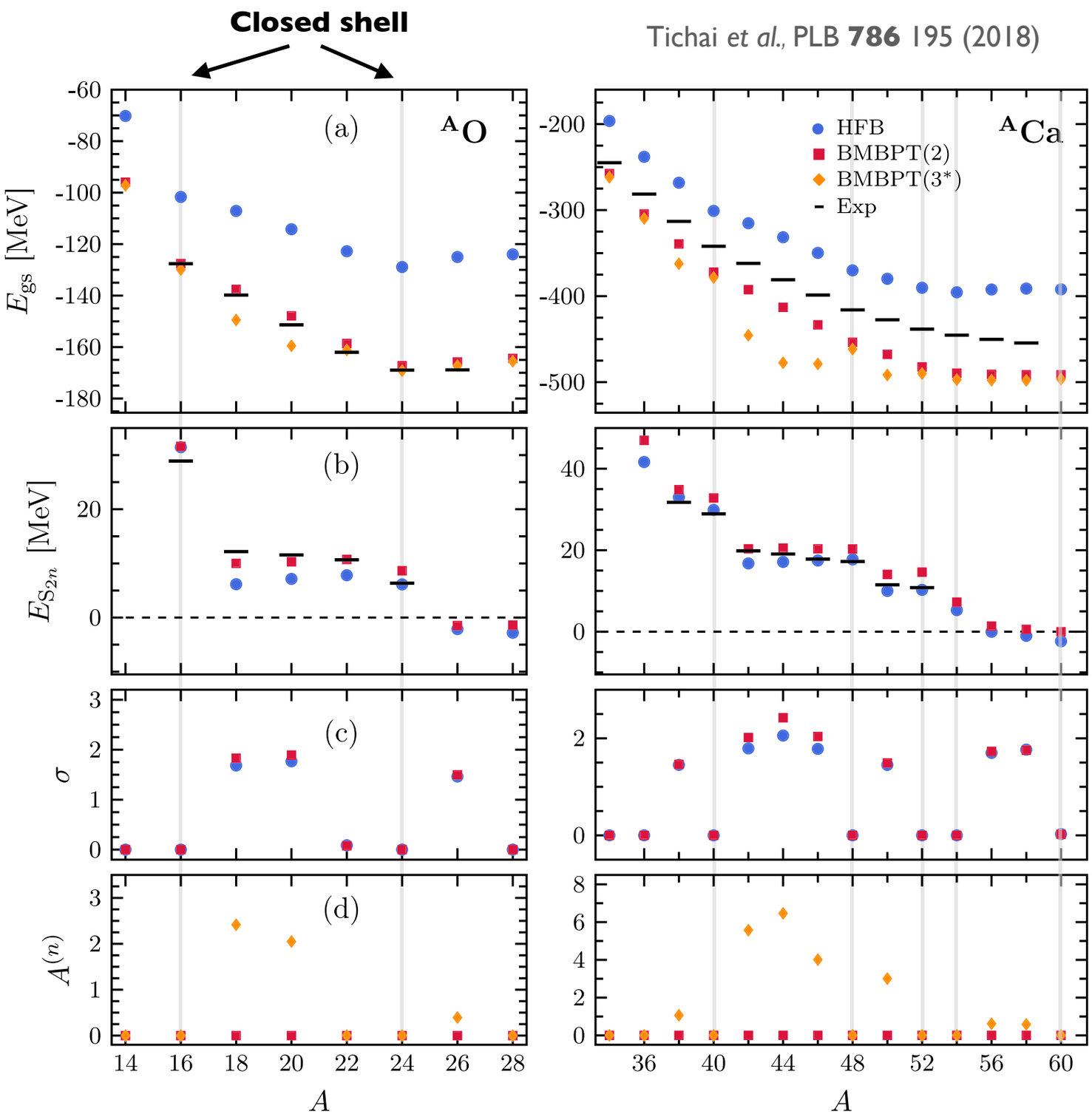
- **All summations run over the entire one-body Hilbert space: no particle and hole states!**

BMBPT - isotopic chains



Calculation details

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

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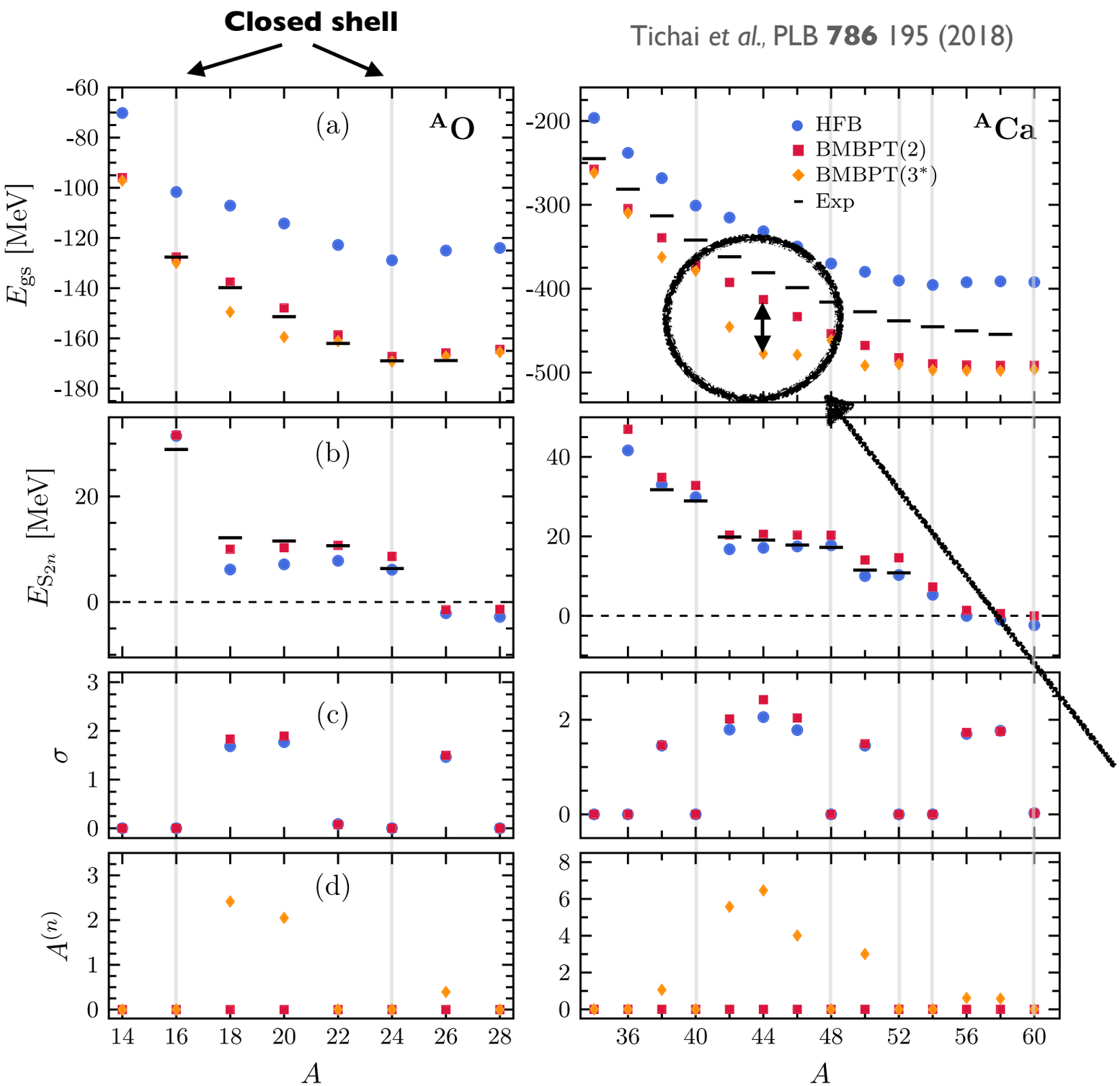

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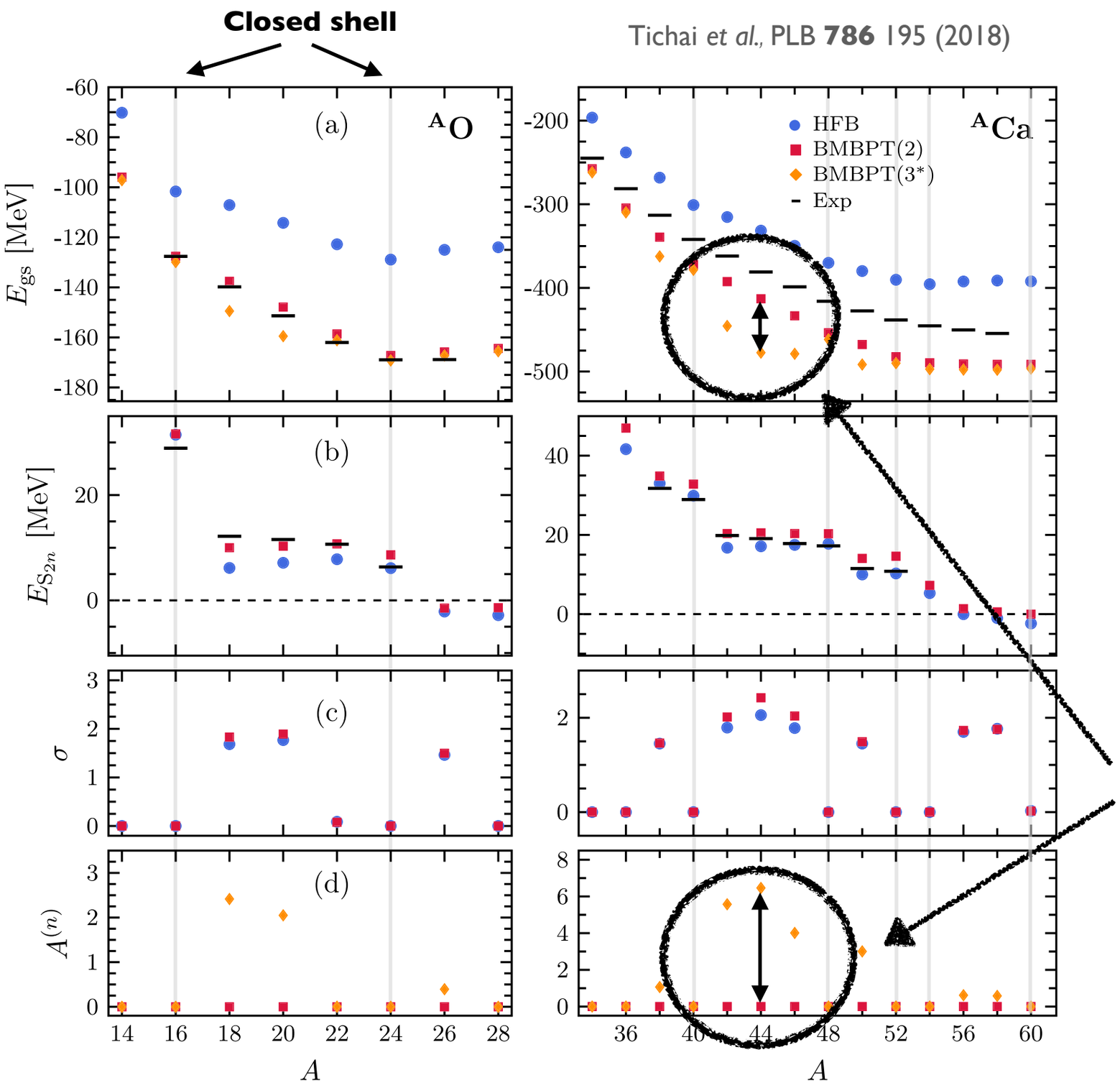
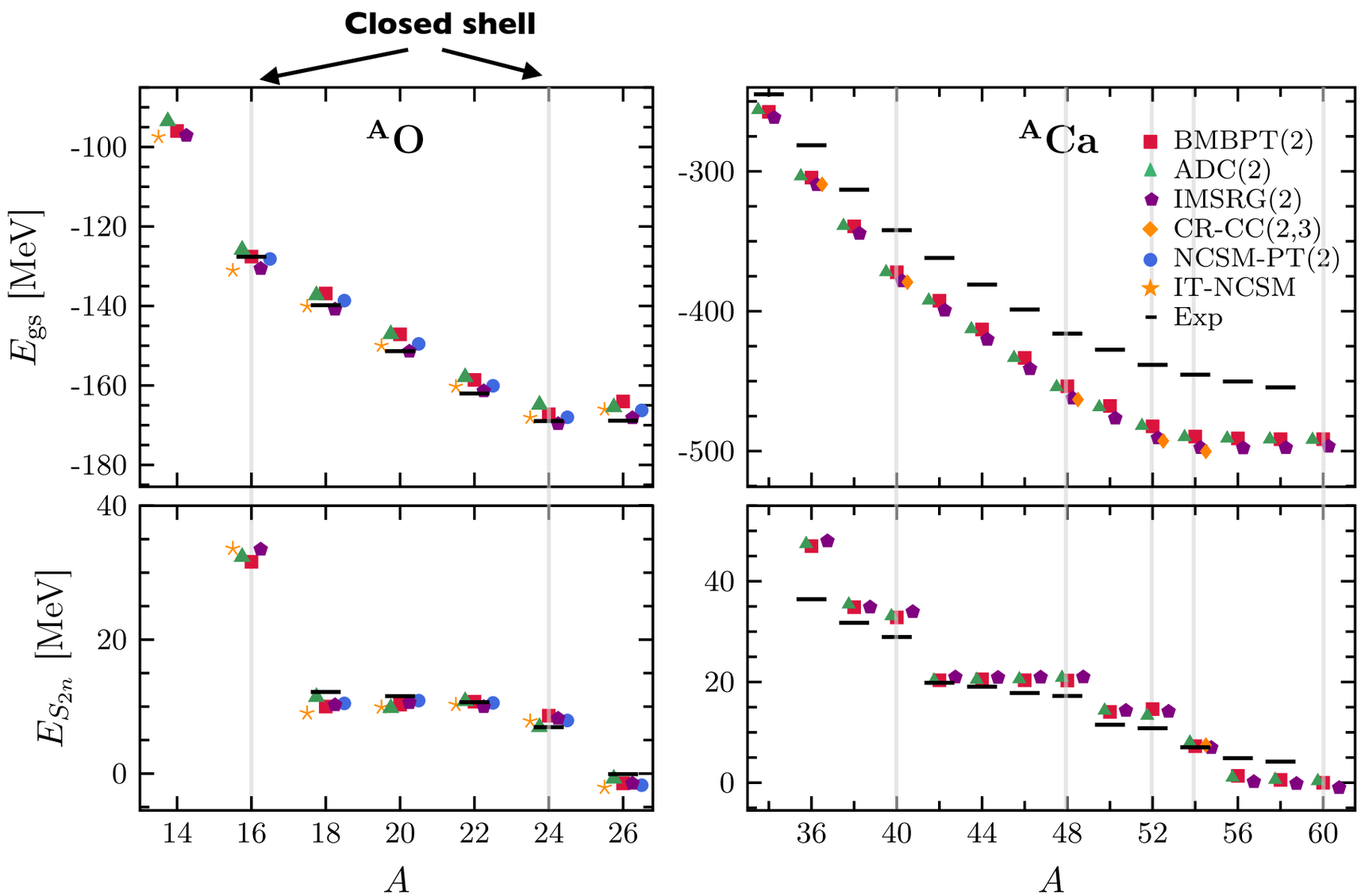


Calculation details

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

- **Bulk correlation effects from second-order energy correction**
- **Symmetry-breaking does not affect quality of separation energies (shell structure)**
- **Shift in particle-number most pronounced in middle of open shells**
- **Deviation from experiment due to defects in Hamiltonian**

BMBPT - consistency and complexity



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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

Symmetry restoration in a nutshell

- **Symmetry-restored observables obtained via action of projection operator P^A**

$$O^{A_0} = \frac{\langle \Psi | O\, P^{A_0} | \Phi \rangle}{\langle \Psi | P^{A_0} | \Phi \rangle} \qquad P^{A_0} = \frac{1}{2\pi} \int_0^{2\pi} e^{i\varphi(A - A_0)} d\varphi$$

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- Off-diagonal operator kernels as central quantities in many-body formalism

$$\mathcal{O}(\varphi) = \langle \psi | O | \Phi(\varphi) \rangle \quad and \quad \mathcal{N}(\varphi) = \langle \psi | \Phi(\varphi) \rangle$$

- Projected observable (for given IRREP A_0) obtained from integration of operator kernels

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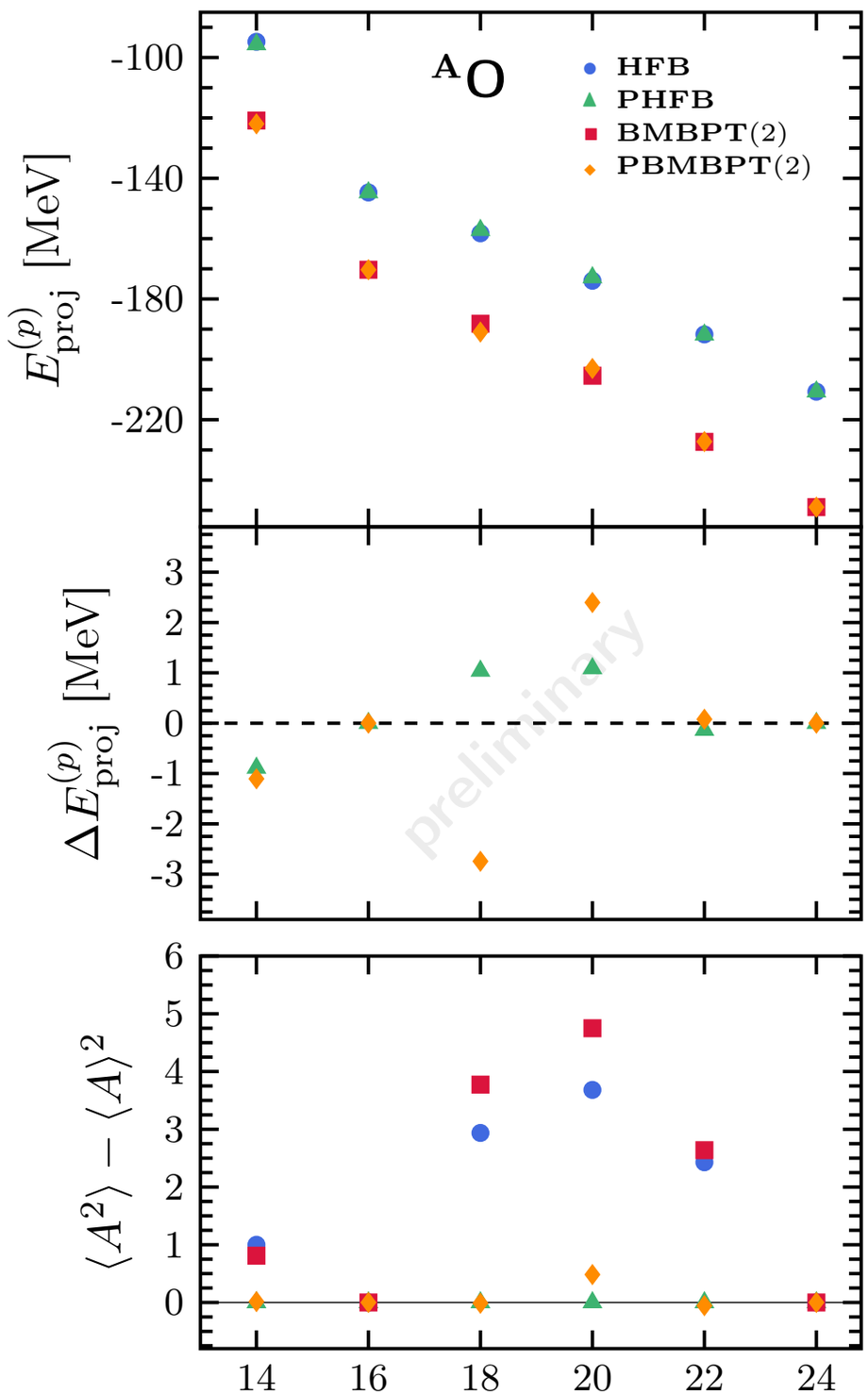
- Value of projected particle number is equal to eigenvalue of target IRREP by construction

Oxygen isotopic chain



Very naive (!) runtime:
300 CPU hours

Correction from projection:

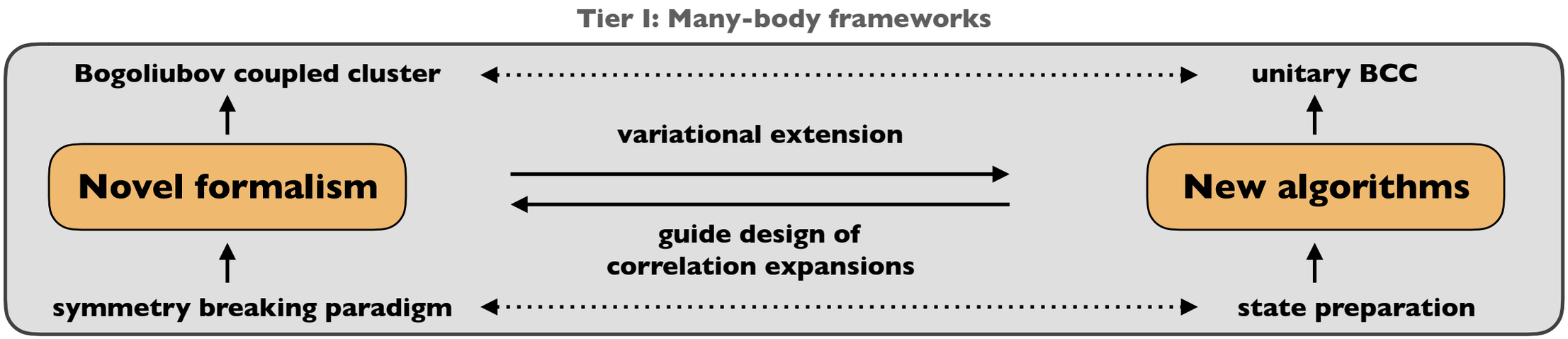
$$\Delta E^{(p)}_{\rm proj} \equiv E^{(p)}_{\rm proj} - E^{(p)}$$

Calculation details

Chiral NN Hamiltonian
SRG: α = 0.08 fm^4
11 major shells (1144 s.p. states)
canonical HFB reference
200 meshpoints

- Additional static correlation effects from projection at mean-field and second order
- Projected particle number yields target IRREP in all cases (sanity check fulfilled!)
- PBMBPT reduces to BMBPT in closed-shell systems (which itself collapses to HFMBPT)
- Proj. PN variance is almost zero in open-shell systems
- Systematic account of non-perturbative physics at low computational cost
- Computational cost is independent of mass number since quasiparticle formulation is employed

Perspectives on quantum computing



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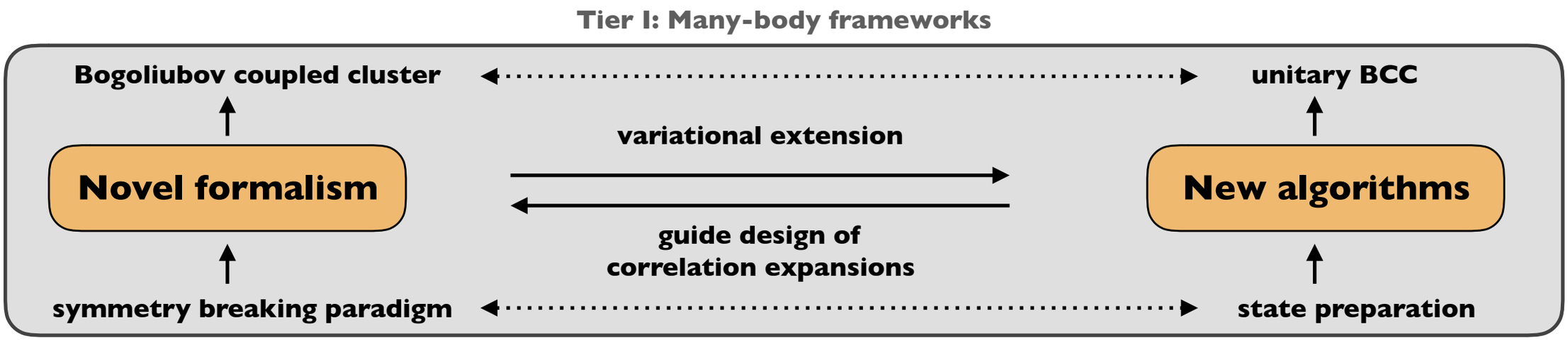

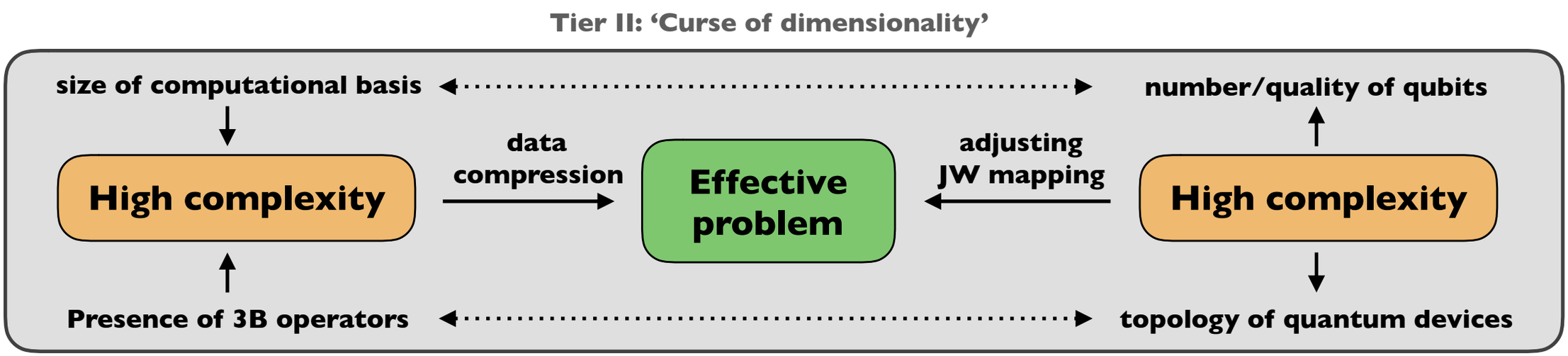

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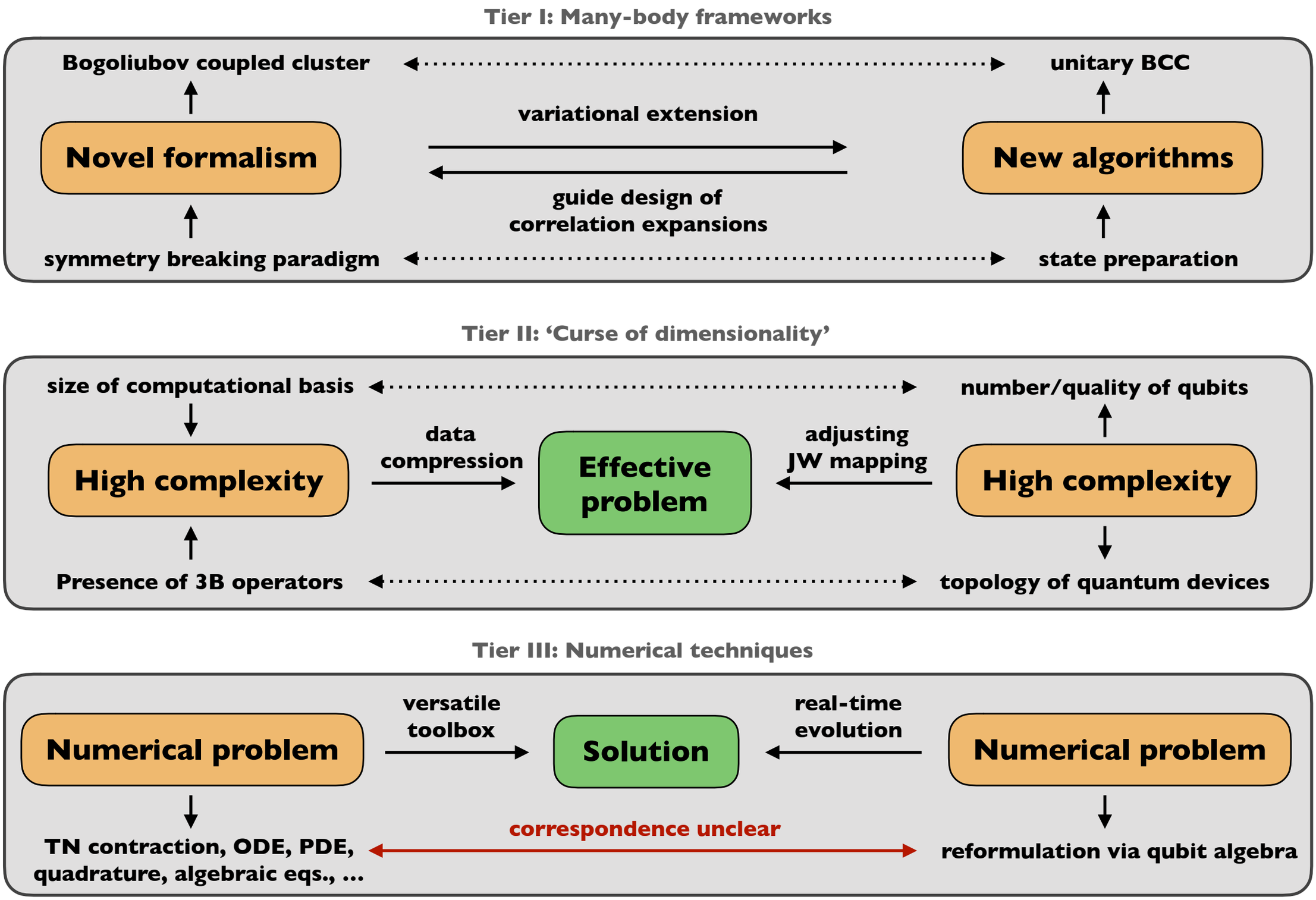

Theoretical perspectives

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
- Proper inclusion of continuum degrees of freedom from Berggren ensembles

Symmetry-broken many-body theory

- Extension of BMBPT to non-perturbative coupled-cluster framework (BCC)
- Systematic account of nuclear deformation from breaking *SU(2)* symmetry
- Improved understanding of symmetry restoration procedures in finite systems
- Odd nuclei and low-lying spectroscopy from equation-of-motion techniques

Towards quantum computing

- Pre-processing of Hilbert space to lower dimension in many-body simulations
- Extension of Bogoliubov coupled cluster framework to its unitary counterpart
- Formulation of symmetry restoration protocol using a quantum device

Epilogue

- **CEA group**
  - T. Duguet, M. Frosini, F. Raimondi, V. Somà
    CEA Saclay, France

- **Collaborators**
  - P. Arthuis, C. Barbieri
    University of Surrey, UK
  - J.-P. Ebran, J. Ripoche
    CEA DAM DIF, France
  - H. Hergert, R. Wirth
    Michigan State University, USA
  - P. Demol
    KU Leuven, Belgium
  - J. Müller, R. Roth, K. Vobig
    Technische Universität Darmstadt, Germany
  - G. Scuseria, J. Zhao
    Rice University, USA
  - R. Schutski
    Skoltech, Russia

Towards a diagrammatic expansion

- **Introduction of rotated quasiparticle operators and reference state**

$$|\Phi(\varphi)\rangle = S(\varphi)|\Phi\rangle \qquad \beta_k^\dagger(\varphi) = S(\varphi)\beta_k^\dagger S^{-1}(\varphi) \qquad \beta_k(\varphi) = S(\varphi)\beta_k S^{-1}(\varphi)$$

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$$\mathcal{R}(\varphi) = \begin{pmatrix} R^{+-}(\varphi) & R^{--}(\varphi) \\ R^{++}(\varphi) & R^{-+}(\varphi) \end{pmatrix} = \begin{pmatrix} 0 & R^{--}(\varphi) \\ 0 & 1 \end{pmatrix}$$

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Balian, Brézin, Nuovo Cimento **64**, 37 (1969)

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- **Important change: off-diagonal propagators allow for self-contractions (loops) in diagrams**