Particle-number-projected Bogoliubov Many-body Perturbation Theory

Breaking and restoration of *U(1)* symmetry beyond mean field

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
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Outline

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

Part II - Diagonal Bogoliubov MBPT

Part III - Restoration of *U(1)* symmetry

Ab Initio and Symmetry Breaking

Part I
Theoretical uncertainties

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

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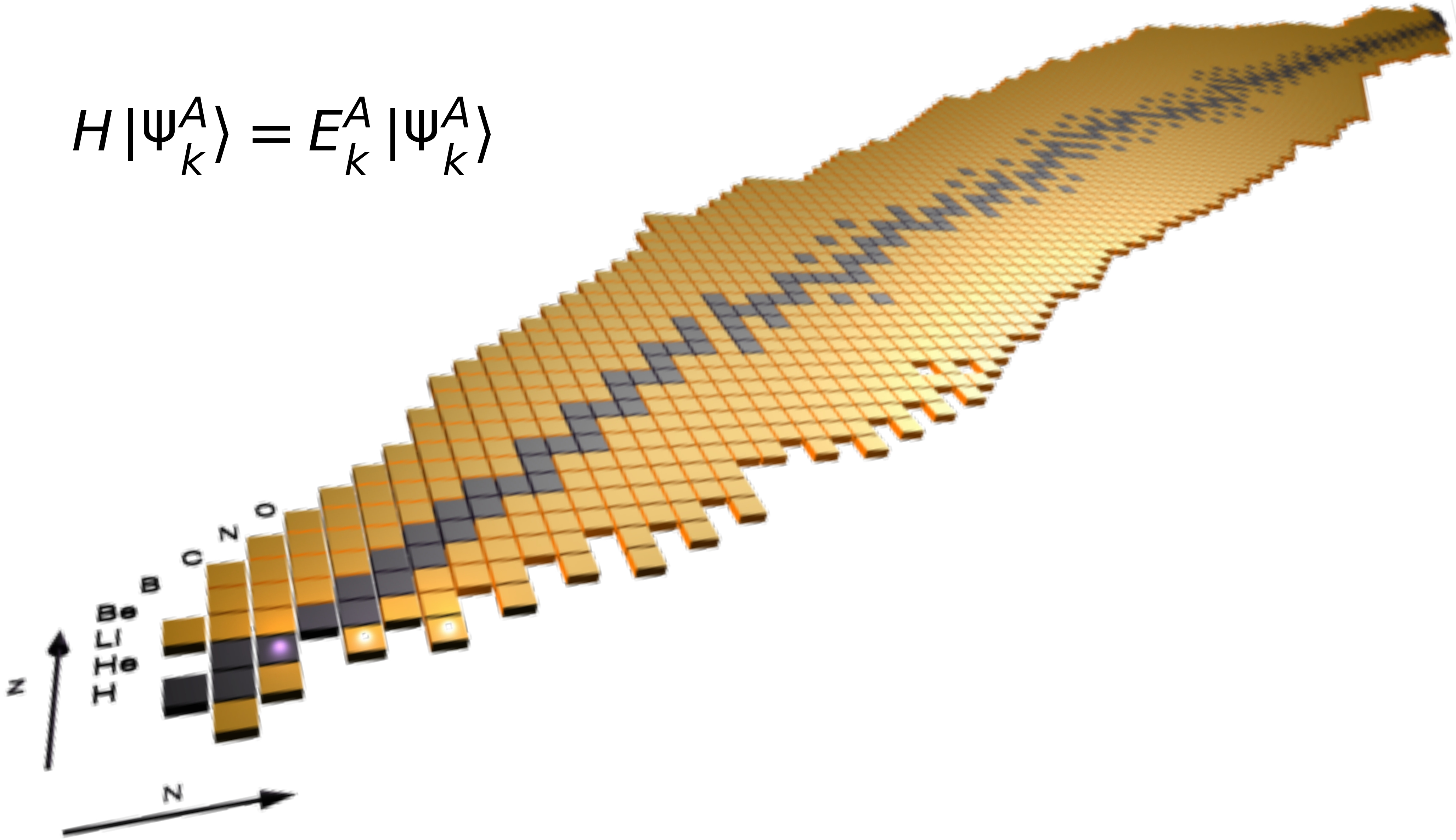

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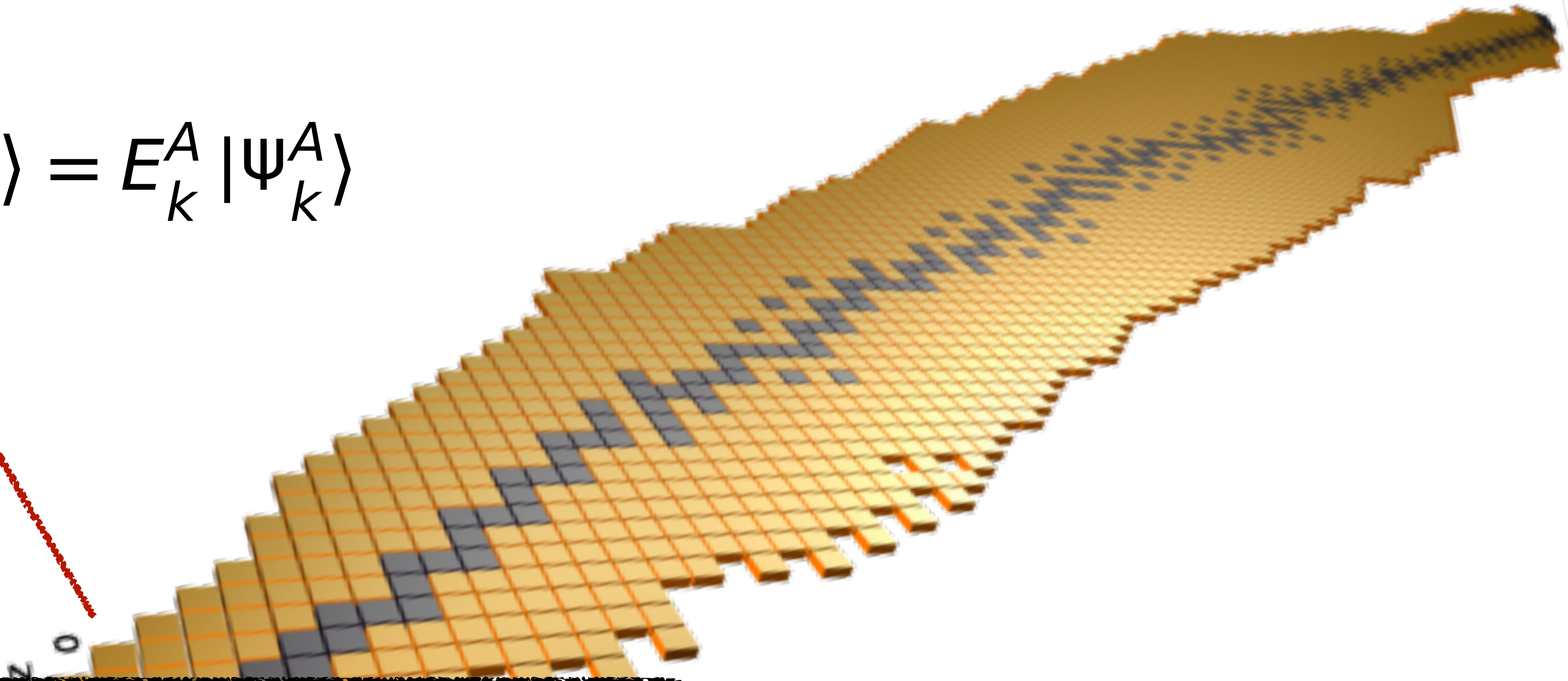

Input Hamiltonian

- 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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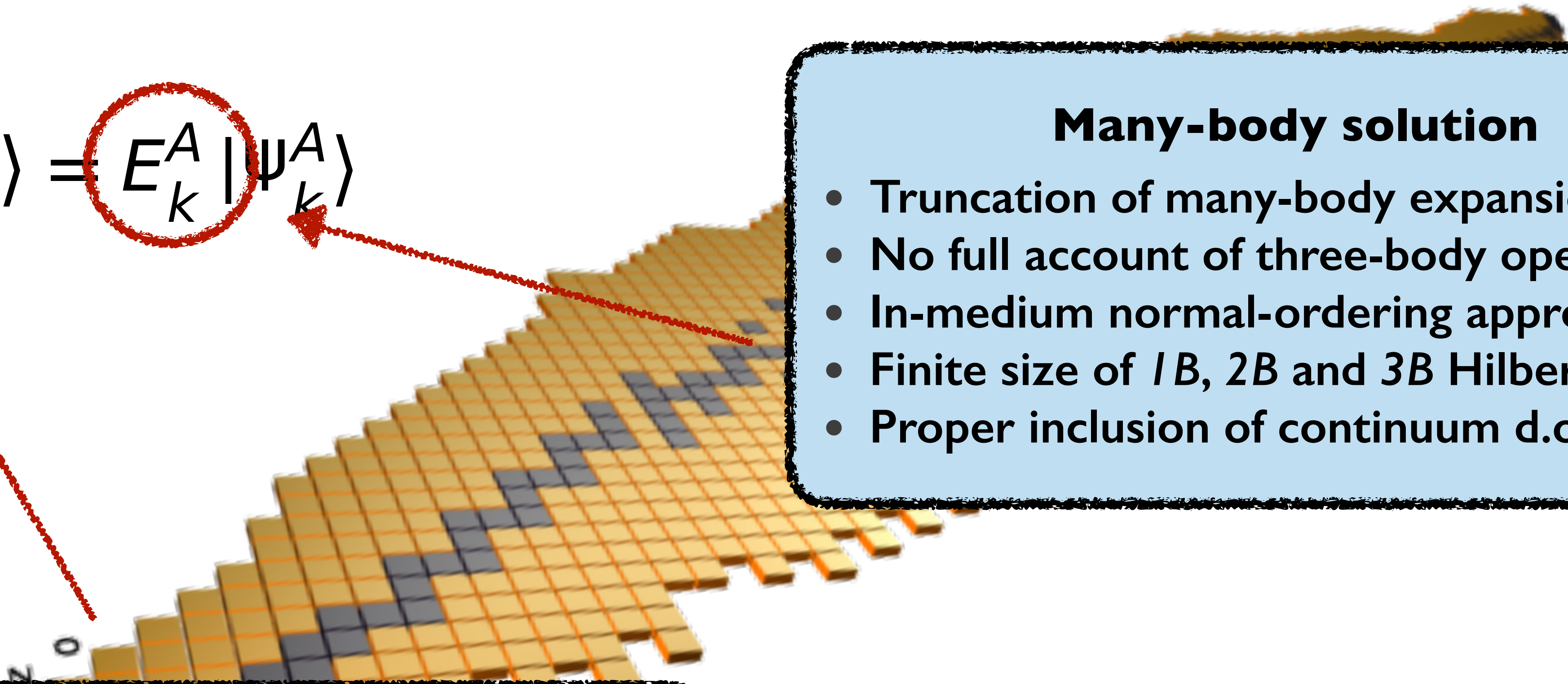

Many-body solution

- 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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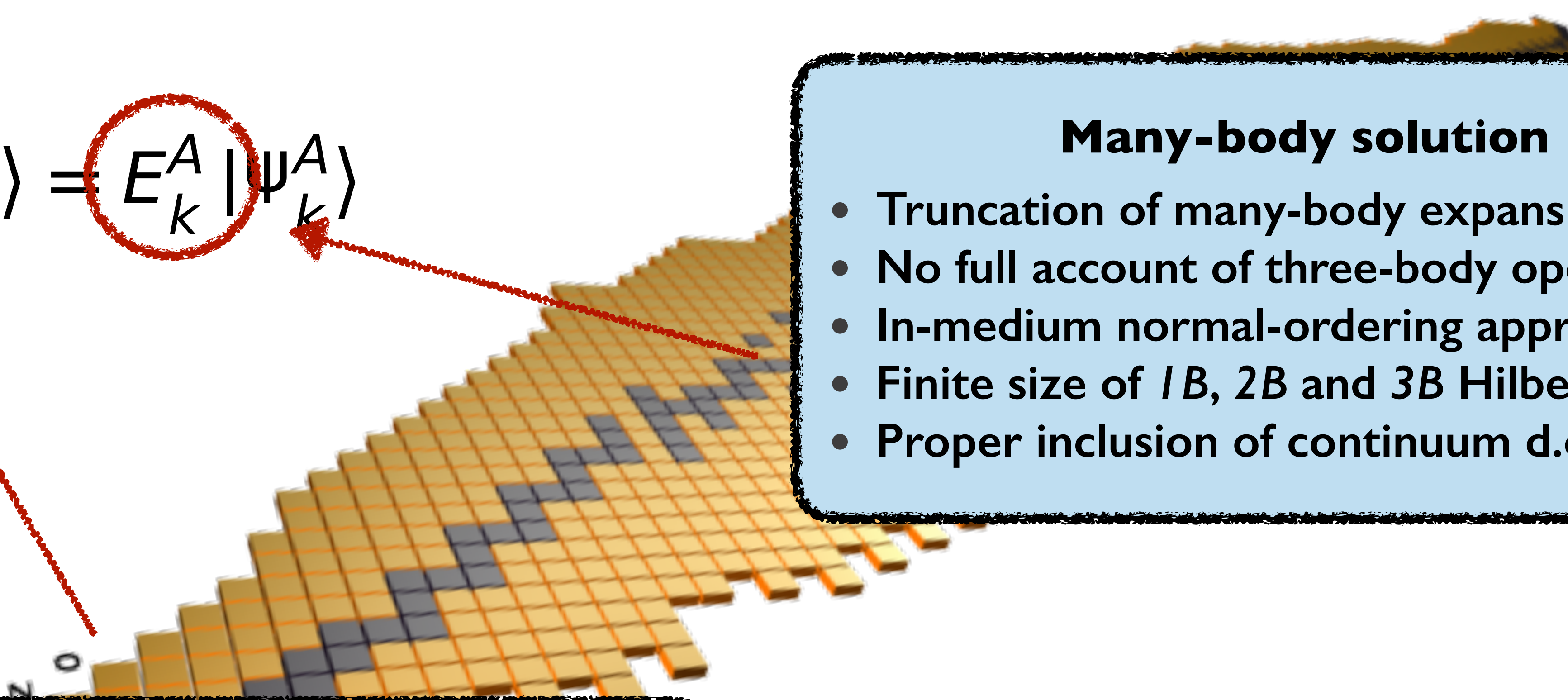

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Typical error on observables

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

Many-body expansions

Horizontal expansion

- Authorize breaking of symmetry group *G*

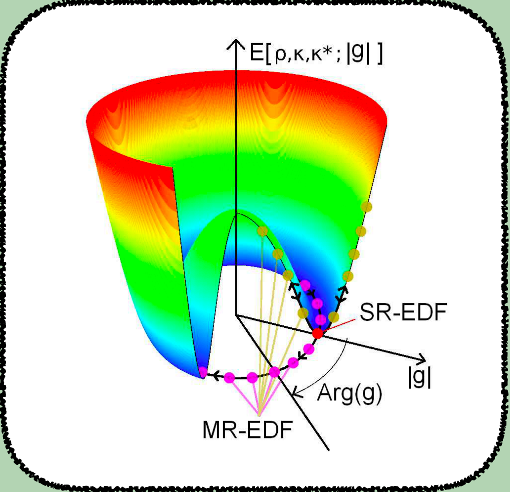
  U(1) : pairing correlations

  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



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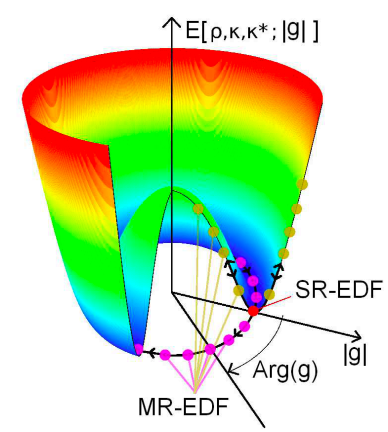

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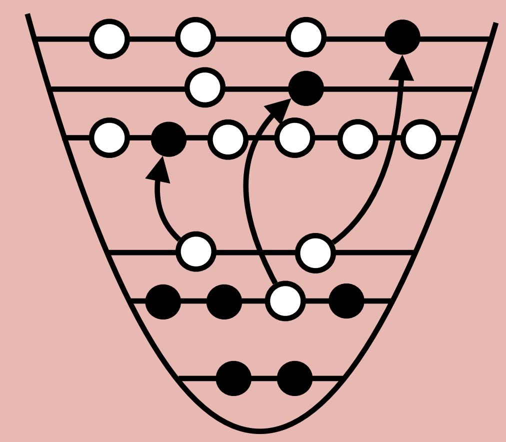
Vertical expansion

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



- Goal: determine wave-function coefficients

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

- 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

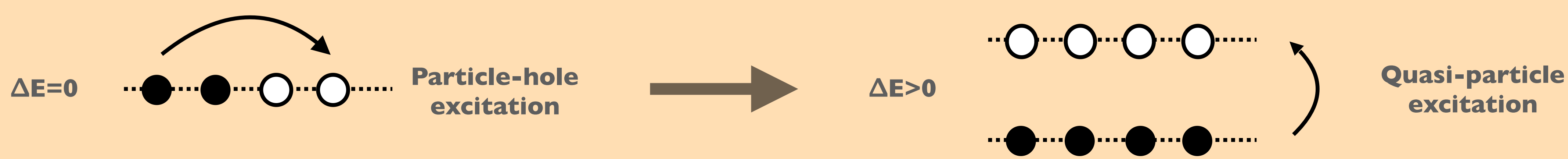
Many-body expansions

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 mean field (see talk of Thomas Duguet)

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

Bogoliubov Many-Body Perturbation Theory

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)

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

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

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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

Perturbative expansion

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

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

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- Various **non-perturbative schemes** formulated and/or in use …

… but symmetry has never been restored in realistic applications!

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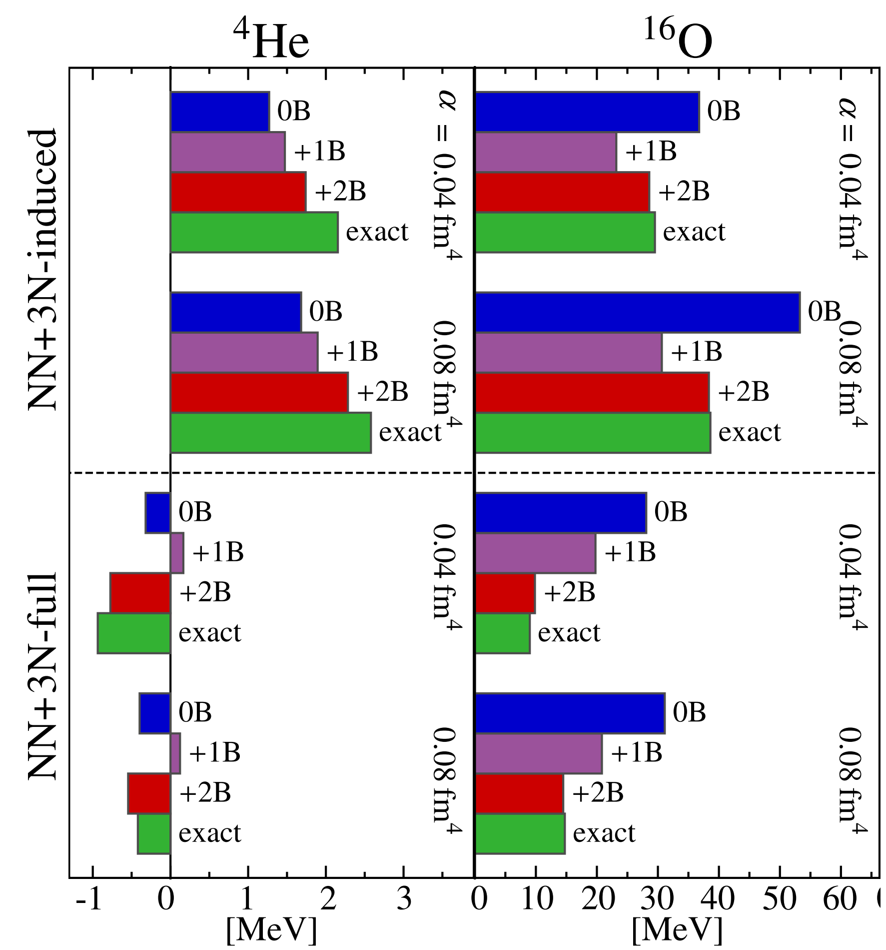

Roth *et al.*, PRL **109** 052501

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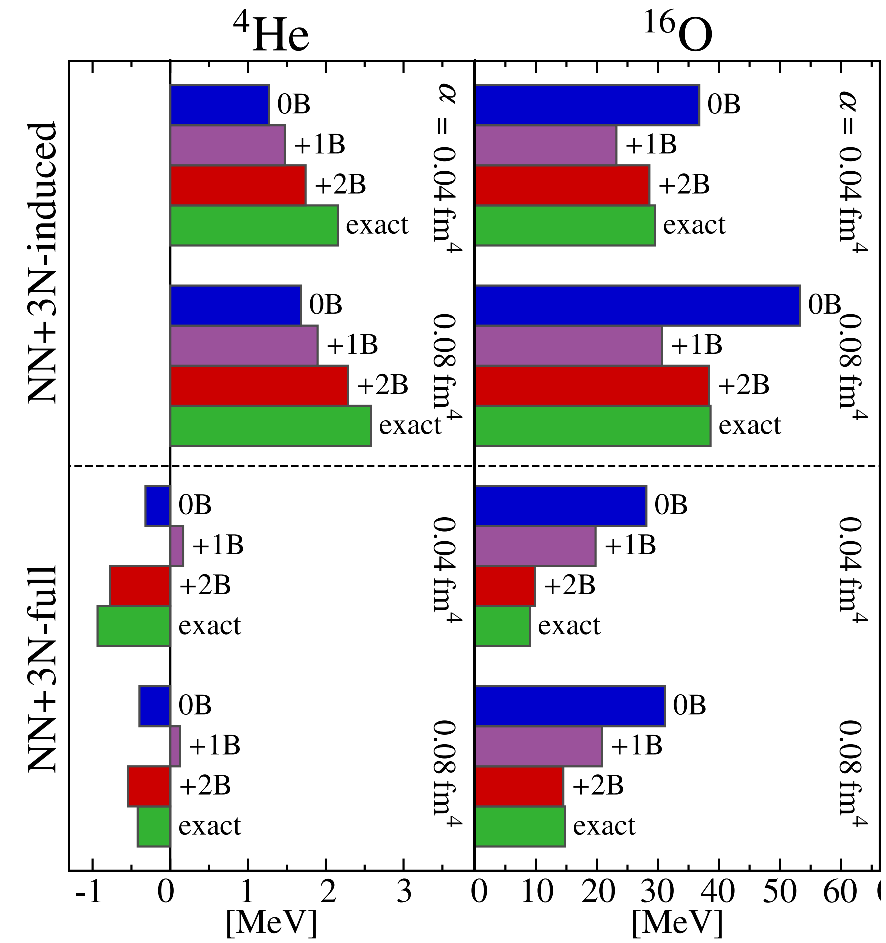
- Particle-number-broken vacua yield additional challenges

$$[O, A] = 0 \quad \not\Rightarrow \quad [O^{NOkB}, A] = 0$$

- For detailed discussion see talk of Julien Ripoche !



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particle number and higher moments A^k (but they are k-body operators)

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- Alternative to projection: readjustment of particle number in high-order BMPT

$$|\Phi\rangle, A_0(N_0, Z_0) \xrightarrow{\text{order } p} |\Psi^{(p)}_{\text{approx}}\rangle \quad \text{with} \quad A' \neq A_0 \xrightarrow{\text{constrained HFB}} |\Phi_{\text{constr.}}\rangle \quad \text{with} \quad A_{\text{constr.}} \neq A_0$$

non-canonical BMBPT calculation (more diagrams)

see talk of Mikael Frosini !

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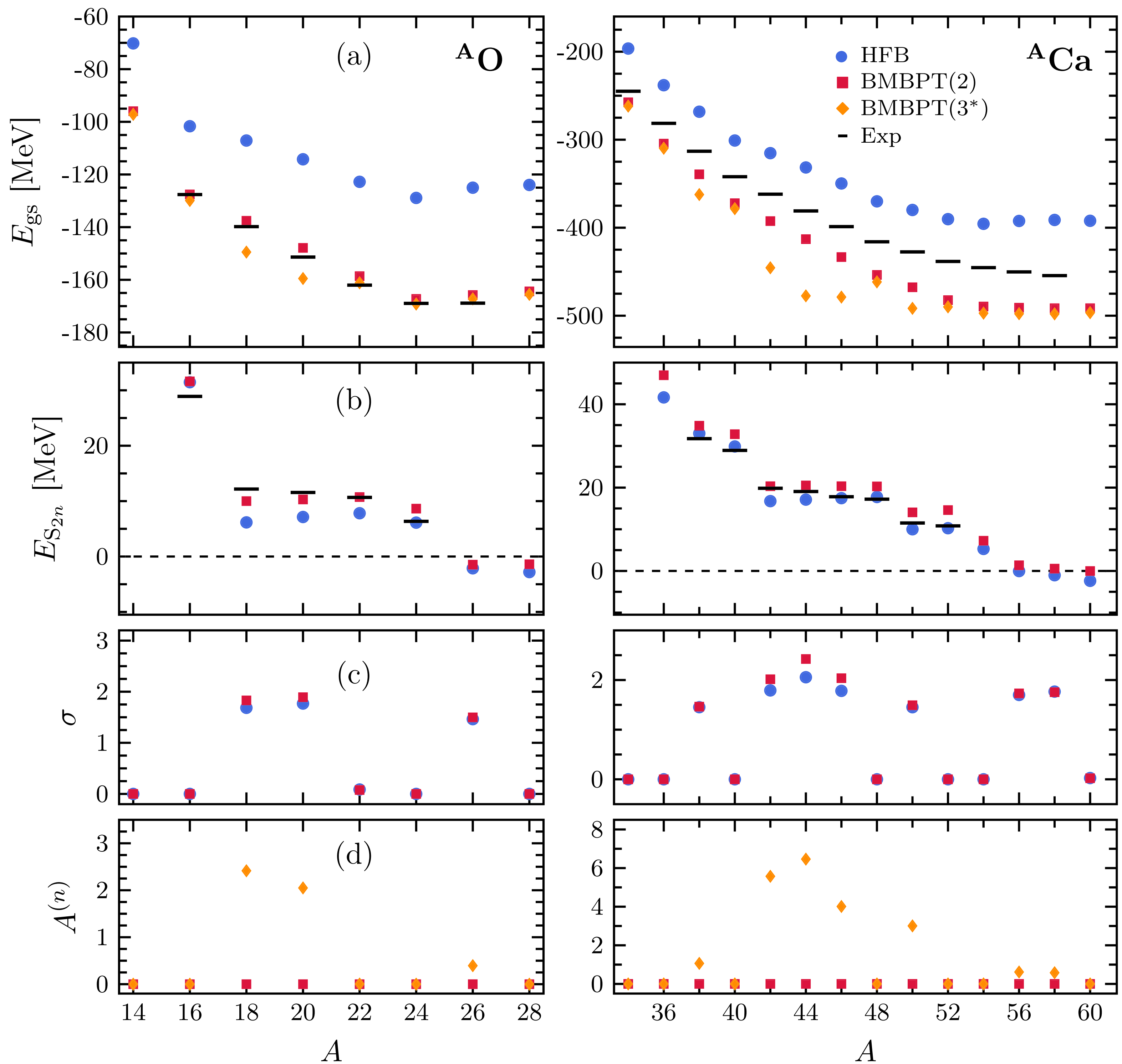
- Good news: no particle-number shift at second order when using canonical HFB reference state

BMBPT - isotopic chains

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



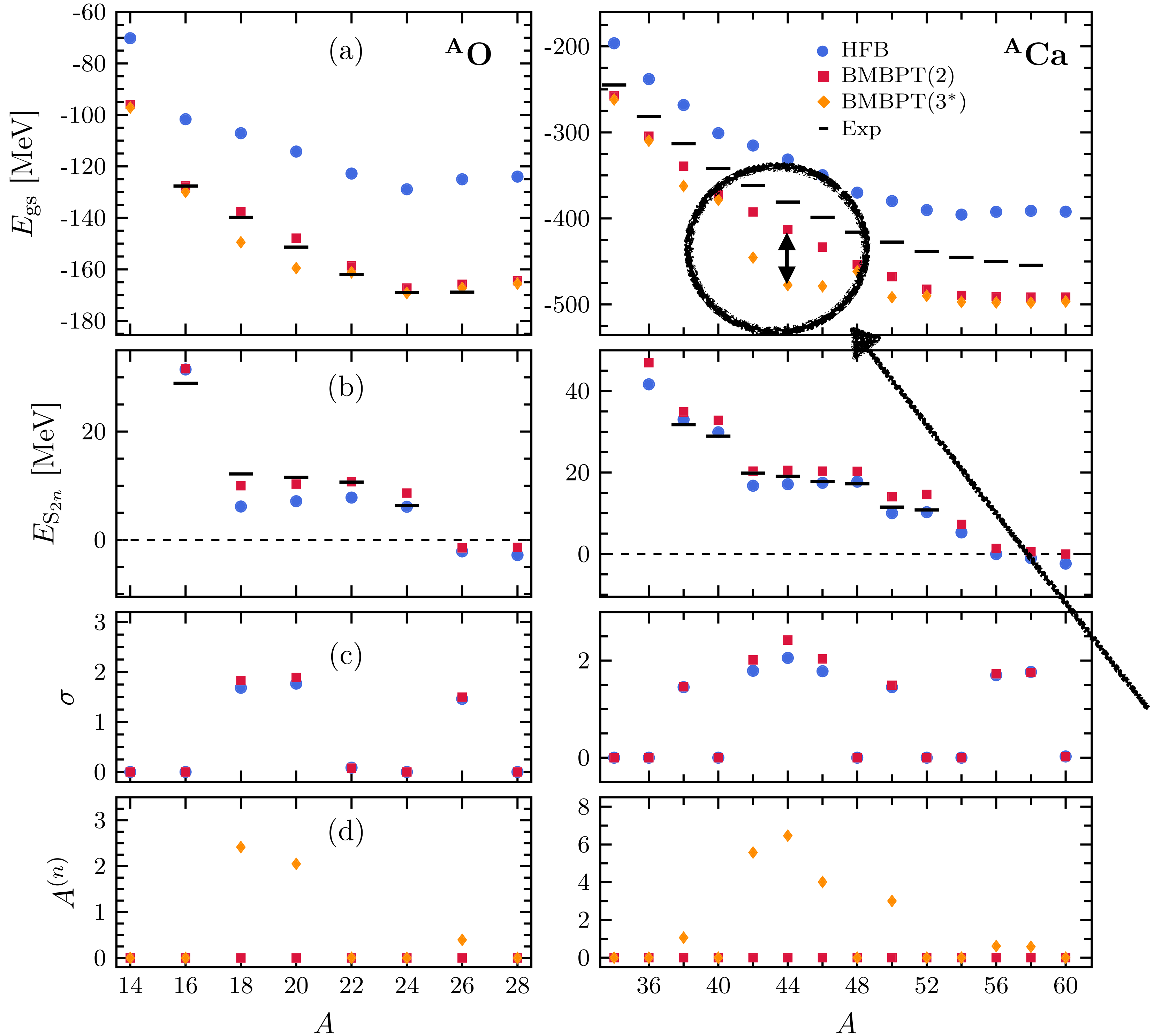
Calculation details

Chiral NN+3N Hamiltonian
NO2B approximation
SRG: α = 0.08 fm⁴
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 - isotopic chains

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



Calculation details

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

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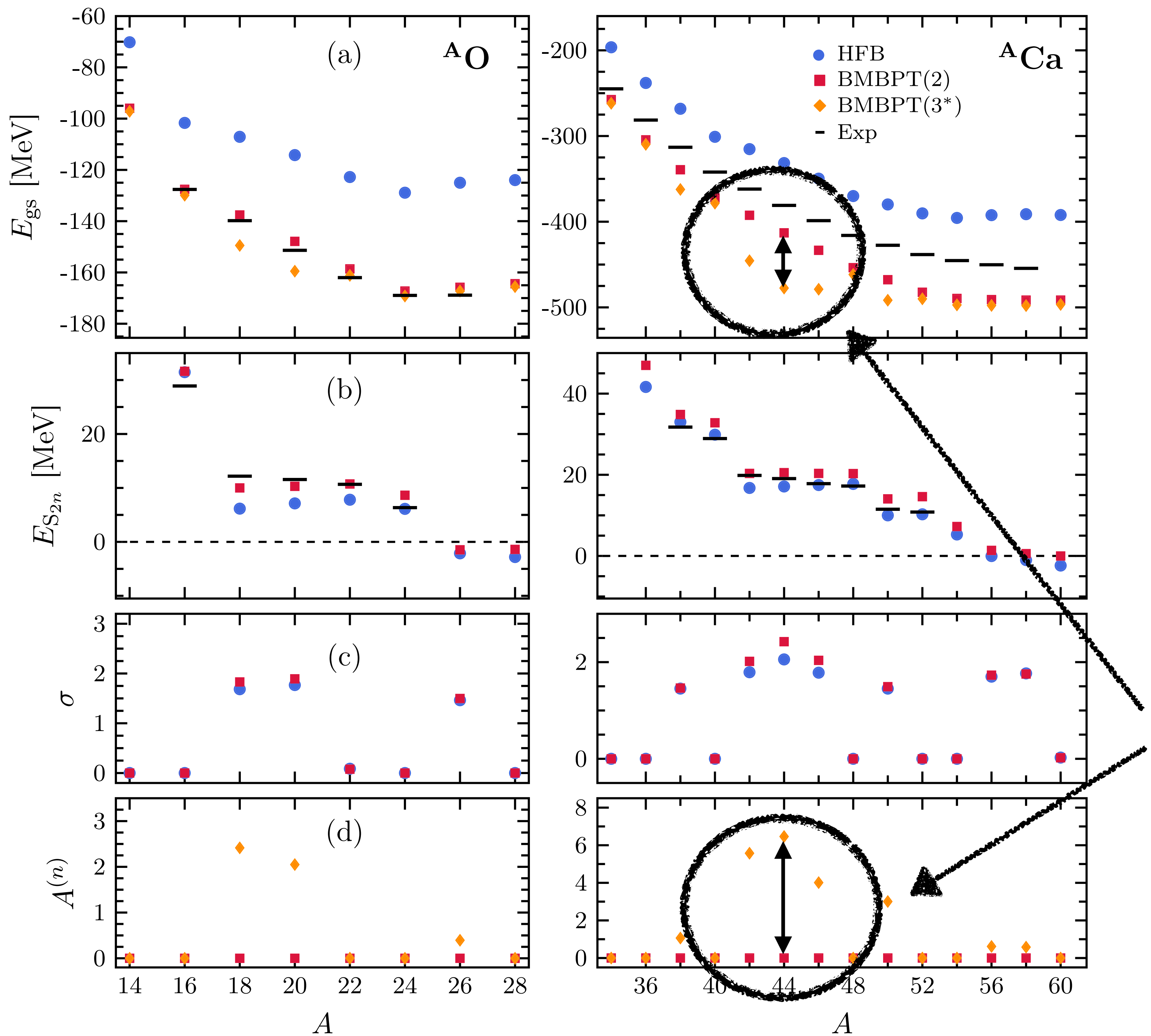

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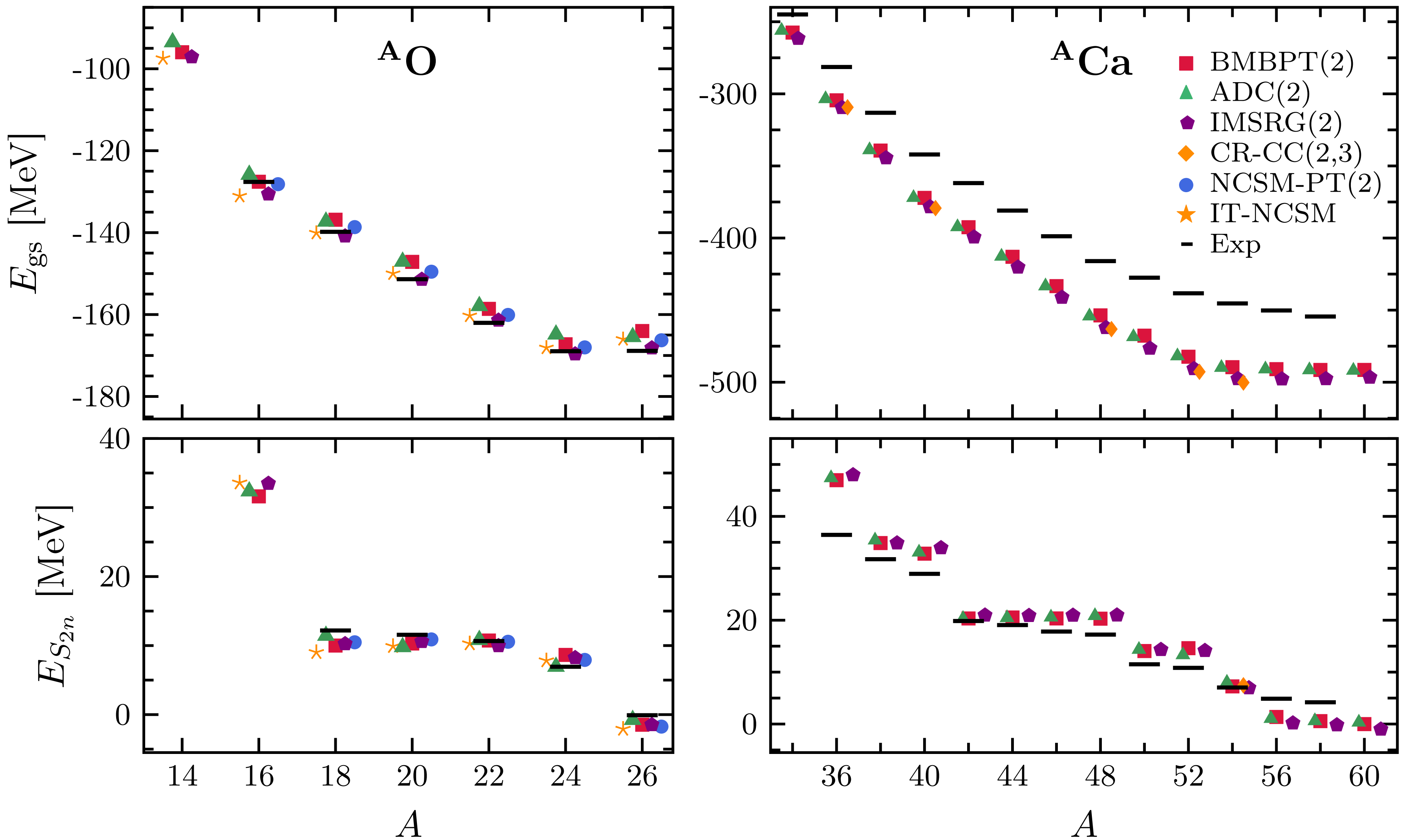
BMBPT - consistency and complexity



Calculation details

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SRG: α = 0.08 fm^4
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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

Projected BMBPT
Restoration of *U(1)* symmetry

Part III
Consistent symmetry restoration beyond HFB

Tichai, Ripoche, Duguet, (2019) in preparation
Ripoche, Tichai, Duguet, (2019) in preparation

Projective eigenequations

- **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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$$\frac{d}{d\varphi} \mathcal{N}(\varphi) - i\, a(\varphi) \mathcal{N}(\varphi) = 0 \quad with \quad \mathcal{N}(0) = 1 \quad \Longrightarrow \quad \mathcal{N}(\varphi) = \exp i \int_0^{\varphi} a(\phi) d\phi$$

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

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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- **Four different types of quasi-particle propagators for symmetry-broken vacuum**

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

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Taylor expansion

$$(-1)^p\frac{1}{p!}\int_0^\infty\cdots\int_0^\infty d\tau_1\ldots d\tau_p\,\langle\Phi|\mathrm{T}\big[\Omega_1(\tau_1)\ldots\Omega_1(\tau_p)O(0)\big]|\Phi(\varphi)\rangle_c$$

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Off-diagonal Wick theorem

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

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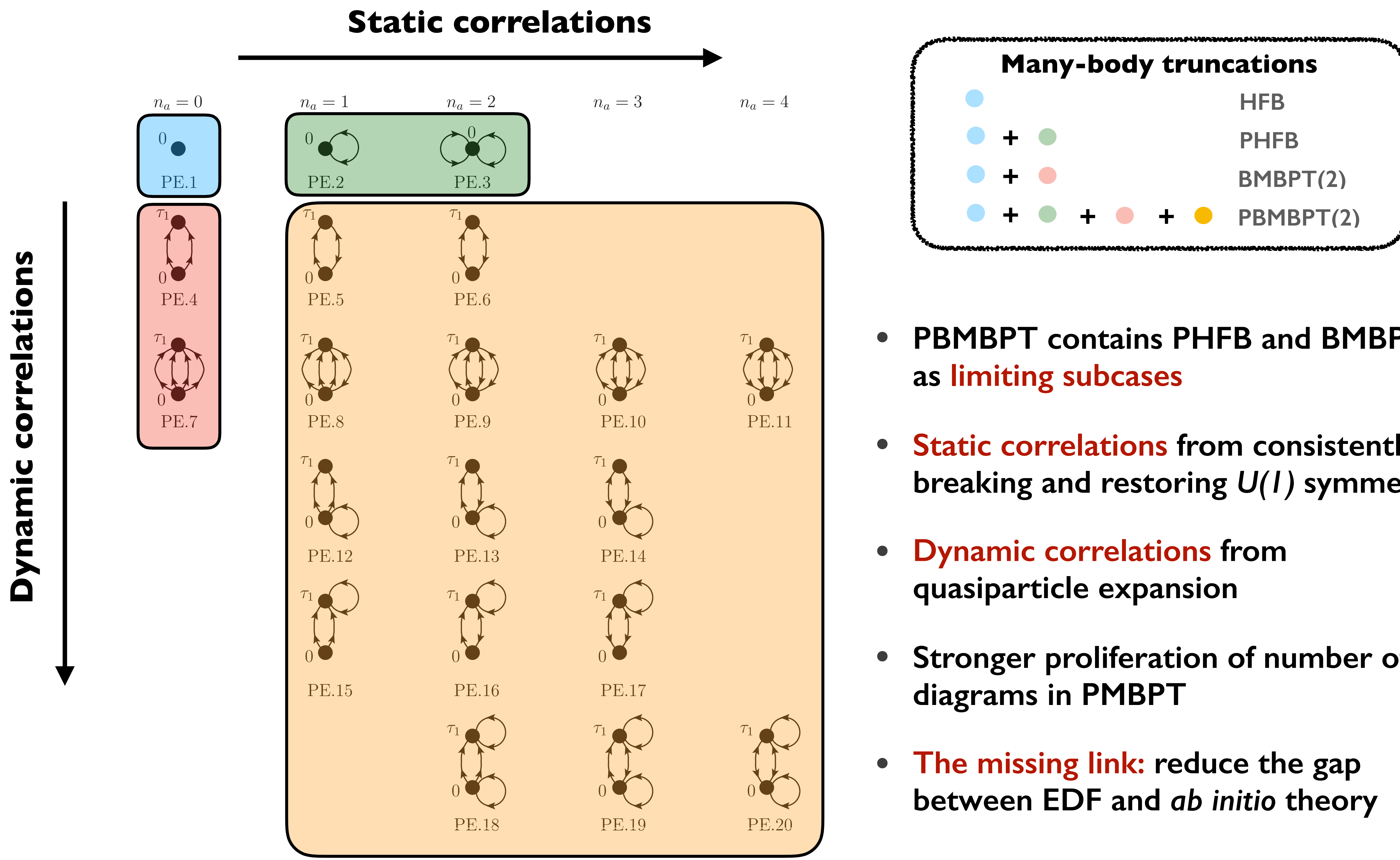
Off-diagonal Wick theorem
Balian, Brézin, Nuovo Cimento **64**, 37 (1969)

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

'More than the sum of its parts'



- PBMBPT contains PHFB and BMBPT as limiting subcases
- Static correlations from consistently breaking and restoring *U(1)* symmetry
- Dynamic correlations from quasiparticle expansion
- Stronger proliferation of number of diagrams in PMBPT
- The missing link: reduce the gap between EDF and *ab initio* theory

‘Intermediates’ - rotated matrix elements

- Introduce non-unitary Bogoliubov transformation yielding new set of quasiparticle operators

$$\begin{pmatrix} \tilde{\beta} \\ \beta^\dagger \end{pmatrix} = M(\varphi) \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} M^{-1}(\varphi) = \mathcal{M}^\dagger(\varphi) \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \qquad with \qquad \begin{pmatrix} 1 & 0 \\ R^{--\star}(\varphi) & 1 \end{pmatrix}$$

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$$O(\varphi) = M(\varphi) O M^{-1}(\varphi)$$

- Rotated operator has the decomposition as initial operator but with rotated matrix elements

$$O(\varphi) \equiv O^{00}(\varphi) + O^{20}(\varphi) + O^{11}(\varphi) + O^{02}(\varphi) + O^{40}(\varphi) + O^{31}(\varphi) + O^{22}(\varphi) + O^{13}(\varphi) + O^{04}(\varphi)$$

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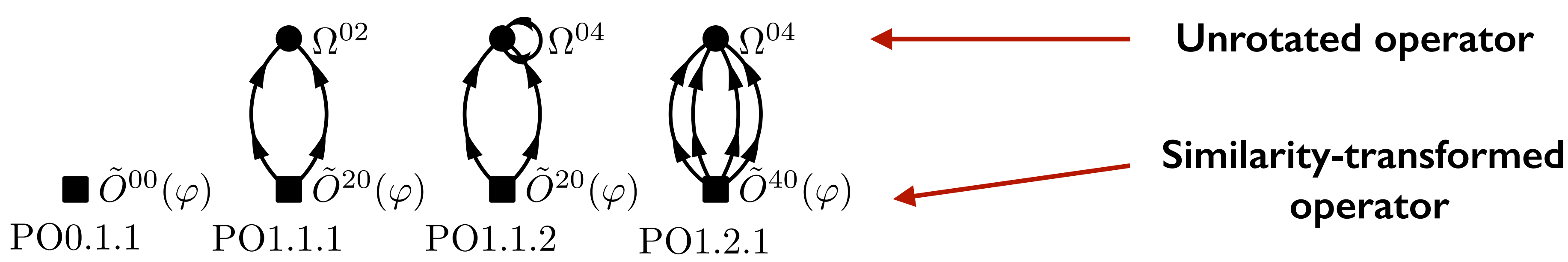

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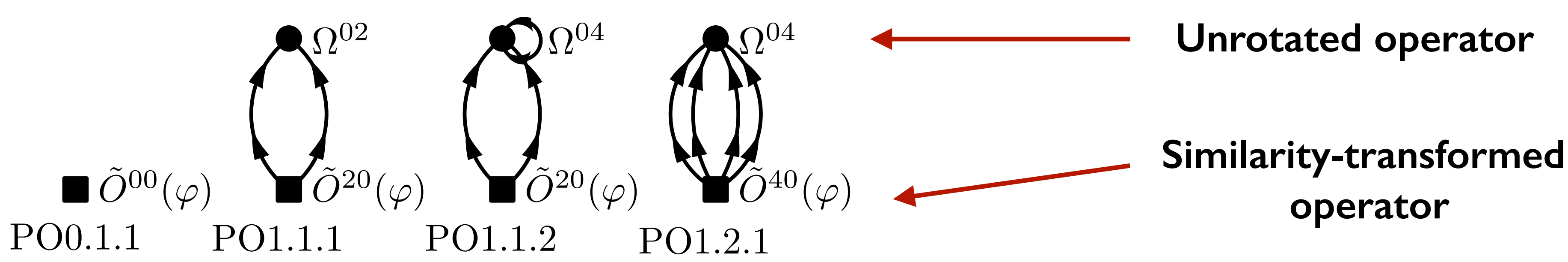
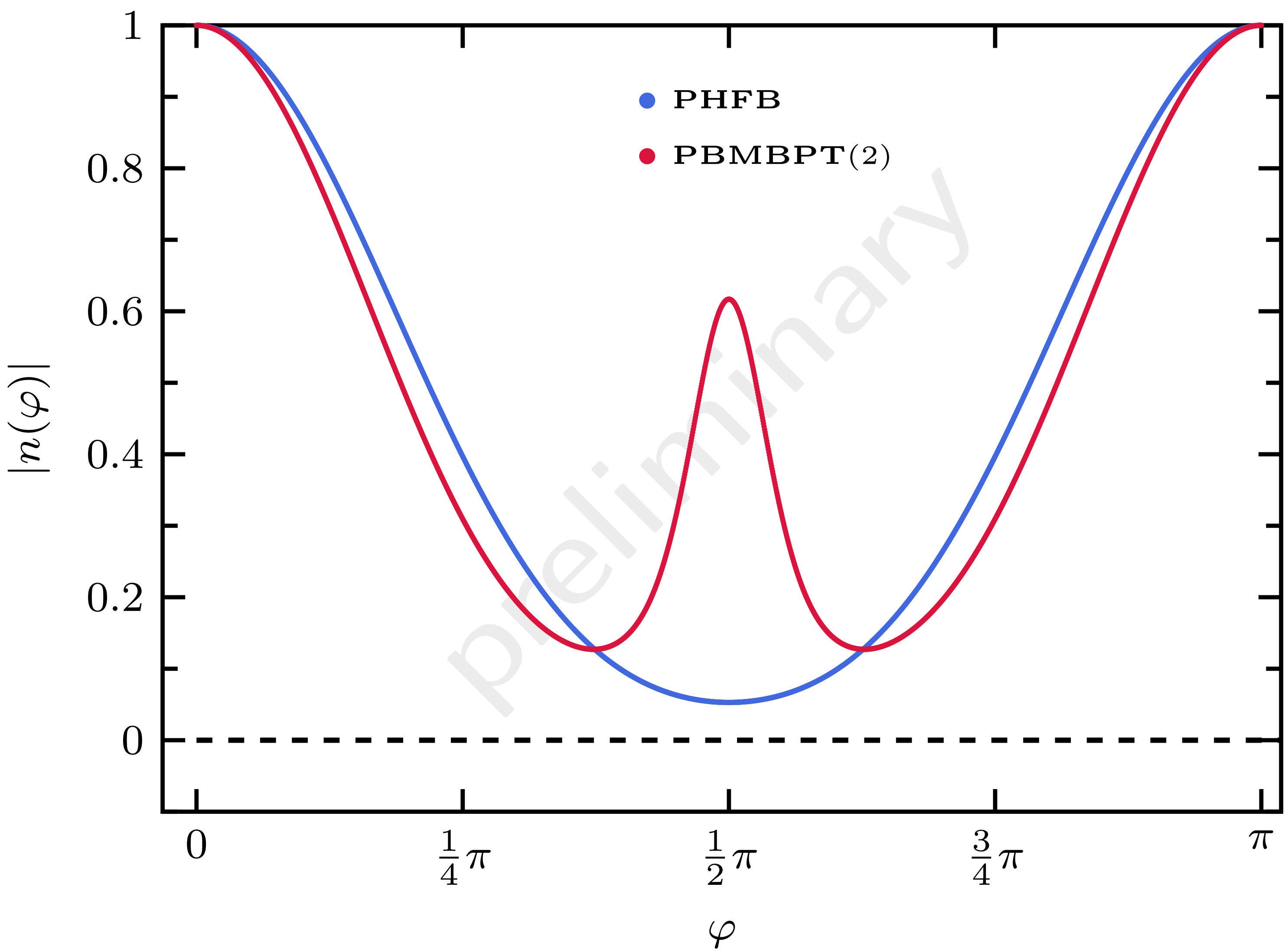


- Complexity conserved: less diagrams at the price of more complex matrix-element handling

Norm kernels



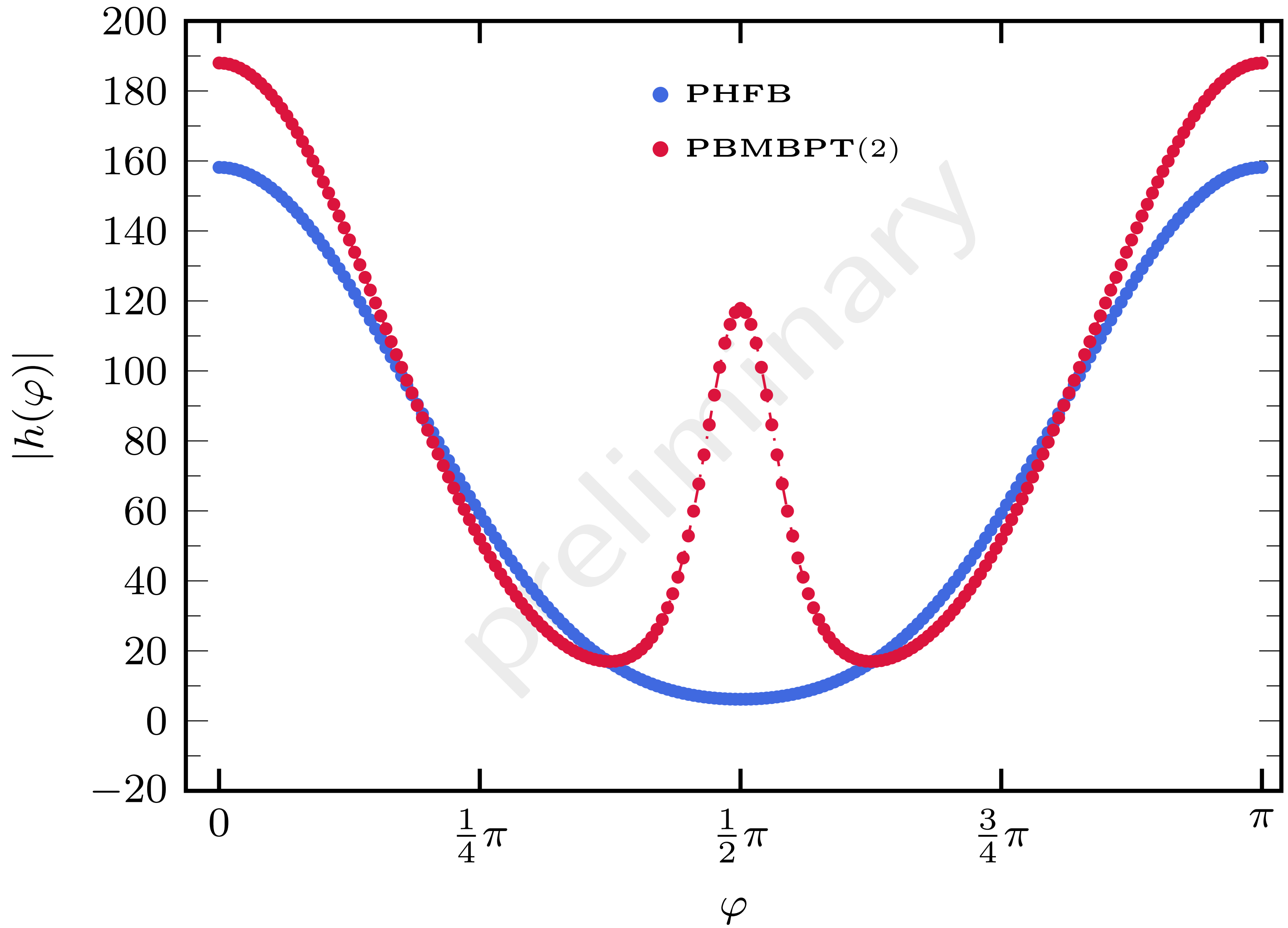
Calculation details

Chiral NN Hamiltonian
SRG: $\alpha = 0.08$ fm^4
9 major shells (660 s.p. states)
canonical HFB reference
O^{18} (proton shell closure)
2000 meshpoints

$$\mathcal{N}(\varphi) = \exp i \int_0^{\varphi} a(\phi) d\phi$$

- Kernels are **π-periodic** (number-parity conservation) and symmetric with respect to π/2
- Projected particle number coincides with A_0 of target IRREP up to numerical precision
- Peak of second-order norm kernel at π/2 *(*not observed in PBCC using pairing Hamiltonian*)*
- Evaluation of norm kernel is **computationally very cheap** since *A* is a *1B* operator

Hamiltonian kernels



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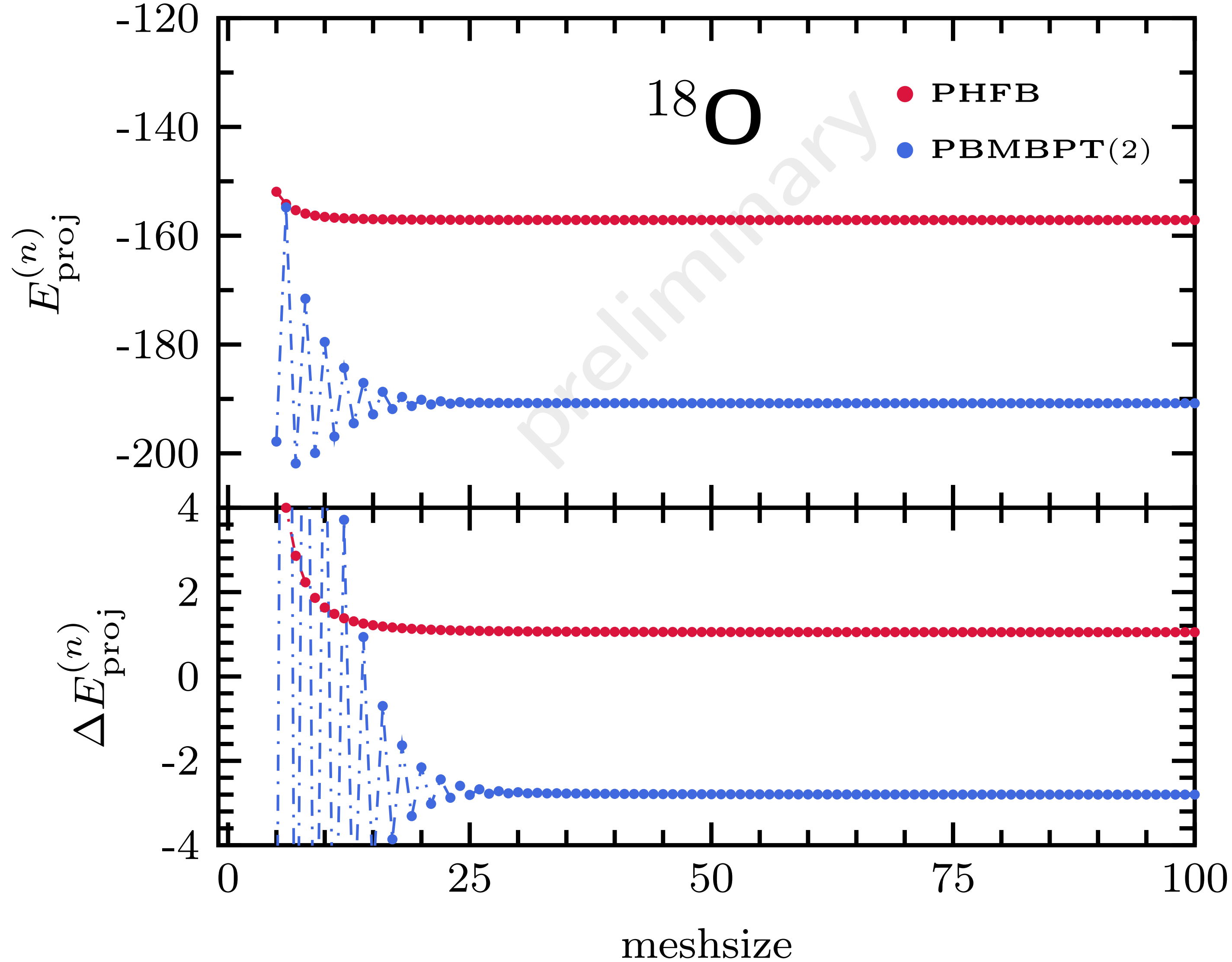
- **Kernels are π-periodic (number-parity conservation) and symmetric with respect to π/2**
- **Mean-field projection coincides with other PHFB codes to numerical precision**
- **Peak of second-order norm kernel at π/2 (not observed in PBCC using pairing Hamiltonian)**

Dependence on the meshsize



Calculation details

Chiral NN Hamiltonian
SRG: $\alpha = 0.08\ \text{fm}^4$
5 major shells (140 s.p. states)
canonical HFB reference

Numerical procedure

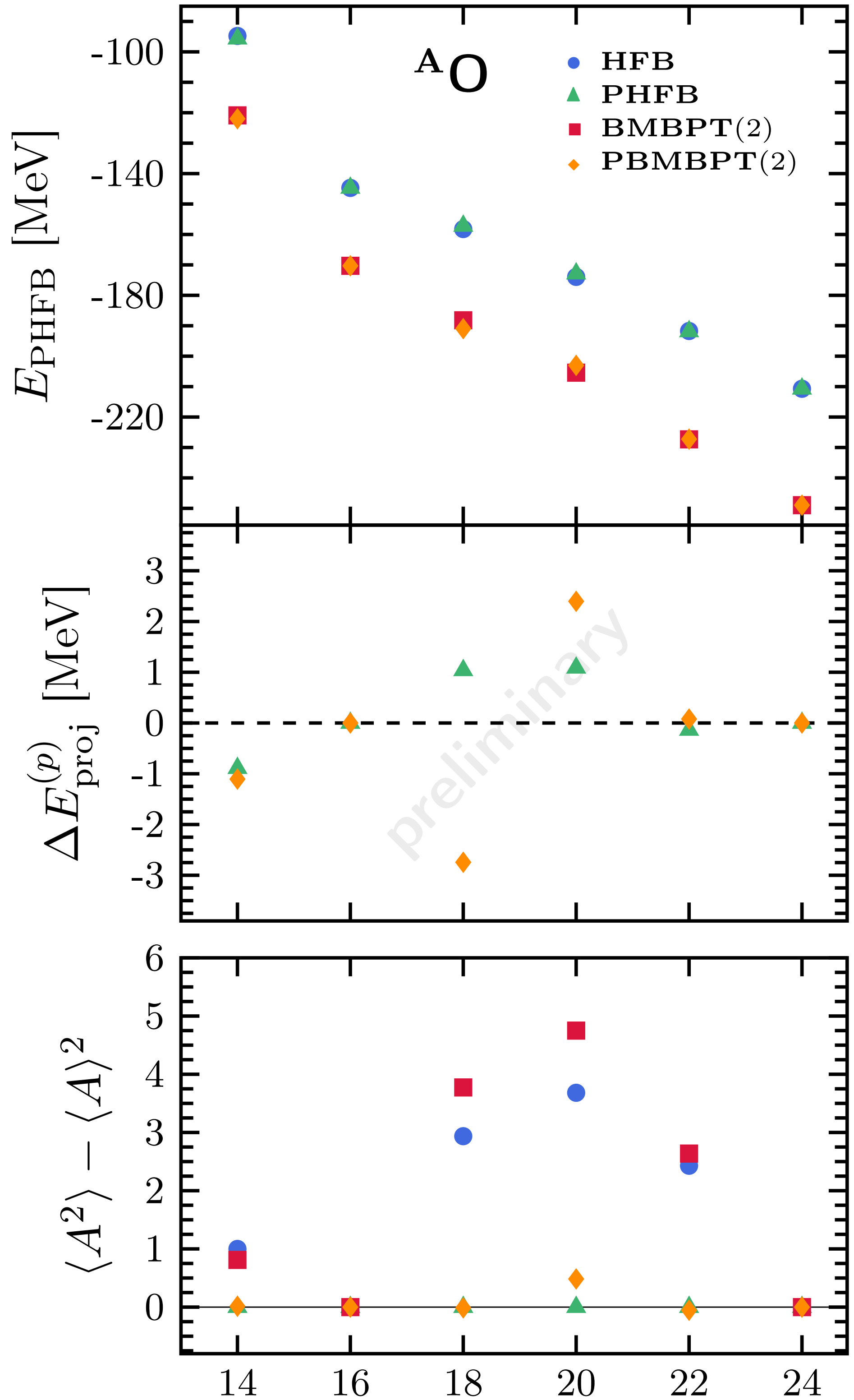
Separate integration of real/imag. part
Interpolation using cubic spline
Equidistant mesh points
Reduced interval *[0,π]*

Correction from projection:

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

- Monotonic dependence on number of mesh points at both truncation levels
- Restoration at second order requires higher number of mesh points than PHFB
- Projection is less efficient than typical 'Pfaffian with Fromenko discretization' employed in EDF

Oxygen isotopic chain



Very naive (!) runtime:
300 CPU hours

Correction from projection:

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

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)
- Projected particle-number variance is almost zero in open-shell systems (see talk of Thomas Duguet)

This feature is not built in!

- Systematic account of non-perturbative physics at low computational cost
- Computational cost is independent of mass number

Related projects

- Study of the impact of normal ordering in particle-number breaking theories

Normal-ordered *k*-body approximation in particle-number breaking theories

Ripoche, Tichai, Duguet, (2019) in preparation

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- Automized generation and evaluation of Feynman diagrams (including *3B* operators)

ADG: Automated generation and evaluation of many-body diagrams

Arthuis, Duguet, Tichai, Lasseri, Ebran, Comp. Phys. Comm. 240C (2019)

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- Computer-aided angular-momentum coupling in nuclear many-body theory

Symmetry reduction of tensor networks in many-body theory
I Automated symbolic evaluation of *SU(2)* algebra

Ripoche, Wirth, Duguet, Tichai, (2019) in preparation

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Arthuis, Duguet, Tichai, Lasseri, Ebran, Comp. Phys. Comm. 240C (2019)
Ripoche, Arthuis, Duguet, Tichai, Duguet (2019), in preparation

- Computer-aided angular-momentum coupling in nuclear many-body theory

Symmetry reduction of tensor networks in many-body theory
I Automated symbolic evaluation of *SU(2)* algebra

Ripoche, Wirth, Duguet, Tichai, (2019) in preparation

- Control the computational scaling via tensor-decomposition techniques for operators

Tensor-decomposition techniques for *ab initio* nuclear structure calculations:
From chiral nuclear potentials to ground-state energies

Tichai, Schutski, Scuseria, Duguet, Phys. Rev. C **99**, 034320

Related projects

- Study of the impact of normal ordering in particle-number breaking theories

Normal-ordered *k*-body approximation in particle-number breaking theories

Ripoche, Tichai, Duguet, (2019) in preparation

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- Data compression of many-body tensors using importance-sampling approaches

Pre-processing the nuclear many-body problem:
Importance truncation *vs.* tensor factorisation techniques

Tichai, Ripoche, Duguet, arXiv:1902.09043, accepted at EPJA

Theoretical perspectives

Solving the *A*-body Schrödinger equation

- Fully consistent restoration of broken *U(1)* gauge symmetry
- Doubly open-shell nuclei from simultaneously breaking *SU(2)* symmetry
- Going to heavier systems: treatment of *3B* forces is a computational bottleneck
- Systematic account of spectroscopy and electromagnetic response

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 NO*k*B approximation for symmetry-broken vacua

Symmetry-restored many-body theory

- Numerical improvements accounting for evaluation of operator kernels
- Alternative projection from solving group-specific differential equation
- Extended formalisms ensuring proper behaviour of higher-order moments
- Benchmarking of technical aspects like shift invariance beyond mean-field level

Epilogue

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