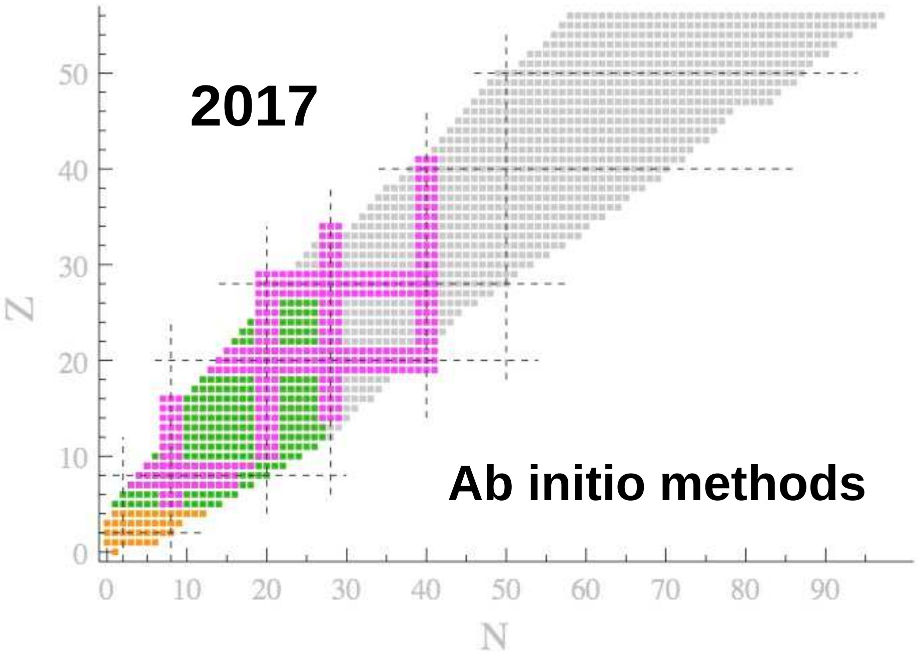
Symmetry broken&restored MBPT/CC formalisms

One possible strategy for ab-initio calculations of **near-degenerate** and **open-shell** systems

I. Let the reference state spontaneously break symmetry(ies)

II. Safely expand the exact solution around it

III. Restore the symmetry(ies) at any truncation order



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With my warm thank you to Georges Ripka

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T. Duguet, J. Phys. G: Nucl. Part. Phys. 42 (2015) 025107

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◉ Conclusions and perspectives

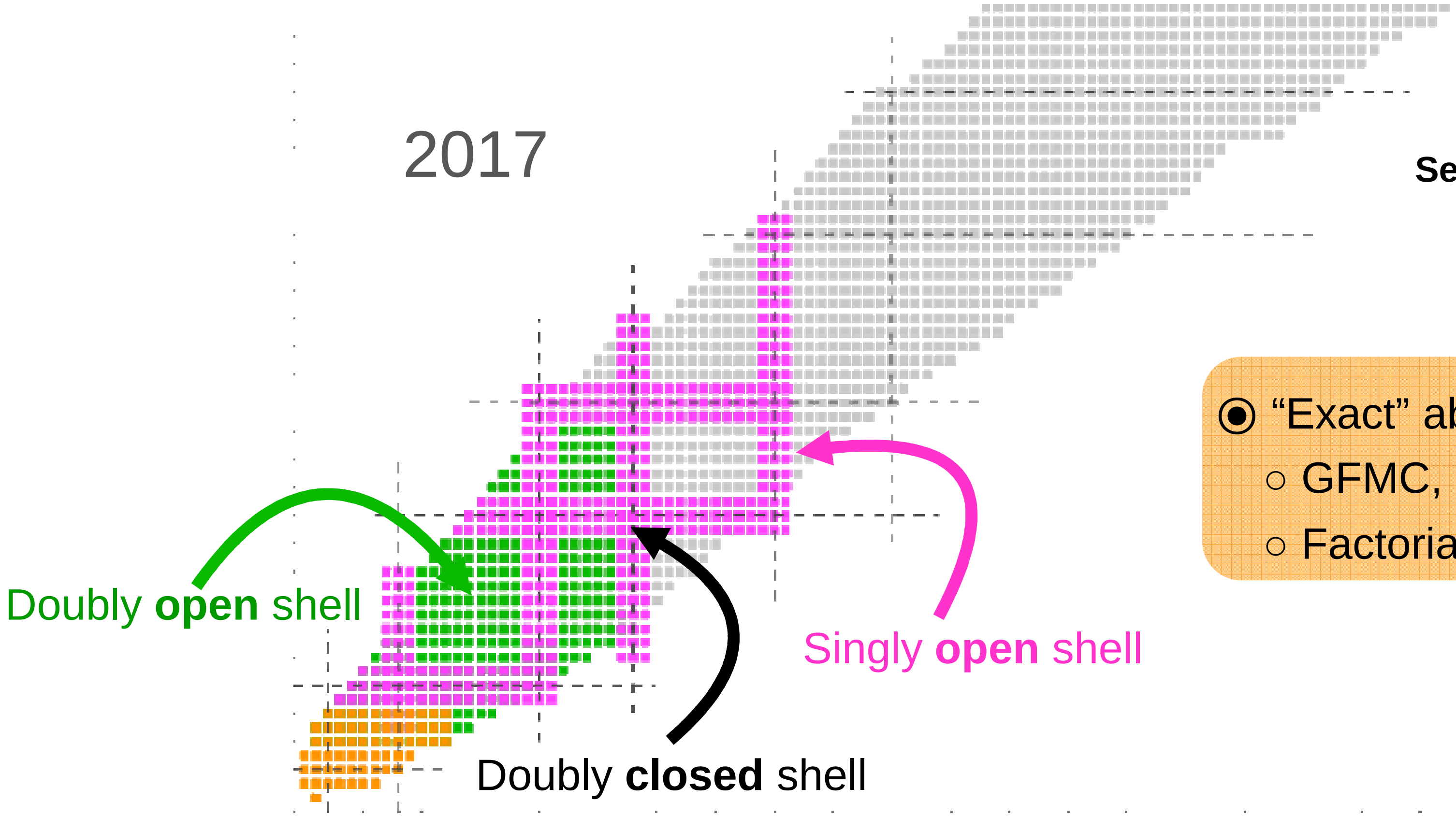
Ab initio nuclear chart

◉ Single-reference expansion methods

- (G)SCGF, (B)CC, IMSRG
- Polynomial scaling

◉ Multi-reference methods

- Valence space CI, MR-IMSRG, MCPT
- Mixed scaling



See V. Somà talk on tuesday

◉ “Exact” ab initio approaches

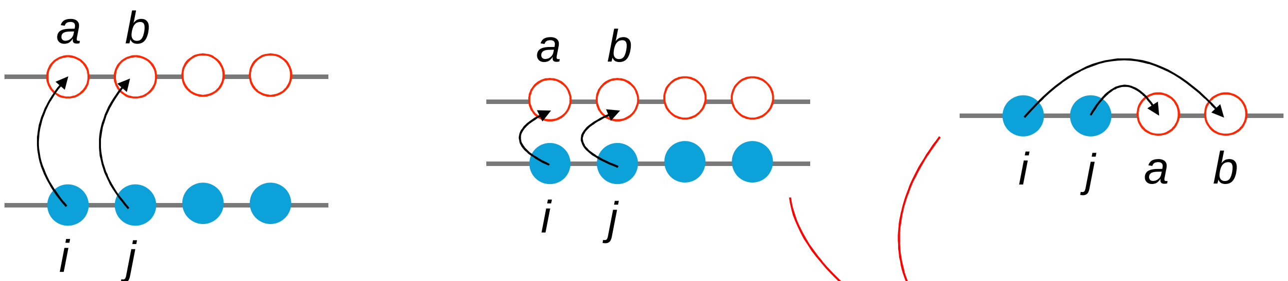
- GFMC, NCSM, FY, HH
- Factorial scaling

Breaking (+ restoring) or not [SU(2) and/or U(1)] symmetries, that is the question/dilemma…

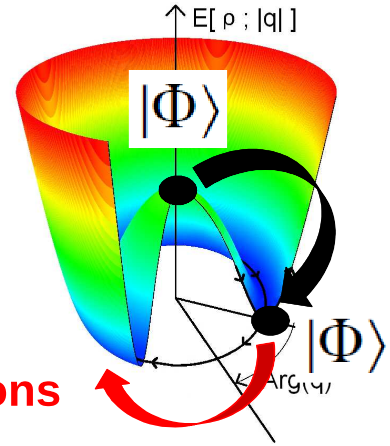
(Near-)degenerate systems via expansion methods

◉ Expansion around a **symmetry adapted determinant** $|\Phi\rangle$ captures correlations via **ph excitations**

Closed-shell | Sub-closed shell | Open-shell



non degenerate | near degenerate | degenerate | ph excitations



E.g. consider MBPT(2) $\Delta E^{(2)} = -\frac{1}{4}\sum_{abij}\frac{|\bar{v}_{abij}|^2}{e_a+e_b-e_i-e_j}$

Expansion **breaks down** when $e_a + e_b \approx e_i + e_j$

Strong correlations

◉ Possible ways out

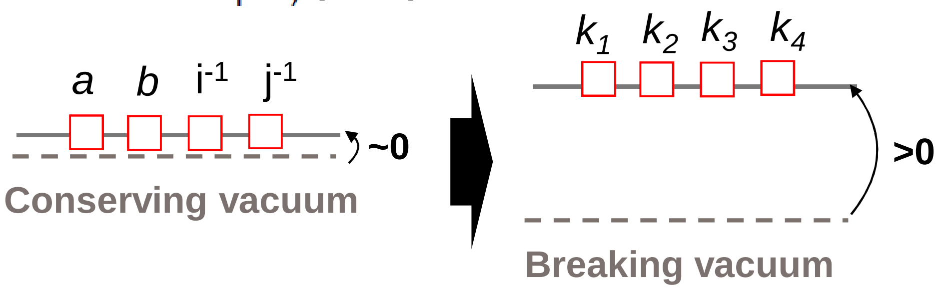
➢ High-order non-perturbative single-determinant method if near-degeneracy = slow convergence

➢ Multi-reference/configuration methods, e.g. MR-MBPT, MR-CC, MR-IMSRG, valence-space CI

➢ Expand around **a symmetry-breaking** reference product state $|\Phi\rangle$ **(non-perturbative static correlations)**

➞ **Lifts the degeneracy, e.g. BMBPT(2)** [U(1) group]

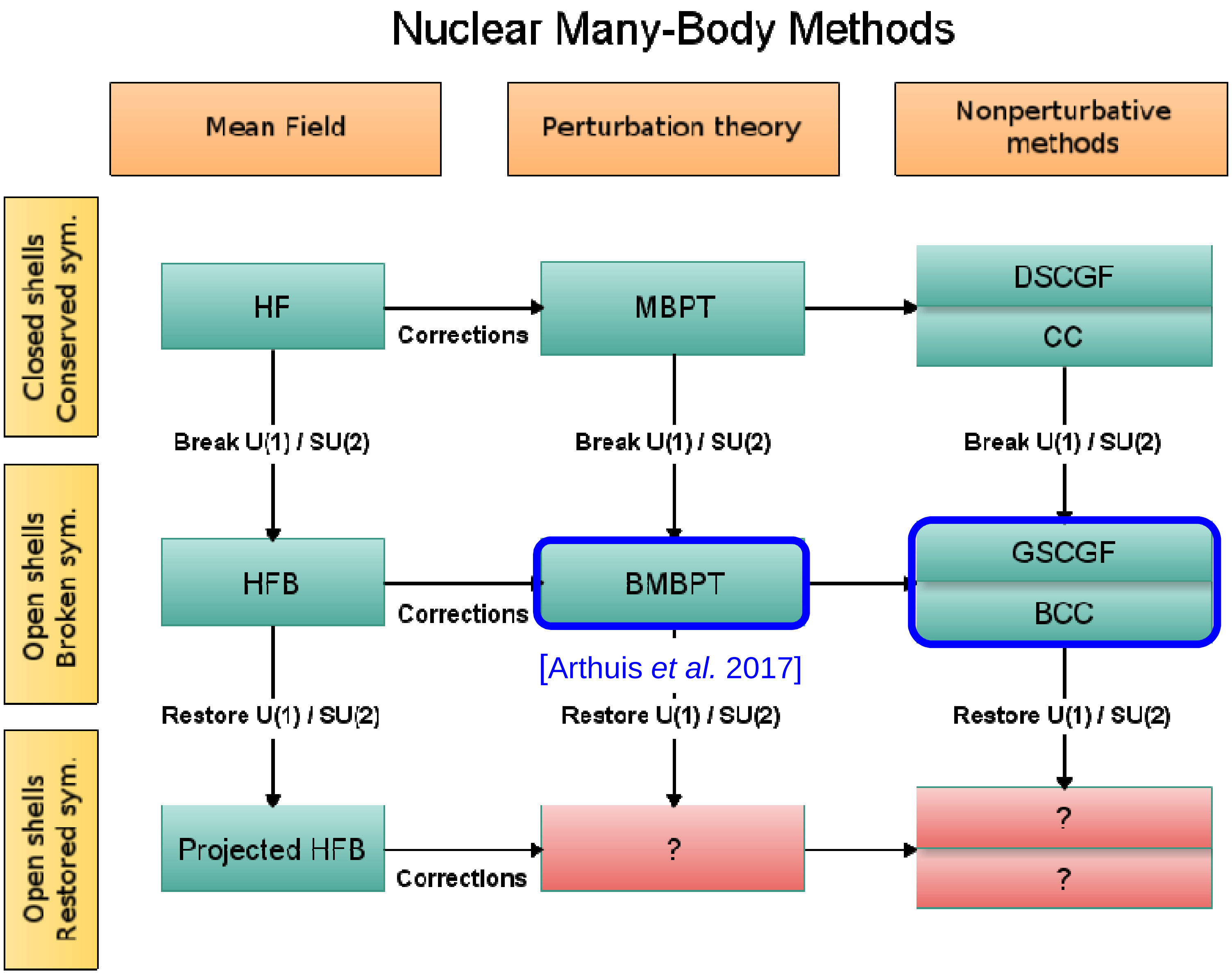
$$\Delta E^{(2)} = -\frac{1}{4!}\sum_{k_1k_2k_3k_4}\frac{|\Omega^{40}_{k_1k_2k_3k_4}|^2}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}} > 0$$



➞ **Symmetries** must be **restored** in finite quantum systems (non-perturbative static correlations)

1) Lowest reference energy 2) Expansion well behaved again

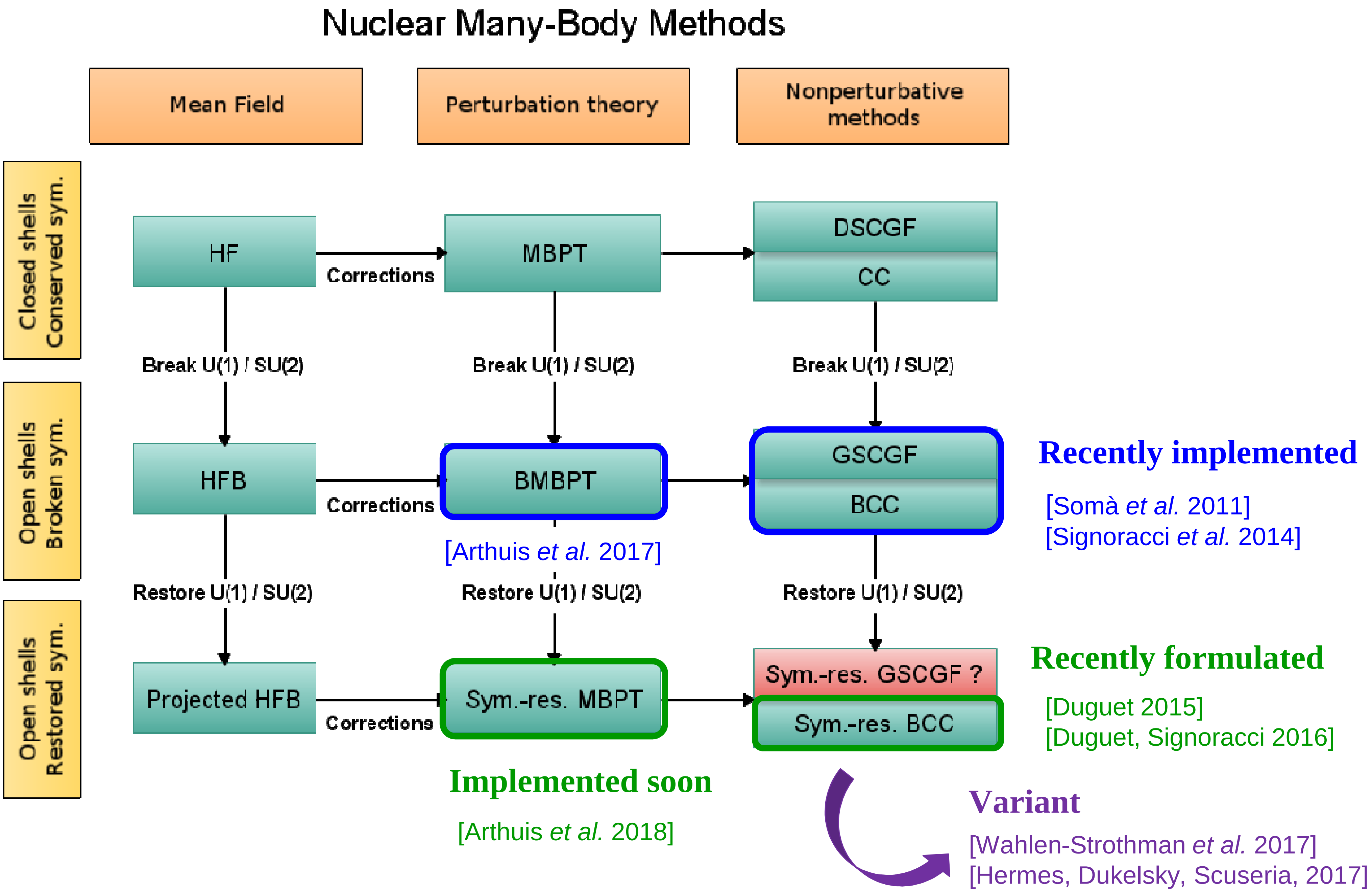
Single-reference many-body methods and symmetries



Recently implemented

[Somà *et al.* 2011]
[Signoracci *et al.* 2014]

Single-reference many-body methods and symmetries



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- ◉ **Conclusions and perspectives**

Basic ingredients

Nuclear Hamiltonian

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

Nuclear grand potential

$$\Omega \equiv H - \lambda A$$

$$[H, S(\varphi)] = [A, S(\varphi)] = [\Omega, S(\varphi)] = 0$$

Schroedinger equation

$$\begin{cases} \Omega|\Psi_\mu^{\mathrm{A}}\rangle = \Omega_\mu^{\mathrm{A}}|\Psi_\mu^{\mathrm{A}}\rangle \\ A|\Psi_\mu^{\mathrm{A}}\rangle = \mathrm{A}|\Psi_\mu^{\mathrm{A}}\rangle \end{cases}$$

with $\Omega_\mu^{\mathrm{A}} \equiv \mathrm{E}_\mu^{\mathrm{A}} - \lambda \mathrm{A}$

U(1) symmetry group

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

$$\langle \Psi_\mu^{\mathrm{A}} | S(\varphi) | \Psi_{\mu'}^{\mathrm{A}'} \rangle \equiv e^{i\mathrm{A}\varphi}\, \delta_{\mathrm{AA}'}\, \delta_{\mu\mu'}$$

Bogoliubov vacuum

$$|\Phi\rangle \equiv C \prod_\alpha \beta_\alpha |0\rangle$$

$$\beta_k |\Phi\rangle = 0 \;\forall k$$

$A|\Phi\rangle \neq \mathrm{A}|\Phi\rangle$

Breaks U(1) symmetry

Bogoliubov transformation

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

Quasi-particle excitations

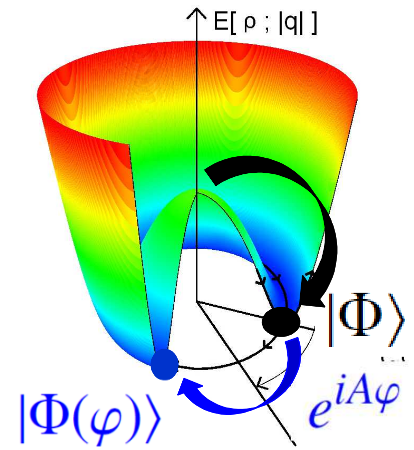
$$|\Phi^{\alpha\beta\ldots}\rangle \equiv \beta_\alpha^\dagger \beta_\beta^\dagger \ldots |\Phi\rangle$$

1p1h <-> 2qp
2ph2h <-> 4qp
⋮

Manifold of gauge-rotated Bogoliubov states

$$\mathcal{M}_{U(1)} \equiv \left\{ |\Phi(\varphi)\rangle \equiv S(\varphi)|\Phi\rangle; \varphi \in [0, 2\pi] \right\}$$

$|\Phi^{\alpha\beta\ldots}(\varphi)\rangle \equiv \beta_\alpha^\dagger \beta_\beta^\dagger \ldots |\Phi(\varphi)\rangle$ **Unrotated quasi-particle creation operators**



Master equations

A of interest

Ground-state $|\Psi_0^{A}\rangle \equiv \frac{\mathcal{U}(\infty)|\Phi\rangle}{\langle\Phi|\mathcal{U}(\infty)|\Phi\rangle}$ with $\mathcal{U}(\tau) \equiv e^{-\tau\Omega}$

Bogoliubov reference state

Off-diagonal kernels

$$\mathcal{N}(\varphi) \equiv \langle\Phi(\varphi)|\Psi_0^{A}\rangle$$

$$\mathcal{A}(\varphi) \equiv \langle\Phi(\varphi)|A|\Psi_0^{A}\rangle$$

$$\Omega(\varphi) \equiv \langle\Phi(\varphi)|\Omega|\Psi_0^{A}\rangle$$

$$\mathcal{H}(\varphi) = \Omega(\varphi) + \lambda\mathcal{A}(\varphi)$$

Gauge-rotated Bogoliubov states

- IRREPs mixed
- The good symmetry is lost
- Symmetry contaminants

Exact off-diagonal kernels

$$\mathcal{N}(\varphi) = e^{-iA\varphi}$$

$$\mathcal{A}(\varphi) = Ae^{-iA\varphi} = A\mathcal{N}(\varphi)$$

$$\Omega(\varphi) = \Omega_0^{A} e^{-iA\varphi} = \Omega_0^{A}\mathcal{N}(\varphi)$$

- Proper IRREP of U(1) selected
- Coefficient delivers g.s. eigenvalue

Expanded + truncated around $|\Phi\rangle$

$$\mathcal{N}(\varphi) \approx \sum_{A'\in\mathbb{N}} N_{app}^{A'} e^{-iA'\varphi}$$

$$\mathcal{A}(\varphi) \approx \sum_{A'\in\mathbb{N}} A_{app}^{A'} N_{app}^{A'} e^{-iA'\varphi}$$

$$\Omega(\varphi) \approx \sum_{A'\in\mathbb{N}} \Omega_{app}^{A'} N_{app}^{A'} e^{-iA'\varphi}$$

Standard methods

$$\mathcal{N}(0) \approx \sum_{A'\in\mathbb{N}} N_{app}^{A'} \otimes$$

$$\mathcal{A}(0) \approx \sum_{A'\in\mathbb{N}} A_{app}^{A'} N_{app}^{A'} \otimes$$

$$\Omega(0) \approx \sum_{A'\in\mathbb{N}} \Omega_{app}^{A'} N_{app}^{A'} \otimes$$

Symmetry-restored observables

$$E_0^{A} \approx E_{app}^{A} = \frac{\int_0^{2\pi} d\varphi\, e^{iA\varphi}\,\mathcal{H}(\varphi)}{\int_0^{2\pi} d\varphi\, e^{iA\varphi}\,\mathcal{N}(\varphi)}$$

$$A = A_{app}^{A} = \frac{\int_0^{2\pi} d\varphi\, e^{iA\varphi}\,\mathcal{A}(\varphi)}{\int_0^{2\pi} d\varphi\, e^{iA\varphi}\,\mathcal{N}(\varphi)}$$

Orthogonality of IRREPs

Extract good IRREP

Design linked MBPT and CC expansions of off-diagonal kernels

Symmetry is restored

-No fingerprint of mixing left to be used

Superfluous in exact limit but not after truncation

Benefit of inserting rotation operator in kernels

Bogoliubov coupled cluster scheme – end result (1)

…after working out BMBPT and CC many-body expansions (derivations, diagrammatics etc see [T. Duguet, A. Signoracci (2016)]**)…**

Off-diagonal operator kernels

$$\mathcal{A}(\varphi) \equiv a(\varphi)\mathcal{N}(\varphi)$$

$$\Omega(\varphi) \equiv \omega(\varphi)\mathcal{N}(\varphi)$$

Linked/connected kernels

Gauge-rotated Bogoliubov coupled cluster amplitudes

$$\mathcal{T}(\varphi) \equiv \sum_{n\in\mathbb{N}} \mathcal{T}_n(\varphi)$$

S <-> 2qp
D <-> 4qp
T <-> 6qp
⋮

$$\mathcal{T}_n(\varphi) \equiv \frac{1}{(2n)!} \sum_{k_1\ldots k_{2n}} \mathcal{T}_{k_1\ldots k_{2n}}(\varphi)\, \beta^\dagger_{k_1} \ldots \beta^\dagger_{k_{2n}}$$

Off-diagonal linked-connected energy and amplitude equations

Linked/terminating BCC expansion
Off-diagonal Wick theorem

Diagonal (standard) Wick theorem

$$\omega(\varphi) = \frac{\langle \Phi(\varphi)|\Omega e^{\mathcal{T}(\varphi)}|\Phi\rangle_c}{\langle \Phi(\varphi)|\Phi\rangle} \qquad \Phi|\tilde{\Omega}(\varphi)e^{\mathcal{T}(\varphi)}|\Phi\rangle_c$$

$$0 = \frac{\langle \Phi^{\alpha\beta\ldots}(\varphi)|\Omega e^{\mathcal{T}(\varphi)}|\Phi\rangle_c}{\langle \Phi(\varphi)|\Phi\rangle} = \langle \Phi^{\alpha\beta\ldots}|\tilde{\Omega}(\varphi)e^{\mathcal{T}(\varphi)}|\Phi\rangle_c$$

Off-diagonal Bogoliubov coupled cluster kernels with original Hamiltonian

Rich algebraic form
e.g. ω(φ) contains 20 diagrams

Diagonal (standard) Bogoliubov coupled cluster kernels with gauge-rotated Hamiltonian!

Same algebraic form as BCC
e.g. ω(φ) contains 4 diagrams

Gauge-rotated operators

$$\tilde{\Omega}(\varphi) \equiv M(\varphi)\Omega M^{-1}(\varphi)$$

$$\tilde{A}(\varphi) \equiv M(\varphi) A M^{-1}(\varphi)$$

Non-unitary transformation

Coupled cluster scheme – end result (2)

Off-diagonal norm kernel

$$\frac{d}{d\varphi}\mathcal{N}(\varphi) + i\,a(\varphi)\,\mathcal{N}(\varphi) = 0 \quad \Rightarrow \quad \boxed{\mathcal{N}(\varphi) = e^{-i\int_0^{\varphi} d\phi\, a(\phi)}}$$

$i\,a(\varphi)\,\mathcal{N}(\varphi)$ → $\mathcal{A}(\varphi)$

ln$\mathcal{N}(\varphi)$ has a terminating BCC expansion
linked
↓
BCC truncated $a(\varphi)$

Particle-number restored energy

$$h(\varphi) \equiv \omega(\varphi) + \lambda a(\varphi)$$

$$\text{A}= \text{A}^{\text{A}}_{\text{app}} = \frac{\int_0^{2\pi} d\varphi\, e^{i\text{A}\varphi}\,\mathcal{A}(\varphi)}{\int_0^{2\pi} d\varphi\, e^{i\text{A}\varphi}\,\mathcal{N}(\varphi)}$$

$$\text{E}^{\text{A}}_0 \approx \text{E}^{\text{A}}_{\text{app}} = \frac{\int_0^{2\pi} d\varphi\, e^{i\text{A}\varphi}\, h(\varphi)\mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi\, e^{i\text{A}\varphi}\,\mathcal{N}(\varphi)}$$

-Needs typically 10 discretization points in φ
-10 independent BBC-like calculations

Consistent BCC expansions of $h(\varphi)$ and $\mathcal{N}(\varphi)$ (via $a(\varphi)$)

1) BMBPT version of the formalism available
2) A symmetry-restored QRPA method can be extracted

Two important limits

Diagonal formalism at φ = 0 : standard BCC theory

$$\omega(0) = \langle \Phi | \Omega e^{\mathcal{T}} | \Phi \rangle_c$$

$$0 = \langle \Phi^{\alpha\beta\cdots} | \Omega e^{\mathcal{T}} | \Phi \rangle_c$$

Gives directly the energy h(0)=ω(0)+λa(0) as $\mathcal{N}$(0)=1
Off-diagonal theory underlines importance of $\mathcal{N}$(φ)

Missing static correlations

Zeroth-order formalism : projected HFB theory

$$\text{E}^{\text{A}(0)}_0 = \frac{\int_0^{2\pi} d\varphi\, e^{i\text{A}\varphi}\,\langle \Phi(\varphi)|H|\Phi\rangle}{\int_0^{2\pi} d\varphi\, e^{i\text{A}\varphi}\,\langle \Phi(\varphi)|\Phi\rangle} = \frac{\langle \Theta^{\text{A}}|H|\Theta^{\text{A}}\rangle}{\langle \Theta^{\text{A}}|\Theta^{\text{A}}\rangle}$$

$$|\Theta^{\text{A}}\rangle \equiv P^{\text{A}}|\Phi\rangle \equiv \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{-i\text{A}\varphi}\, S(\varphi)|\Phi\rangle$$

No dynamical correlations

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◉ **Conclusions and perspectives**

Conclusions and perspectives

◉ Formulation of symmetry broken&restored BMBPT and BCC theory

○ Offer a consistent way to capture static and dynamical correlations along with their interference

○ The formalism is valid (i.e. can be adapted) to any symmetry

◉ First step is to implement the symmetry broken theory for U(1) in semi-magic nuclei

○ First implementation of BCC [Signoracci *et al.* 2014]

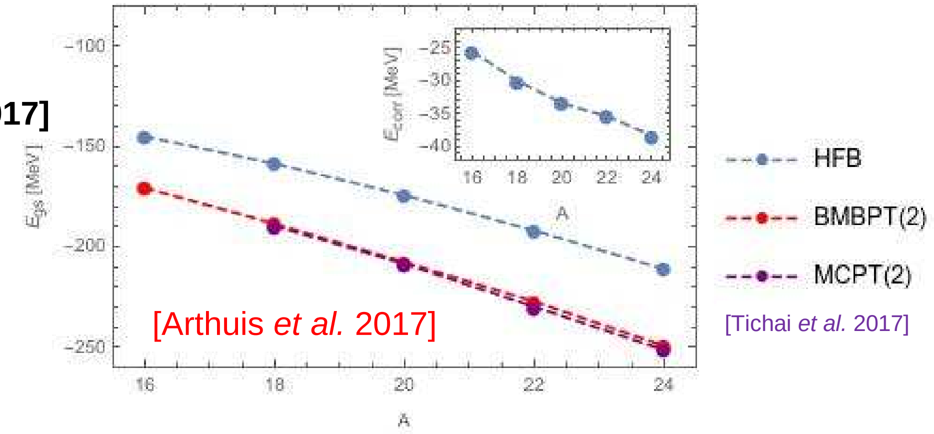
○ **On-going implementation of BMBPT [Arthuis *et al.* 2017]**

◉ Implementation of symmetry restoration step next

○ **Particle-number restored BMBPT [Arthuis *et al.* 2018]**

○ Particle-number restored BCC [next]

BE of $^{16-24}$O at BMBPT(2)



Collaborators on ab initio nuclear many-body calculations

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