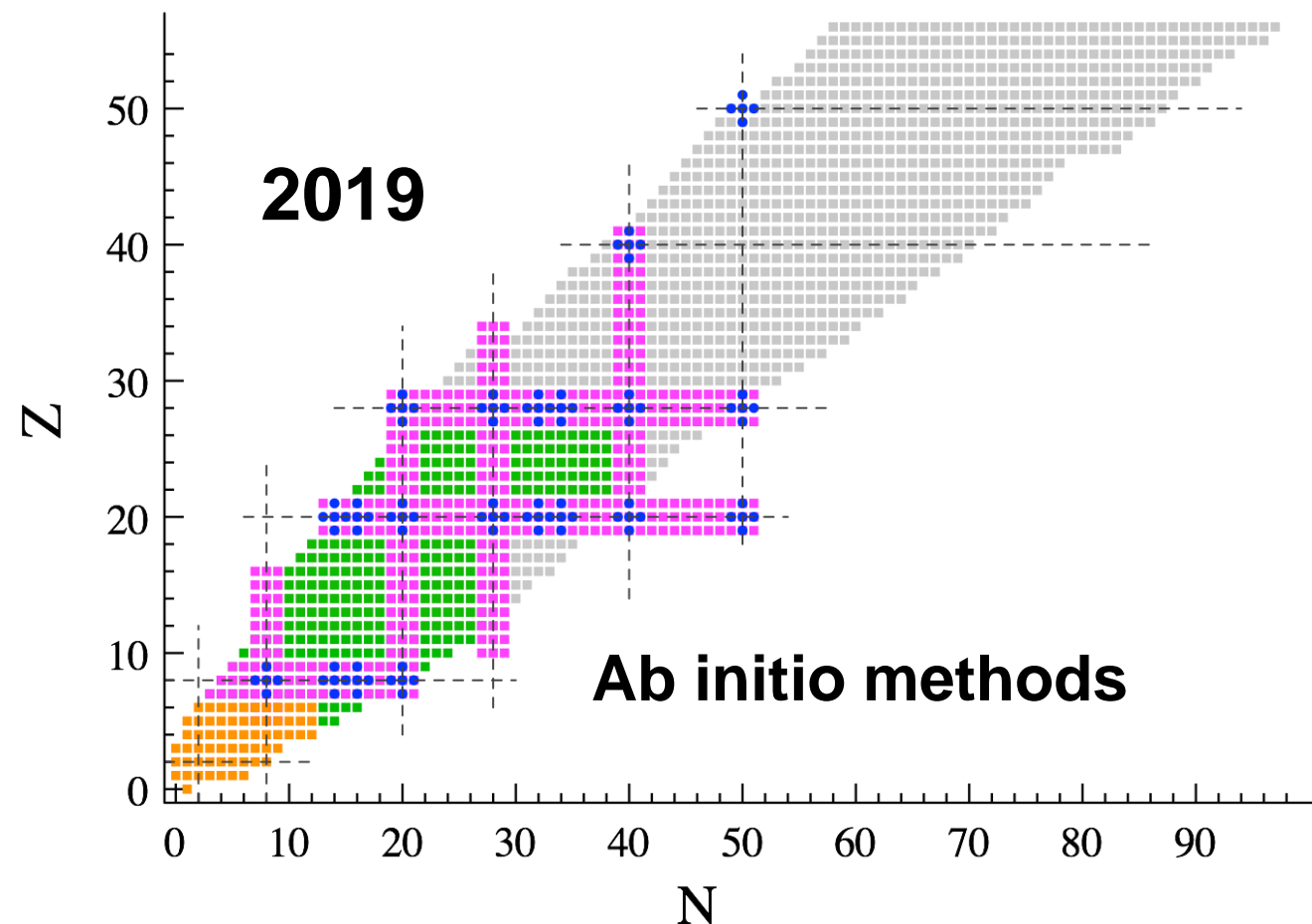


Particle-number projected Bogoliubov coupled cluster formalism

From weakly to strongly correlated systems



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Recent advances on proton-neutron pairing and quartet correlations in nuclei
ESNT workshop, Sept 2-6 2019, Saclay, France

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● Breaking and restoring symmetries in quantum many-body theory

- Prolegomena

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● Application to Richardson/BCS pairing Hamiltonian

● Conclusions

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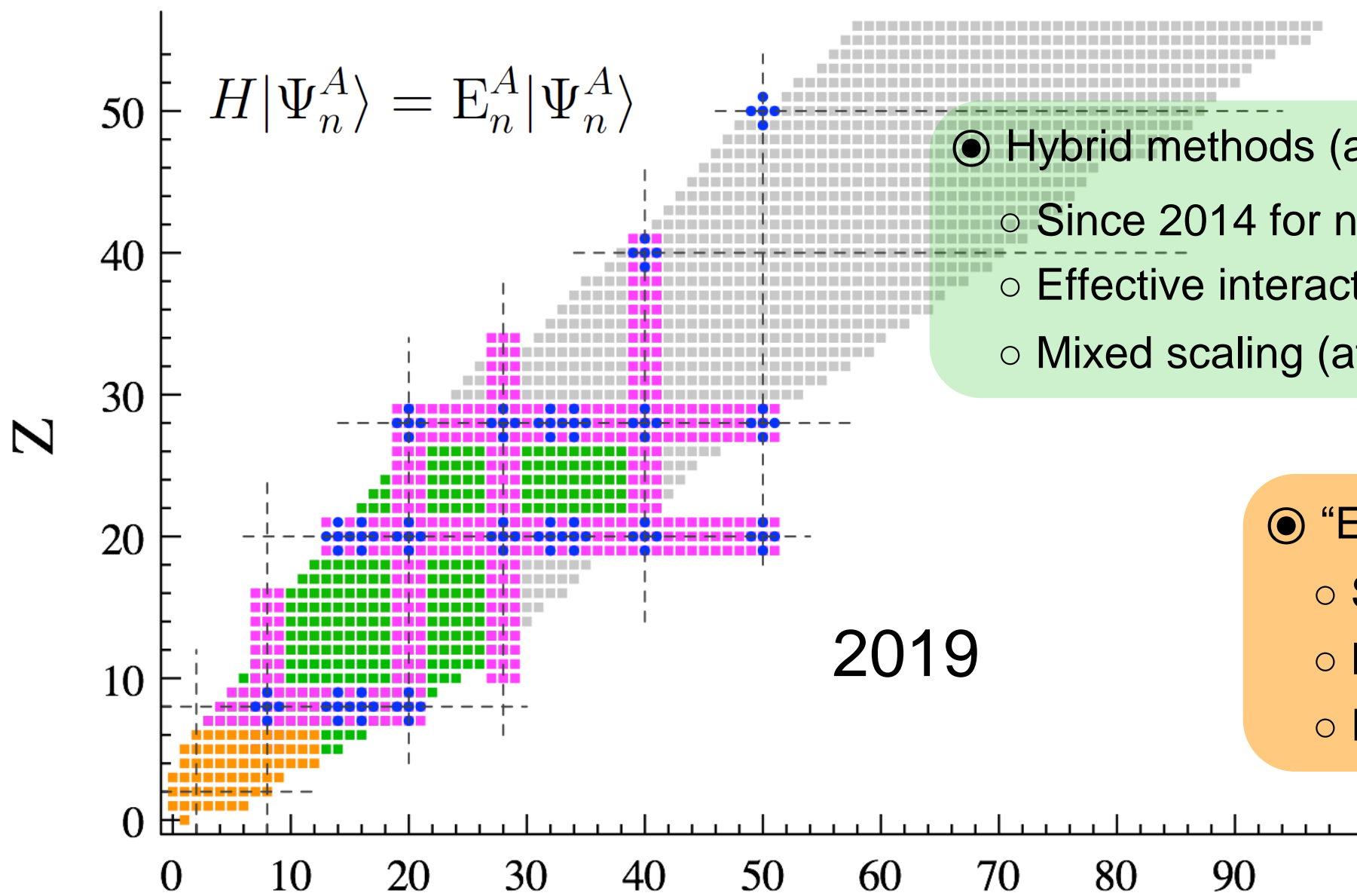
Ab initio nuclear chart

Approximate methods for closed-shells

- Since 2000's
- MBPT, SCGF, CC, IMSRG
- Polynomial scaling

Approximate methods for open-shells

- Since 2010's
- **(P)BMBPT, GGF, (P)BCC**, MR-IMSRG, MCPT
- Polynomial scaling



Hybrid methods (ab initio shell model)

- Since 2014 for non-perturbative methods
- Effective interaction via MBPT/NCSM/CC/IMSRG
- Mixed scaling (at best)

"Exact" methods

- Since 1980's
- Monte Carlo, CI, ...
- Factorial/exponential scaling

N **Bold** = symmetry breaking (& restoration) single-reference methods

Single-reference expansion many-body methods

Nuclear Hamiltonian

$$H = T + V^{2N} + W^{3N}$$

Symmetry group $U(1)$ dealt with today

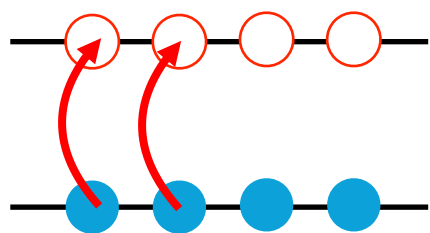
$$[H, S] = 0 \quad \text{where} \quad S \equiv \boxed{A}, J^2, J_z \dots$$

Mean-field reference state

$$H = H_0 + H_1 \quad \text{such that} \quad \begin{aligned} [H_0, S] &= 0 \\ [H_1, S] &= 0 \end{aligned}$$

$$\Rightarrow \underline{H_0 |\Phi_0^S\rangle = \mathcal{E}_0^S |\Phi_0^S\rangle} \quad \text{Exactly solvable}$$

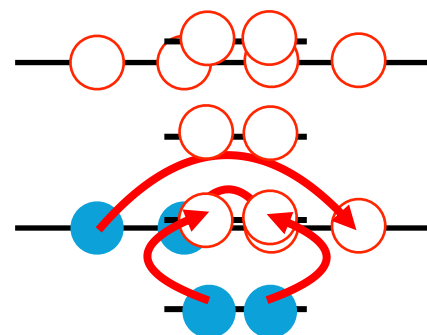
Closed-shell



Non-degenerate

Good starting point

Open-shell



Non-degenerate

Improper starting point

A-body eigenvalue problem

$$H |\Psi_0^S\rangle = E_0^S |\Psi_0^S\rangle \quad N^A \text{ cost where } N = \dim \mathcal{H}_1$$

Many-body expansion

$$H = H_0 + H_1$$

$$|\Psi_0^S\rangle = \underline{U^S(\infty)} \underline{|\Phi_0^S\rangle}$$

Wave operator Reference state

- ▶ Accounts for « weak/dynamical » correlations
- ▶ Expand as a series (MBPT, CC...) + truncate = N^p cost

Symmetry breaking

$$[H'_0, S] \neq 0$$

$$[H'_1, S] \neq 0$$

$$H = H'_0 + H'_1$$

$$|\Psi_0^S\rangle = \underline{U(\infty)} \underline{|\Phi_0\rangle} \quad \text{More general reference state}$$

- ▶ Accounts for “strong/non-dynamical” correlations
- ▶ Expand (BMBPT, BCC...) + truncate = N^p cost

- 1) Truncated series breaks symmetry
- 2) Exact symmetry must eventually be restored

Single-reference expansion many-body methods and symmetries

Nuclear Many-Body Methods

Mean Field

Perturbation theory

Nonperturbative
methods

Hamiltonian H

HF

MBPT

DSCGF

CC

Corrections

1 Break $U(1) / SU(2)$

Break $U(1) / SU(2)$

Break $U(1) / SU(2)$

HFB

BMBPT

GSCGF

BCC

Corrections

Restore $U(1) / SU(2)$

[Henley, Willets, 1964]
[Duguet, Signoracci 2016]
[Tichai *et al.* 2018]

Restore $U(1) / SU(2)$

Projected HFB

?

Corrections

?

?

Closed shells
Conserved sym.

Open shells
Broken sym.

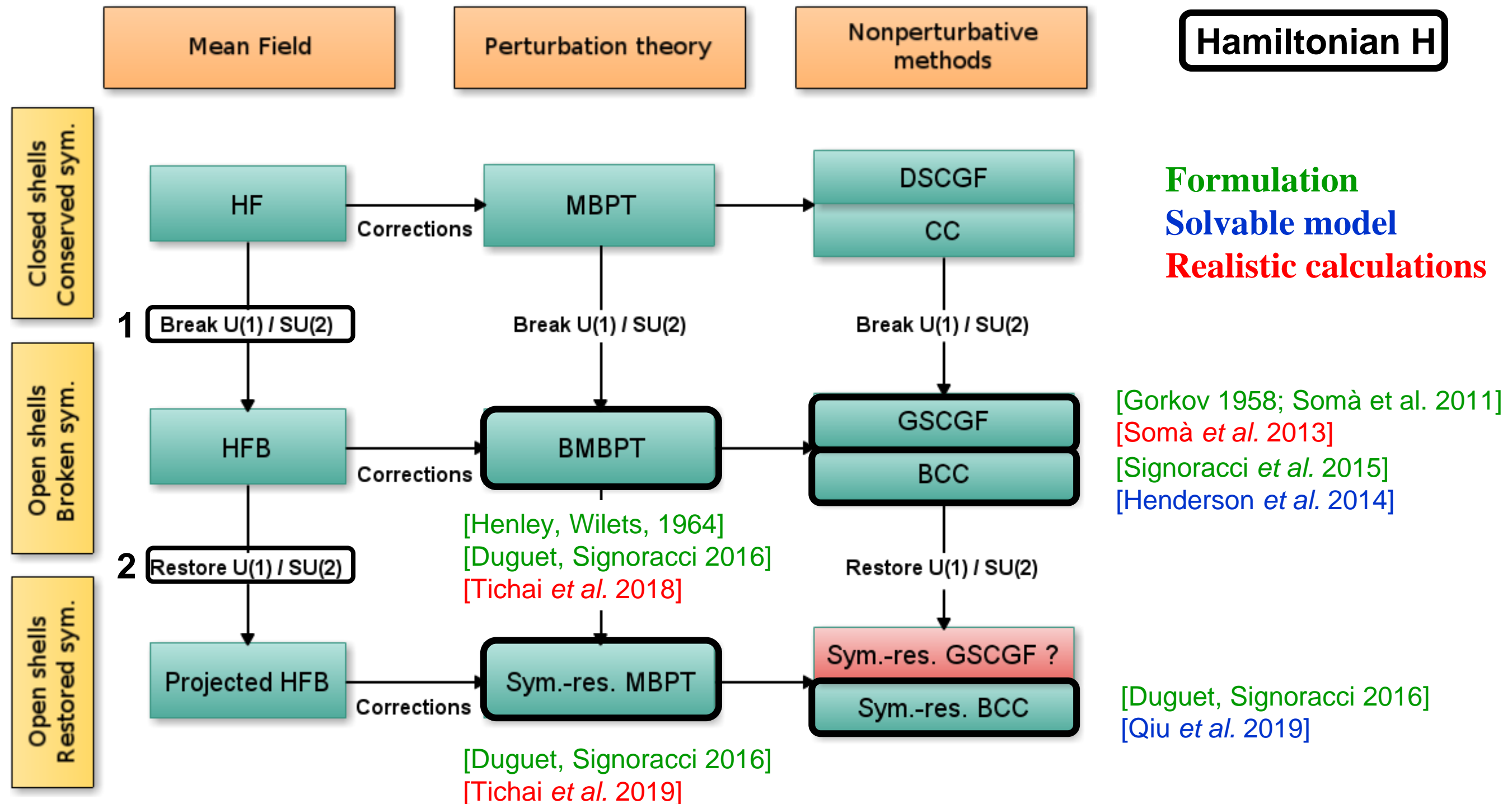
Open shells
Restored sym.

Formulation
Solvable model
Realistic calculations

[Gorkov 1958; Somà *et al.* 2011]
[Somà *et al.* 2013]
[Signoracci *et al.* 2015]
[Henderson *et al.* 2014]

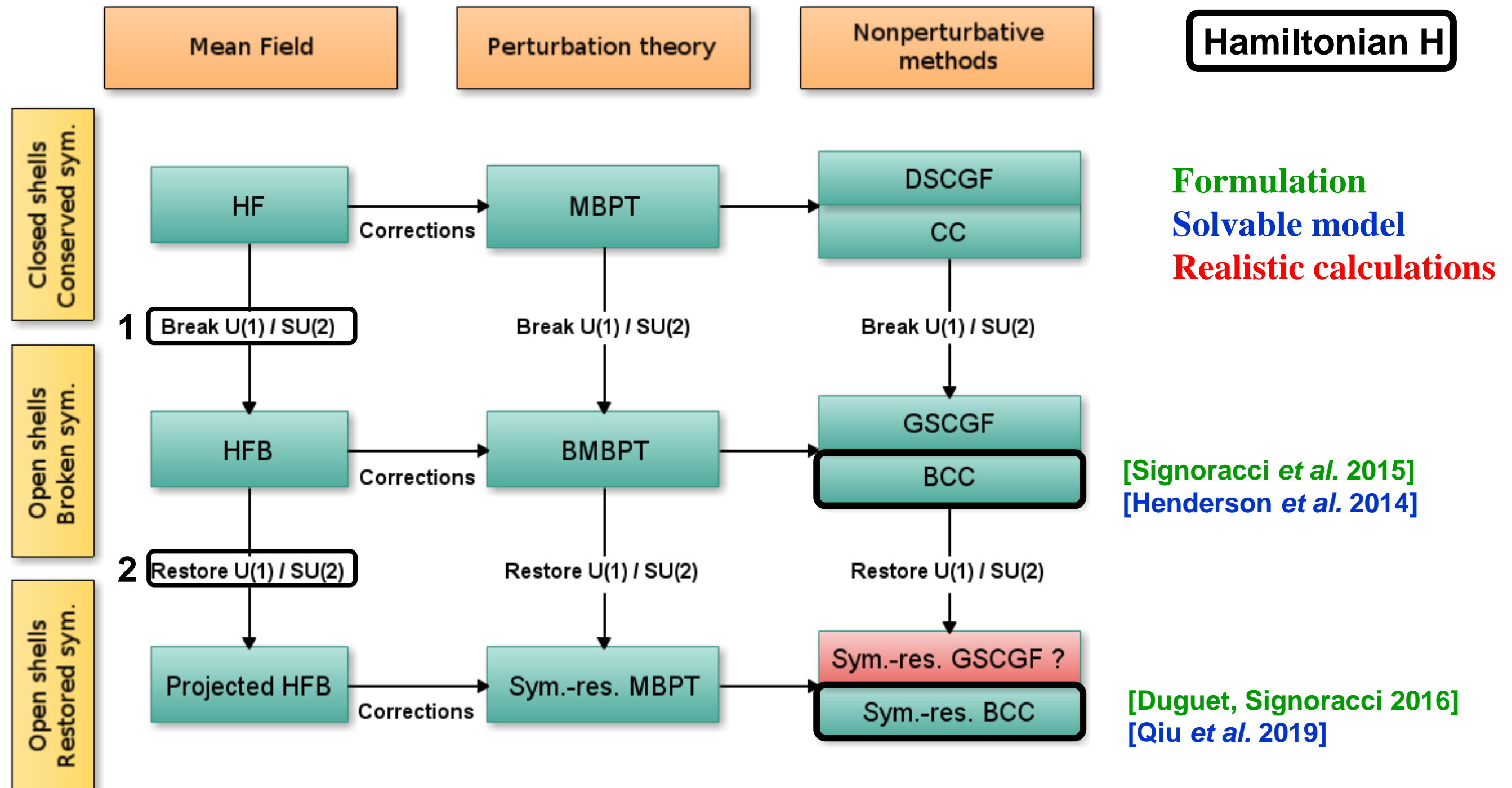
Single-reference expansion many-body methods and symmetries

Nuclear Many-Body Methods



Single-reference expansion many-body methods and symmetries

Nuclear Many-Body Methods



Today: BCC and Projected BCC formalism applied to the pairing (Richardson) Hamiltonian

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Operators

Nuclear Hamiltonian

$$\begin{aligned}
 H \equiv & \frac{1}{(1!)^2} \sum_{pq} t_{pq} c_p^\dagger c_q \\
 & + \frac{1}{(2!)^2} \sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r \\
 & + \frac{1}{(3!)^2} \sum_{pqrst} \bar{w}_{pqrst} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s \left. \vphantom{\sum_{pqrst}} \right\}
 \end{aligned}$$

Genuine 3N interaction / six-legs vertex

Grand potential

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

When working in Fock space

Chemical potential



Controls the average particle number in the system

Particle number

$$A \equiv \sum_p c_p^\dagger c_p$$

k-body force



Mode-2k tensor



Basis representation dim N



Storage cost N^{2k}

Bogoliubov reference state and normal ordering

Bogoliubov reference state

$$\beta_k = \sum_p U_{pk}^* c_p + V_{pk}^* c_p^\dagger$$

$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p$$

$$|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$$

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

Vacuum state
Reduces to SD in \mathcal{H}_A for closed-shell

Breaks U(1) symmetry

$$A|\Phi\rangle \neq A|\Phi\rangle$$

Normal ordering via Wick's theorem in quasi-particle basis

$$H \equiv \sum_{n=0}^3 \sum_{i+j=2n} \frac{1}{i!j!} \sum_{l_1 \dots l_{i+j}} H_{l_1 \dots l_{i+j}}^{ij} \beta_{k_1}^\dagger \dots \beta_{k_i}^\dagger \beta_{k_{i+j}} \dots \beta_{k_{i+1}}$$

H^{ij} matrix elements function of

$$t_{pq} \quad \bar{v}_{pqrs} \quad \bar{w}_{pqrst} \quad U_{pk} \quad V_{pk}$$

$$\equiv \underbrace{H^{00} + [H^{20} + H^{11} + H^{02}]}_{H_0} + [H^{40} + H^{31} + H^{22} + H^{13} + H^{04}] + \boxed{\sum_{i+j=6} H^{ij}}$$

$$\equiv \sum_{n=0}^2 H^{[2n]} \boxed{+ H^{[6]}} \quad \text{6-qp operators}$$

Similarly for A and Ω

➡ **Six-index tensors**
Too expensive to handle

➡ **NO2B approximation**
1-3% error in closed shell
[Roth et al., PRL 109 (2012) 052501]

➡ **PNO2B approximation**
Particle-number conserving
[Ripoche, Tichai, Duguet, arXiv:1908.00765]

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BCC formalism

Bogoliubov reference state

$$|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$$

Quasi-particle excitations

[Signoracci *et al.* PRC 2015]

$$\mathcal{B}^\mu \equiv \mathcal{B}^{k_1 \dots k_{2n}} = \beta_{k_1}^\dagger \dots \beta_{k_{2n}}^\dagger$$

$$|\Phi^\mu\rangle \equiv \mathcal{B}^\mu |\Phi\rangle$$

Orthonormal basis of Fock space

Bogoliubov CC ansatz

$$|\Psi_{\text{BCC}}^A\rangle \equiv e^U |\Phi\rangle \quad \text{with}$$

as soon as U is truncated

$$U = \sum_{n=1} U_n$$

Cluster amplitudes
Unknowns of the problem

$$U_n \equiv \frac{1}{(2n)!} \sum_{k_1 \dots k_{2n}} U_{k_1 \dots k_{2n}}^{2n0} \underbrace{\beta_{k_1}^\dagger \dots \beta_{k_{2n}}^\dagger}_{\text{n-tuple connected cluster operator}}$$

Reduces to npnh excit. in closed-shell

Energy and amplitude equations

$$H|\Psi^A\rangle = E^A |\Psi^A\rangle$$

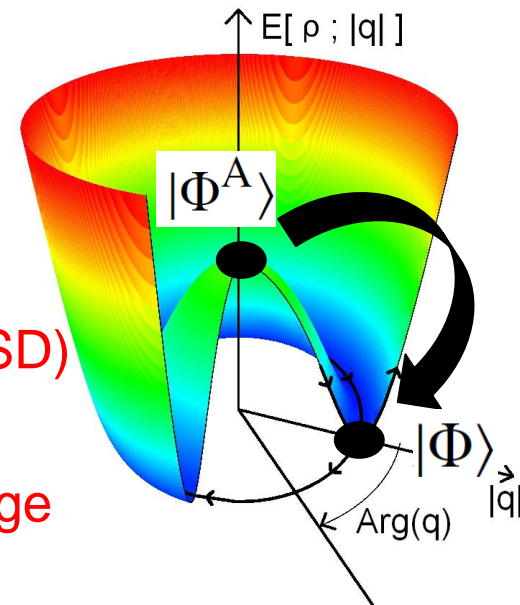
$$A|\Psi^A\rangle = 0$$

$$\begin{aligned} \langle \Phi | & \left| \begin{aligned} E^A &= \langle \Phi | H e^U | \Phi \rangle_C \\ 0 &= \langle \Phi^\mu | H e^U | \Phi \rangle_C \\ A^A &= \langle \Phi | A e^U | \Phi \rangle_C \end{aligned} \right. \end{aligned}$$

Pure excitation operators

Truncate, e.g. $U = U_1 + U_2$ (BCCSD)
Solve for $n=1,2$

Constrained to be true in average



Ex: for the energy

Connected = terminating exponential

Algebraic expression through Wick's theorem/diagrammatic rules

$$E^A = H^{00} + \frac{1}{2} \sum_{k_1 k_2} H_{k_1 k_2}^{02} U_{k_1 k_2}^{20} + \frac{1}{8} \sum_{k_1 k_2 k_3 k_4} H_{k_1 k_2 k_3 k_4}^{04} U_{k_1 k_2}^{20} U_{k_3 k_4}^{20} + \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} H_{k_1 k_2 k_3 k_4}^{04} U_{k_1 k_2 k_3 k_4}^{40}$$

Bogoliubov many-body perturbation formalism

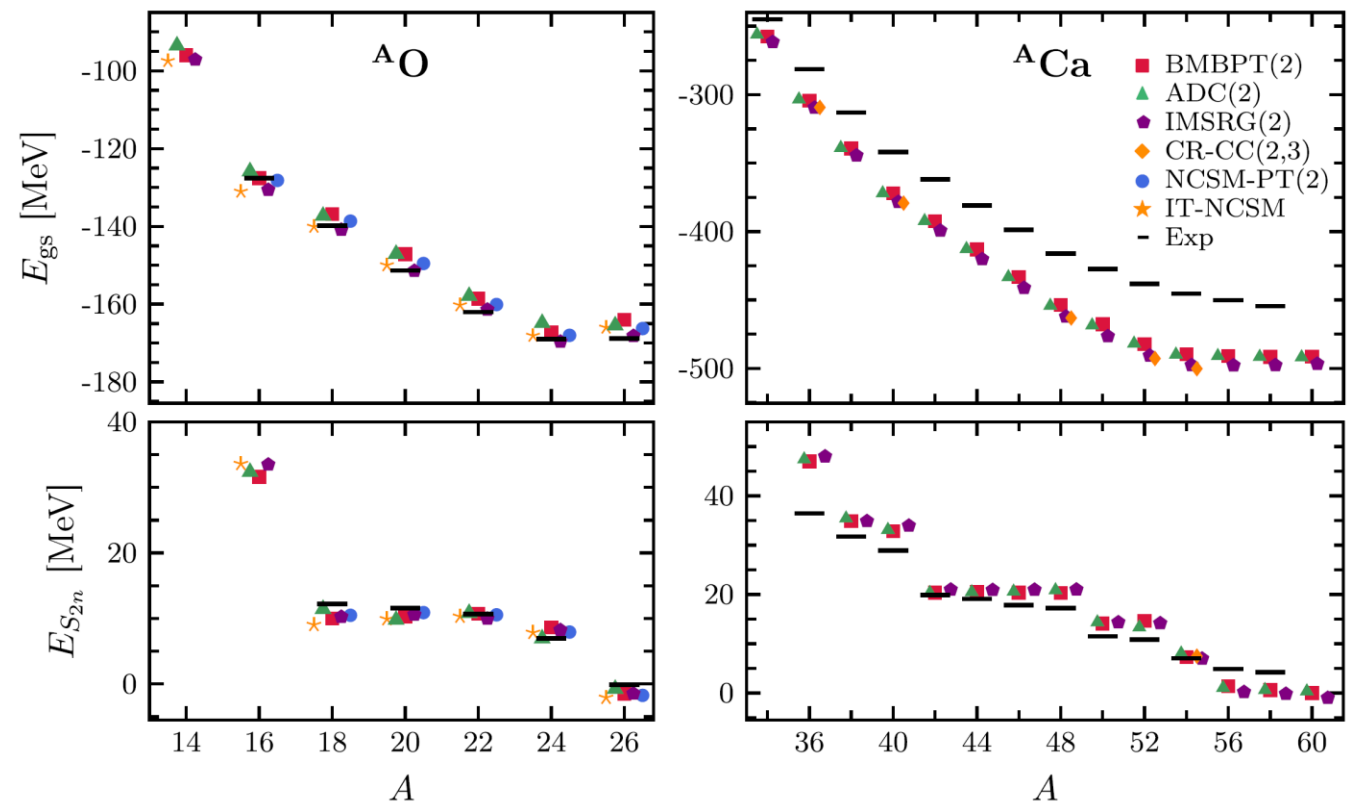
● Perturbative reduction of BCC

[Duguet, Signoracci JPG 2016]

→ Code for automated generation&evaluation of many-body diagrams to arbitrary order [Arthuis et al. CPC 2018]

→ Convergence properties at high orders and resummation methods [Demol et al. to be published 2019]

● **BMBPT(2)** ab initio calculations of mid-mass semi-magic nuclei [Tichai et al. PLB 2018]



Calculation details

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

Runtime

NCSM: 20.000 hours
MCPT: 2.000 hours
IMSRG(2): 1.500 hours
SCGF(2): 400 hours
BMBPT(2): < 1min !

→ 2-3% agreement of all methods with exact results (IT-NCSM)

→ Different truncation schemes yield **consistent description** of open-shell nuclei

→ BMBPT optimal to systematically test **next generation of Chiral EFT nuclear Hamiltonians**

● Future implementation of BCCSD(T) for accurate ab initio calculations of open-shell nuclei

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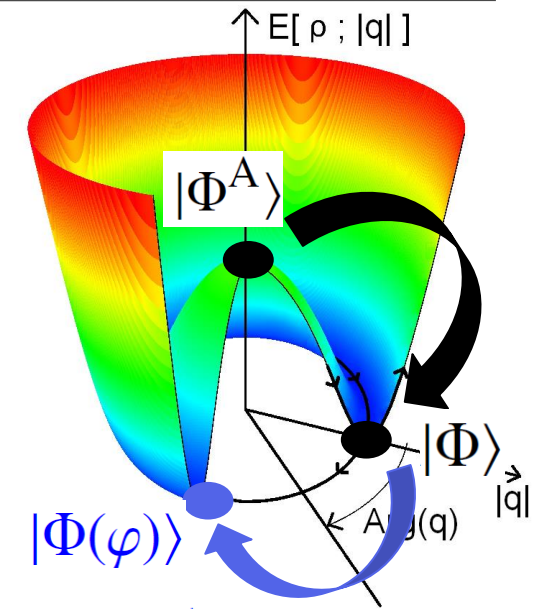
U(1) breaking and projection

Particle-number conserving states, i.e. states belonging to \mathcal{H}_A

Exact eigenstates of H: $|\Psi_\mu^A\rangle$ Slater determinants: $|\Phi^A\rangle = \prod_{i=1}^A a_i^\dagger |0\rangle$

Particle-number breaking states

General states on Fock space: $|\Phi\rangle \Rightarrow A|\Phi\rangle \neq A|\Phi\rangle \Rightarrow |\Phi(\varphi)\rangle \equiv R(\varphi)|\Phi\rangle \neq e^{iA\varphi}|\Phi\rangle$



Particle-number projection operator

Thouless transformation of Bogoliubov states

$$P^A \equiv \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-iA\varphi} R(\varphi)$$

$$\langle \Phi(\varphi) | = \langle \Phi(\varphi) | \Phi \rangle \langle \Phi | e^{Z(\varphi)}$$

Known from (U,V,φ) Pure de-excitation operator

$$\text{with } Z(\varphi) \equiv \frac{1}{2} \sum_{k_1 k_2} Z_{k_1 k_2}^{02}(\varphi) \beta_{k_2} \beta_{k_1}$$

Particle number projection

$$|\Phi\rangle \equiv \sum_{A' \in \mathbb{N}} c_{A'} |\Theta^{A'}\rangle \Rightarrow P^A |\Phi\rangle \equiv \sum_{A' \in \mathbb{N}} \frac{c_{A'}}{2\pi} |\Theta^{A'}\rangle \underbrace{\int_0^{2\pi} d\varphi e^{-i(A-A')\varphi}}_{2\pi\delta_{AA'}} = c_A |\Theta^A\rangle$$

Extracts component in \mathcal{H}_A

Particle-number projected BCC formalism

Projected BCC ansatz

[Duguet, Signoracci JPG 2016]
[Qiu et al. PRC 2019]

$$|\Psi_{\text{PBCC}}^A\rangle \equiv P^A |\Psi_{\text{BCC}}^A\rangle \quad \text{Always true!}$$

Projected BCC energy and particle number

$$\begin{aligned} H|\Psi^A\rangle &= E^A|\Psi^A\rangle \\ A|\Psi^A\rangle &= A^A|\Psi^A\rangle \end{aligned} \quad \xrightarrow{\langle\Phi|} \left\{ \begin{aligned} E^A &= \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{H}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)} \\ A^A &= \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{A}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)} \end{aligned} \right.$$

Not a pure excitation operator...

$$\text{with } \left\{ \begin{aligned} \mathcal{N}(\varphi) &\equiv \langle\Phi(\varphi)|e^U|\Phi\rangle = \langle\Phi(\varphi)|\Phi\rangle\langle\Phi|e^{U_Z(\varphi)}|\Phi\rangle \\ \mathcal{H}(\varphi) &\equiv \langle\Phi(\varphi)|He^U|\Phi\rangle = \langle\Phi(\varphi)|\Phi\rangle\langle\Phi|H_Z(\varphi)e^{U_Z(\varphi)}|\Phi\rangle \\ \mathcal{A}(\varphi) &\equiv \langle\Phi(\varphi)|Ae^U|\Phi\rangle = \langle\Phi(\varphi)|\Phi\rangle\langle\Phi|A_Z(\varphi)e^{U_Z(\varphi)}|\Phi\rangle \end{aligned} \right.$$

Off-diagonal norm, Hamiltonian and particle-number kernels

Similarity transformed operator

$$O_Z(\varphi) \equiv e^{Z(\varphi)} O e^{-Z(\varphi)}$$

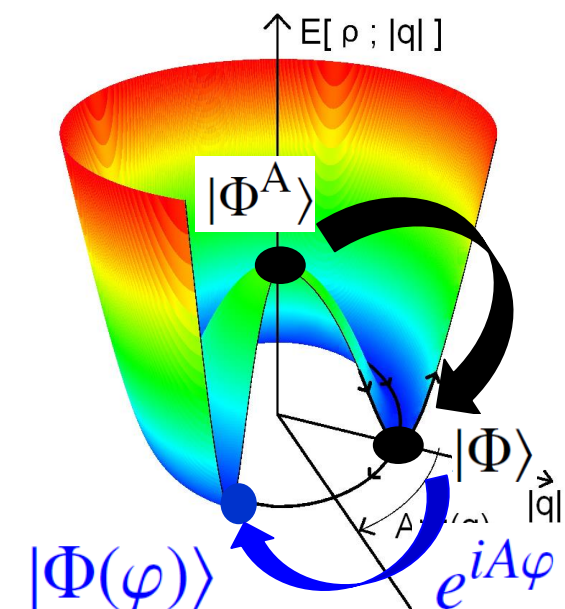


$$\begin{aligned} \begin{pmatrix} \beta(\varphi) \\ \beta^\dagger(\varphi) \end{pmatrix} &\equiv e^{Z(\varphi)} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} e^{-Z(\varphi)} \\ &= \begin{pmatrix} 1 & 0 \\ Z^{20}(\varphi) & 1 \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \end{aligned}$$

Non-unitary Bogoliubov transformation



Normal-ordered operator with ME $O_{k_1 \dots k_{i+j}}^{ij}(\varphi)$



Particle-number projected BCC formalism

Disentangled cluster operators



Disantengling the algebra to extract pure excitation terms

$$e^{U_Z(\varphi)}|\Phi\rangle \equiv e^{W(\varphi)}|\Phi\rangle$$



$$W(\varphi) = \sum_{n=0} W_n(\varphi) \equiv \underbrace{W_0(\varphi)}_{\text{Constant}} + \underbrace{\mathcal{T}(\varphi)}_{\text{Standard cluster operator form}}$$

with $W_n(\varphi) \equiv \frac{1}{2n!} \sum_{k_1 \dots k_{2n}} W_{k_1 \dots k_{2n}}^{2n0}(\varphi) \beta_{k_1}^\dagger \dots \beta_{k_{2n}}^\dagger$

- 1) Pure excitation operator **BUT contains a constant term**
- 2) Allows algebraic expressions of kernels following standard steps
- 3) Explicit relation between $W(\varphi)$ and $U_Z(\varphi)$ too complicated (need other approach)

Connected kernels and PBCC energy

$$\mathcal{N}(\varphi) \equiv \underline{e^{W_0(\varphi)}} \langle \Phi(\varphi) | \Phi \rangle$$

$$h(\varphi) \equiv \frac{\mathcal{H}(\varphi)}{\mathcal{N}(\varphi)} = \langle \Phi | H_Z(\varphi) e^{\mathcal{T}(\varphi)} | \Phi \rangle_C = \frac{H^{00}(\varphi)}{2} + \frac{1}{2} \sum_{k_1 k_2} H_{k_1 k_2}^{02}(\varphi) \underline{W_{k_1 k_2}^{20}(\varphi)}$$

But how to determine $W(\varphi)$?

Correlated norm kernel determined by $W_0(\varphi)$

Connected part of energy kernel determined by $\mathcal{T}(\varphi)$
Same algebraic/terminating form as standard BCC kernel!

$$E^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} h(\varphi) \mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)}$$

Consistent dynamical and static correlations

1) Reduction to BCC

$$E^A = \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \langle \Phi | H e^U | \Phi \rangle_C$$

2) Reduction to PHFB

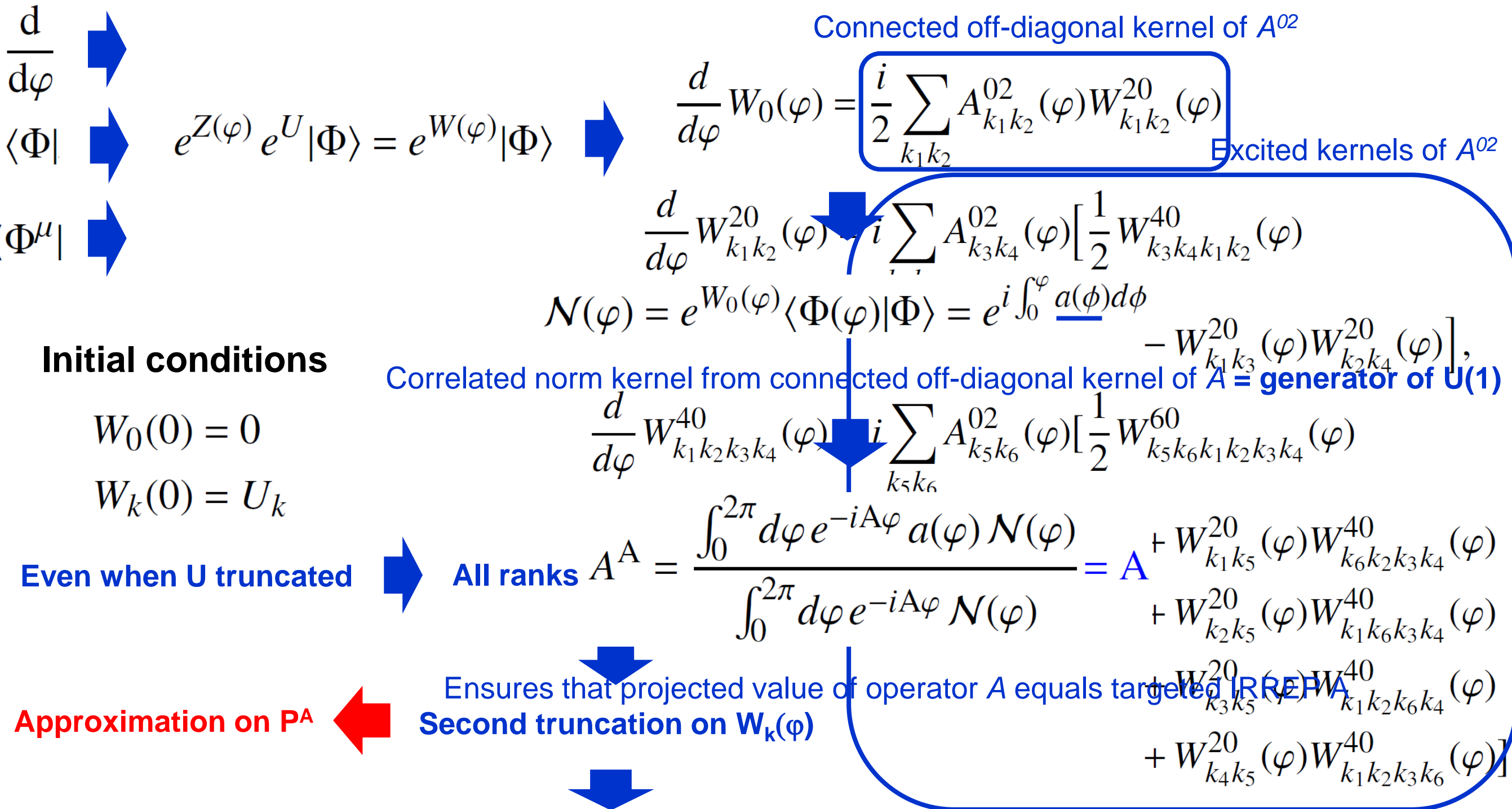
$$\mathcal{N}^{\text{PHFB}}(\varphi) \equiv \langle \Phi(\varphi) | \Phi \rangle$$

$$h^{\text{PHFB}}(\varphi) = \langle \Phi | H_Z(\varphi) | \Phi \rangle_C$$

Particle-number projected BCC formalism

Gauge-rotated cluster amplitudes $W_k(\varphi)$

Coupled ordinary differential equations



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BCS pairing Hamiltonian

Hamiltonian

$$H = \sum_p (\epsilon_p - \lambda) N_p - G \sum_{pq} P_p^\dagger P_q$$

Doubly-degenerate picket fence model

$$\epsilon_p = \epsilon_{\bar{p}} = p \Delta \epsilon$$

Exact ground-state energy

Richardson solution

[R.W. Richardson, PL 1963; PR 1966]

What about BCC? [Henderson *et al.* PRC 2014]

$$\text{BCCSD: } U \approx U_1 + U_2$$

What about PBCC? [Qiu *et al.* PRC 2019]

$$\text{PBCCSD(2): } U \approx U_1 + U_2$$

Operators

$$N_p = c_p^\dagger c_p + c_{\bar{p}}^\dagger c_{\bar{p}}$$

$$P_p^\dagger = c_p^\dagger c_{\bar{p}}^\dagger$$

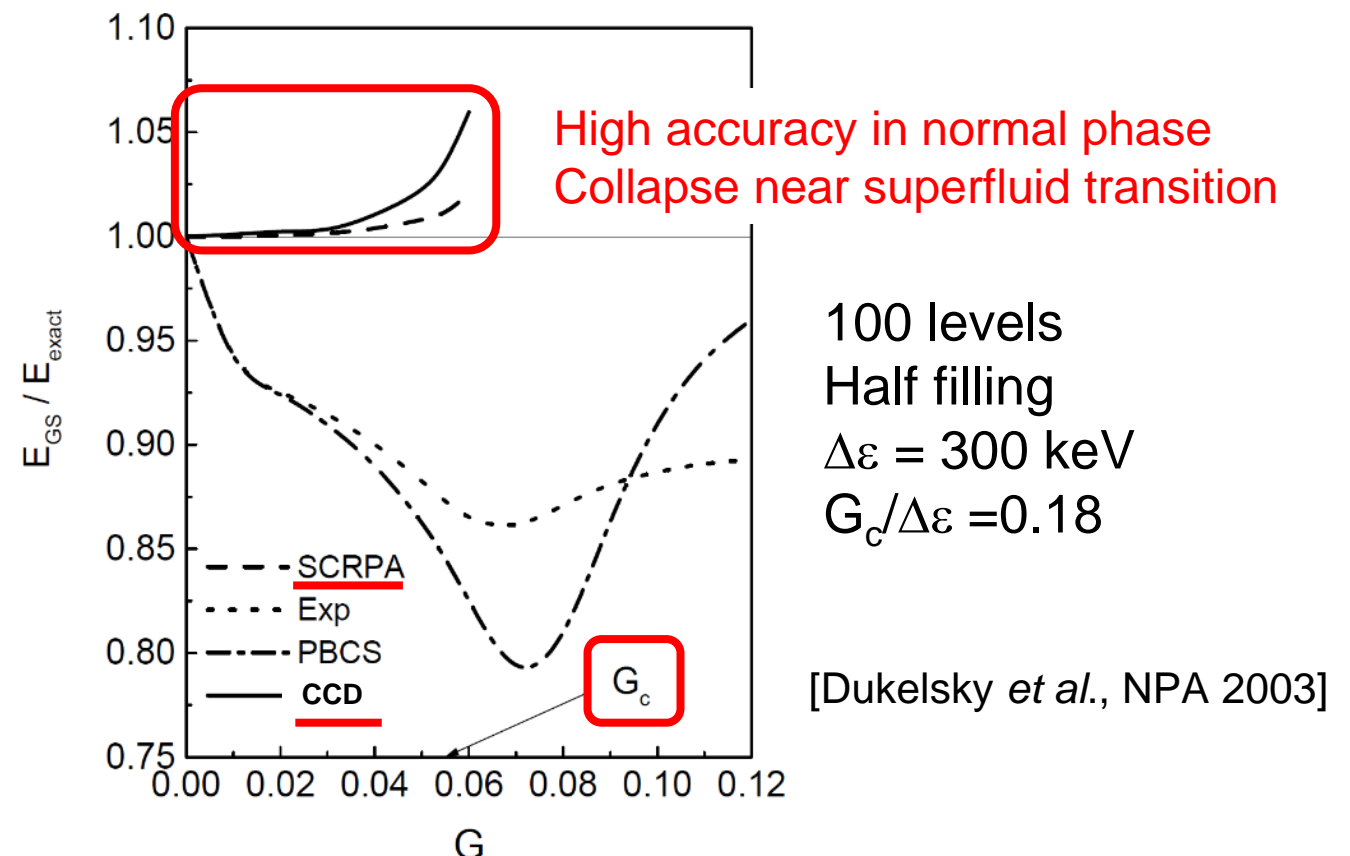
SU(2) algebra

$$[P_p, P_q^\dagger] = \delta_{pq} (1 - N_p)$$

$$[N_p, P_q^\dagger] = 2 \delta_{pq} P_q^\dagger$$

Typical approximate methods

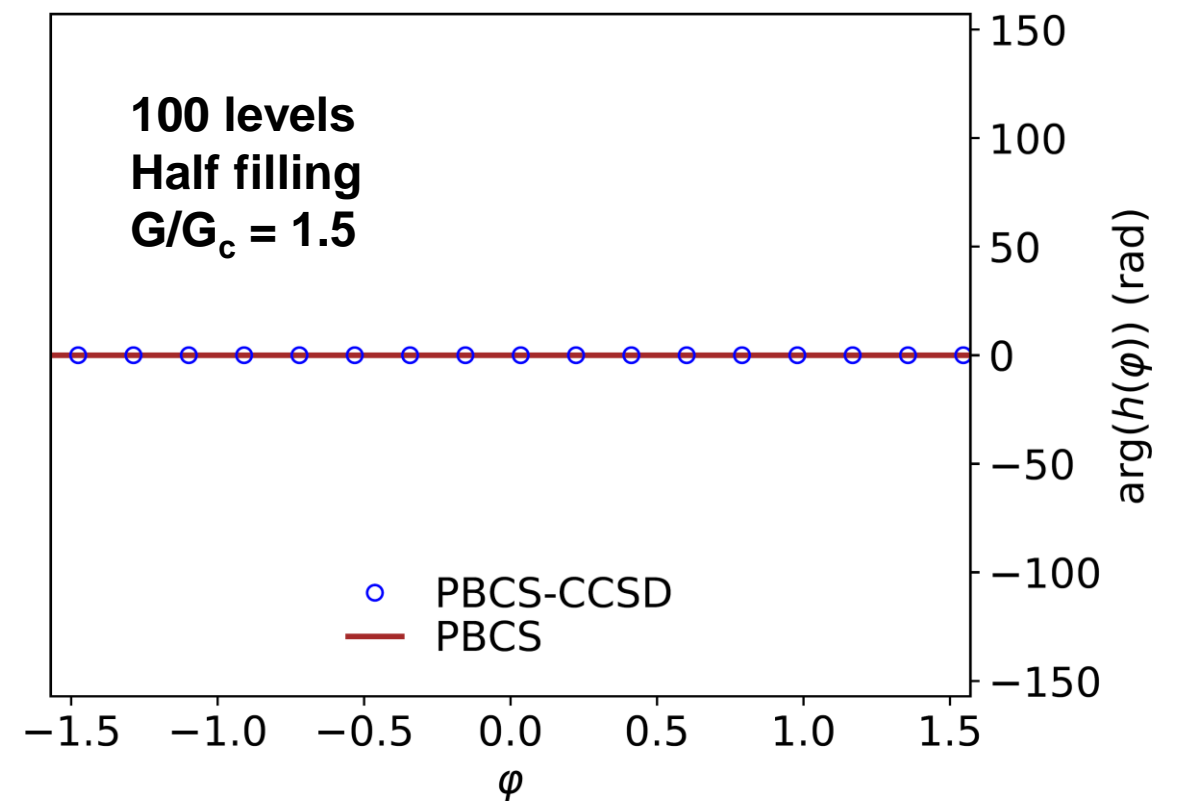
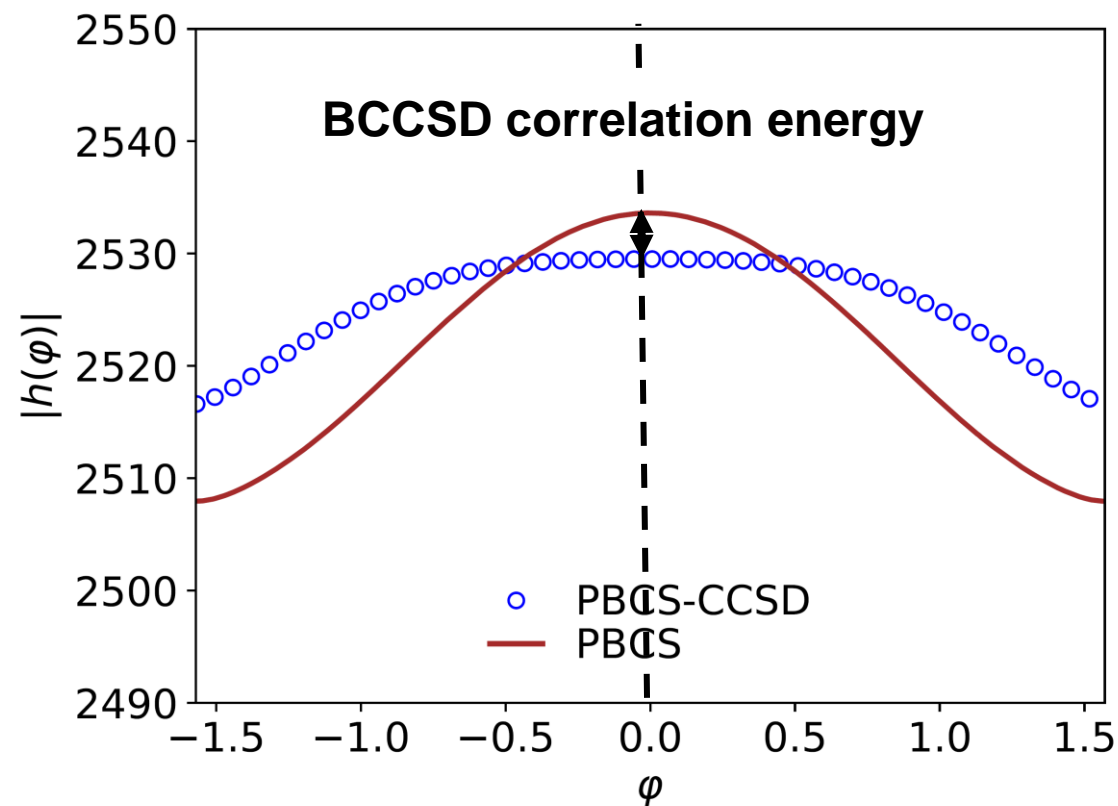
- BCS and projected BCS (before variation)
- Coupled cluster theory with doubles
- Self-consistent RPA



Other recent accurate methods

[Degroote *et al.* PRB 2016; Ripoche *et al.* PRC 2017]

Connected hamiltonian kernel



PBCC energy and kernels

$$E^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} h(\varphi) \mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)} \quad \text{with}$$

$$\mathcal{N}(\varphi) \equiv e^{W_0(\varphi)} \langle \Phi(\varphi) | \Phi \rangle$$

$$h(\varphi) \equiv \frac{\mathcal{H}(\varphi)}{\mathcal{N}(\varphi)} = \langle \Phi | H_Z(\varphi) e^{\mathcal{T}(\varphi)} | \Phi \rangle_C$$

Exact (or symmetry-conserving) limit

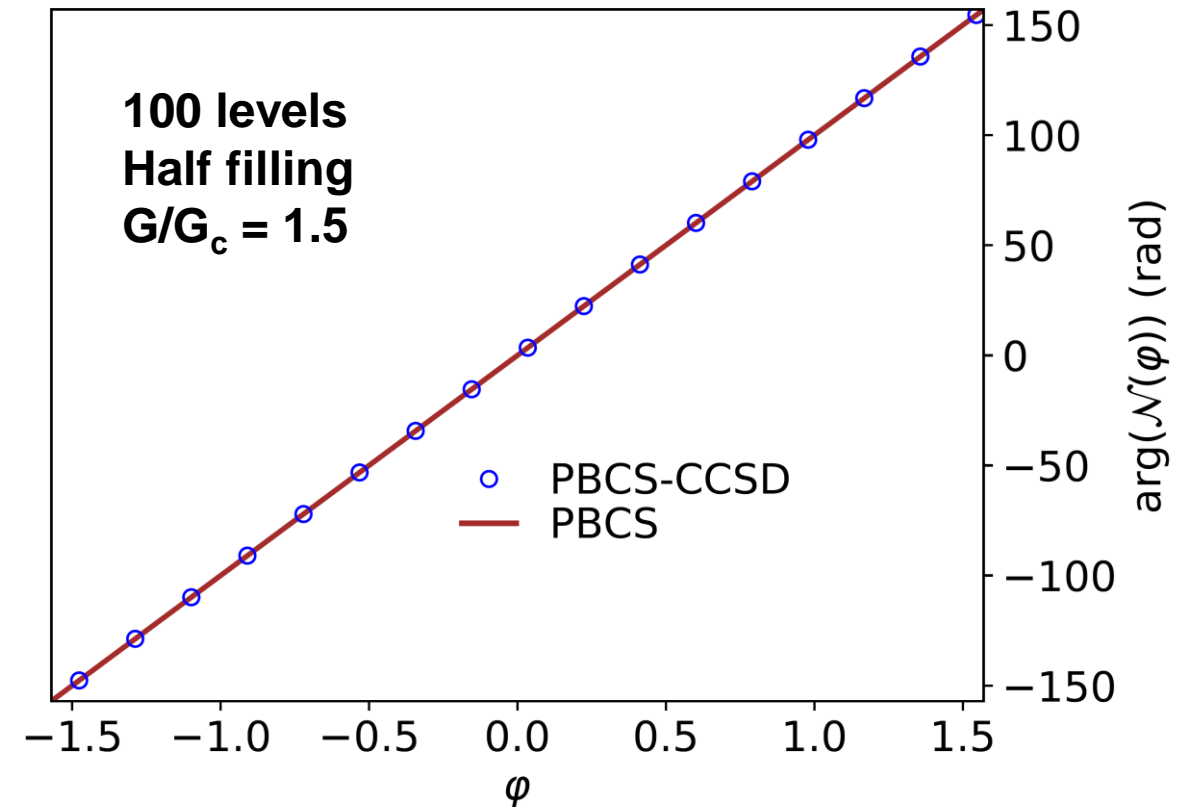
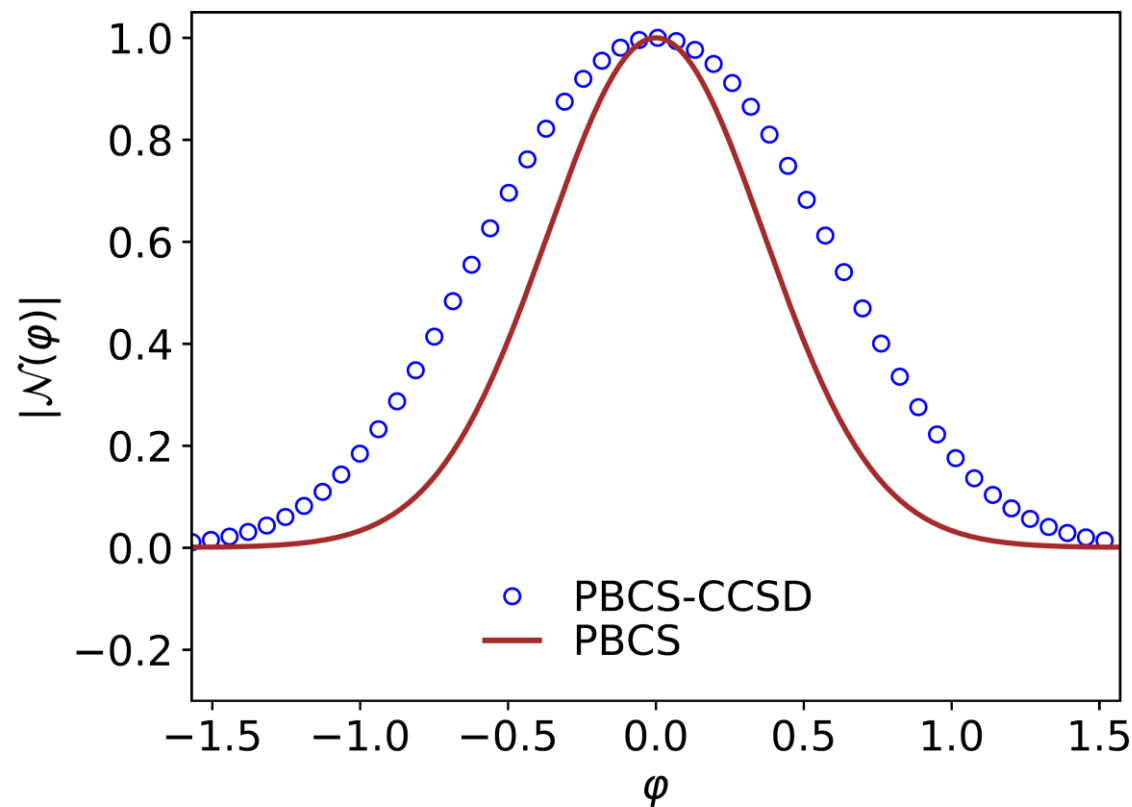
$$\mathcal{N}(\varphi) = e^{iA\varphi}$$

$$\frac{d}{d\varphi} h(\varphi) = 0$$

◎ PBCC ↔ PBCS-CC(S)D here

- $h(\varphi)$ real with typical bell-shape curve
- PBCC brings $h(\varphi)$ closer to constant
- Not constant $h(\varphi)$ induces non-trivial projection

Norm kernel



PBCC energy and kernels

$$E^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} h(\varphi) \mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)} \quad \text{with}$$

$$\mathcal{N}(\varphi) \equiv e^{W_0(\varphi)} \langle \Phi(\varphi) | \Phi \rangle$$

$$h(\varphi) \equiv \frac{\mathcal{H}(\varphi)}{\mathcal{N}(\varphi)} = \langle \Phi | H_Z(\varphi) e^{\mathcal{T}(\varphi)} | \Phi \rangle_C$$

Exact (or symmetry-conserving) limit

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

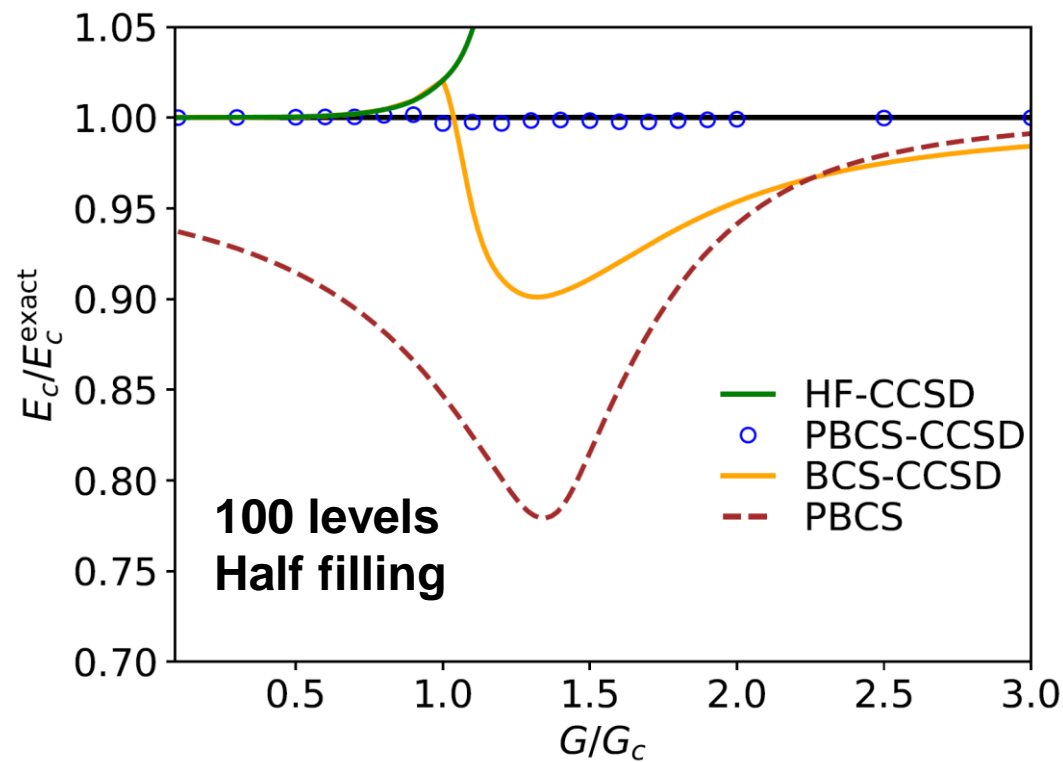
$$\frac{d}{d\varphi} h(\varphi) = 0$$

◎ PBCC ↔ PBCS-CC(S)D here

- $|\mathcal{N}(\varphi)|$ displays bell-shape curve and phase $\propto A$
- PBCC brings $\mathcal{N}(\varphi)$ closer to single IRREP $e^{iA\varphi}$
- $\mathcal{N}(0) = 1 \leftrightarrow$ Intermediate normalization

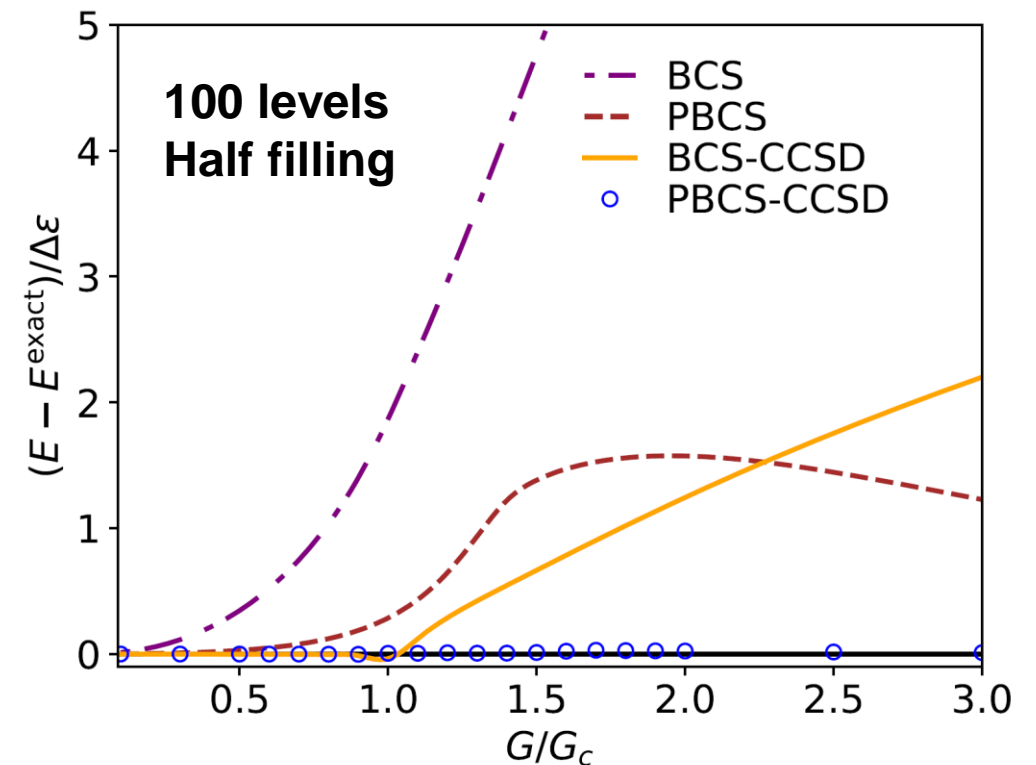
Results - 1

Fraction of correlation energy

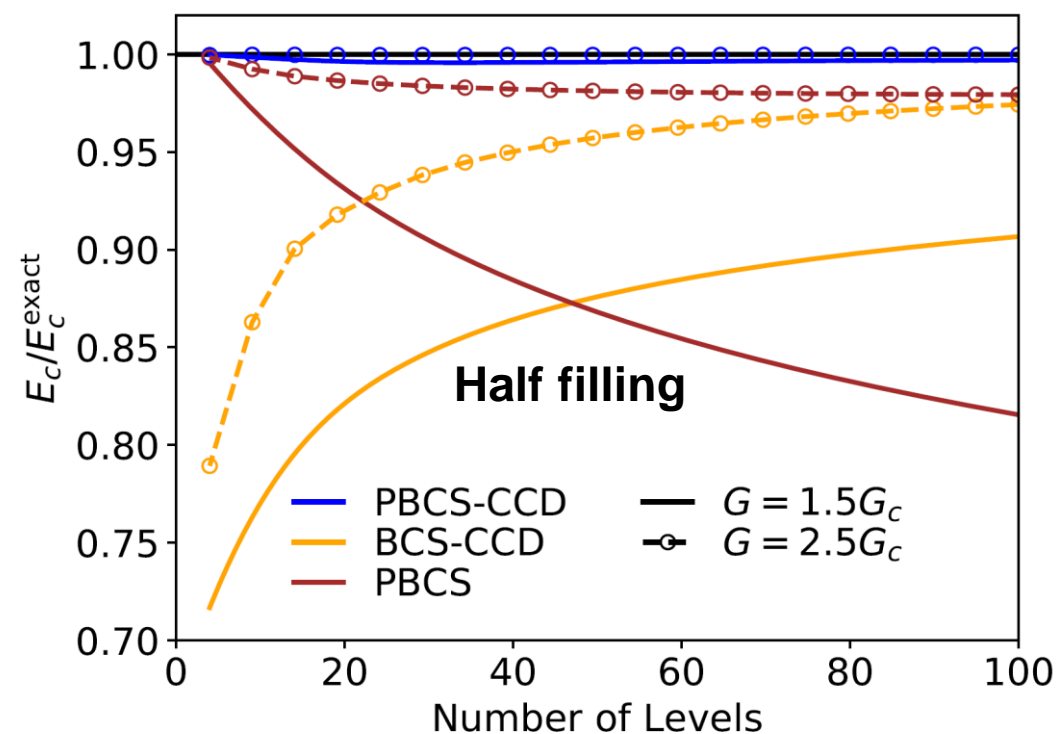


Absolute energy error

[Qiu et al. PRC 2019]



Dependence on system size



● BCC ↔ BCS-CC(S)D here

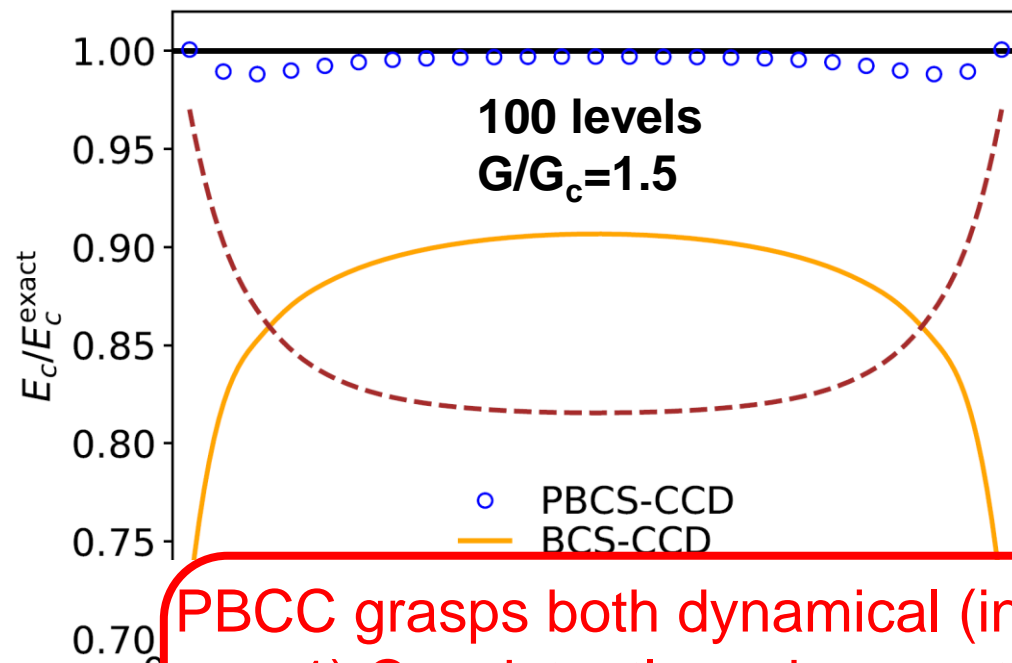
- Extends quality of CC through phase transition
- Better than PBCS except for $G \gg G_c$
- Poor in small systems

● PBCC ↔ PBCS-CC(S)D here

- Perfect from weak to strong coupling
- Perfect from small to large systems
- Dominates all other methods

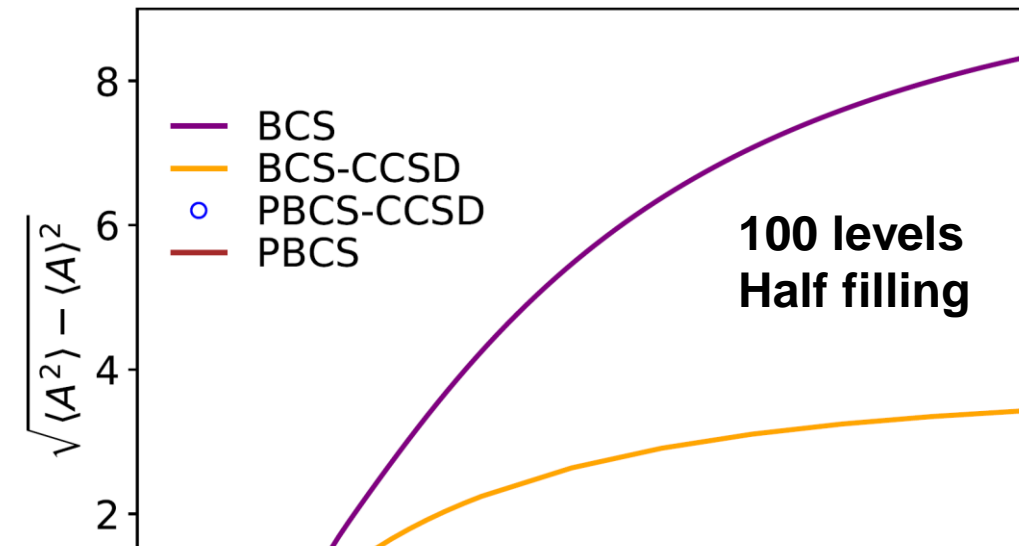
Results - 2

Filling fraction



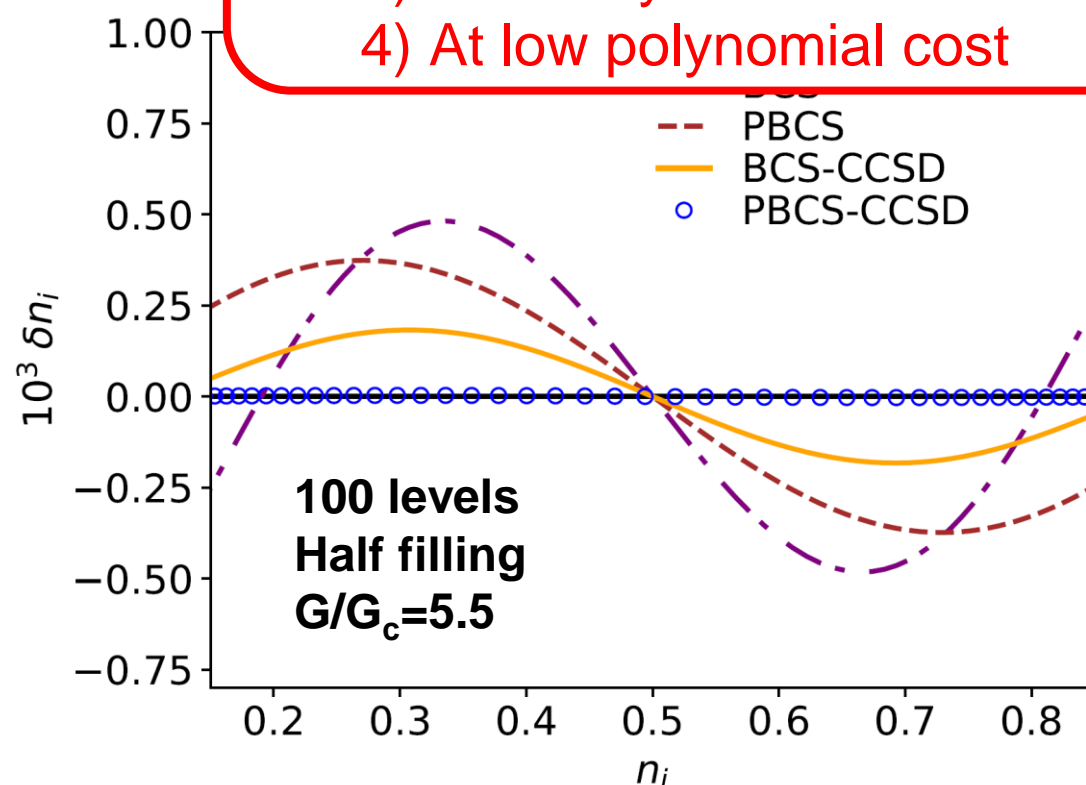
[Qiu et al. PRC 2019]

Particle number dispersion



PBCC grasps both dynamical (ind. excit.) and non-dynamical (def.+proj.) correlations

- 1) Consistently and accurately
- 2) For weak and strong coupling regimes
- 3) For all system sizes
- 4) At low polynomial cost



improves on BCS in the « closed shell »

- Poor near « closed shell »
- Reduce σ_A by factor of 2 compared to BCS

◎ PBCC ↔ PBCS-CC(S)D here

- Perfect « throughout the shell »
- One-body properties are perfect
- $\sigma_A=0$ ($W_3(\varphi)$ to be added for very high precision)

Contents

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● Breaking and restoring symmetries in quantum many-body theory

- Prolegomena

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● Conclusions

Conclusions

◎ Particle-number projected Bogoliubov coupled cluster and many-body perturbation theories

- Extends single-reference CC/MBPT methods to open-shell nuclei via symmetry breaking&restoration
- First consistent formulation of symmetry restoration techniques beyond the mean-field
- Results obtained for U(1) on the solvable Richardson Hamiltonian hold great promises

◎ Future

- Ab initio PBCC and PBMBPT calculations of singly open-shell nuclei

[Tichai, Ripoché, Duguet, in progress]

- Apply to SU(2) (already formulated) for ab initio calculations of doubly open-shell nuclei

[Tichai, Hagen, Duguet, in progress]

- Combine with IT/TF techniques to go to heavier nuclei

[Tichai, Ripoché, Duguet, EPJA 2019]

- Extend BCC and PBCC to excited states

[Demol, Tichai, Duguet, planned]

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