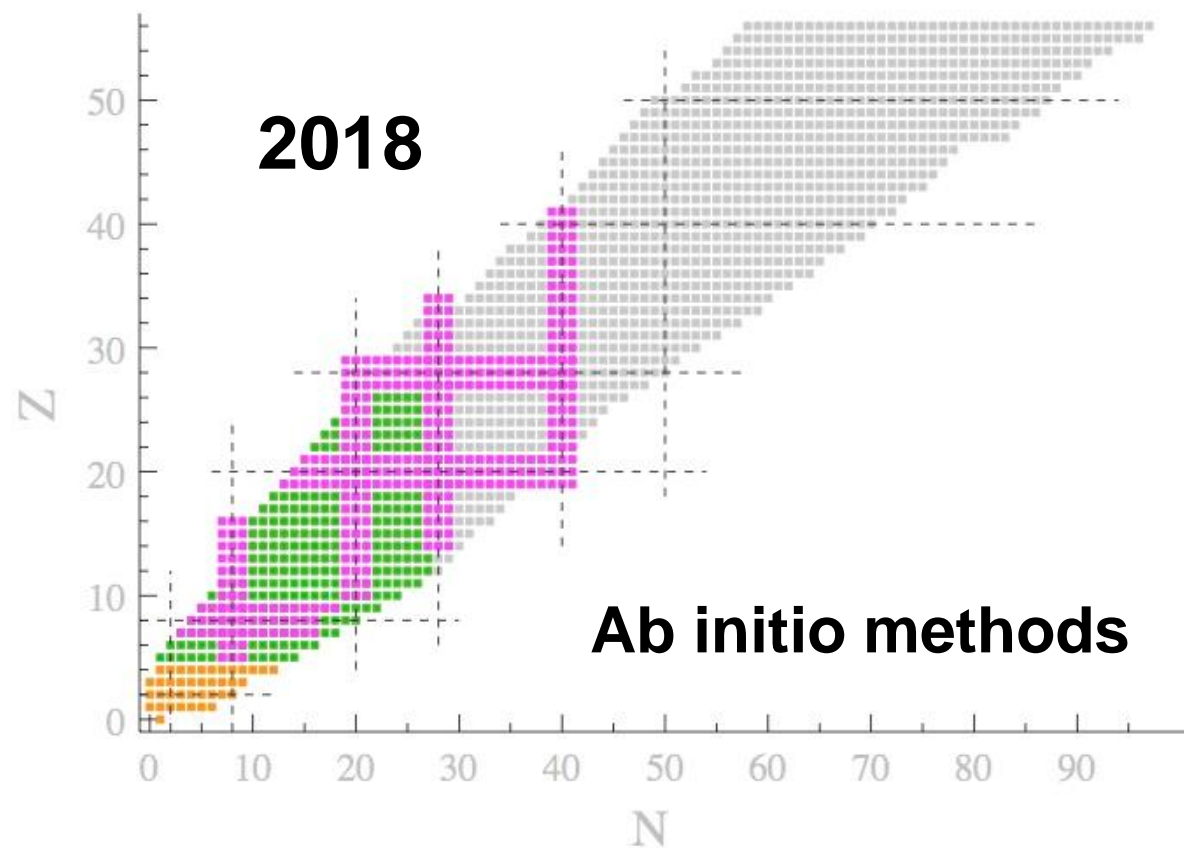


Symmetry broken&restored MBPT

to deal with (near-)degenerate finite many-fermion systems, e.g. open-shell nuclei



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

T. Duguet, A. Signoracci, J. Phys. G: Nucl. Part. Phys. 44 (2016) 015103

ESNT workshop, CEA-Saclay, France, March 26th-30th 2018



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- Nuclear chart and ab initio methods
- Why breaking symmetries?
- On-going developments and projects in this direction

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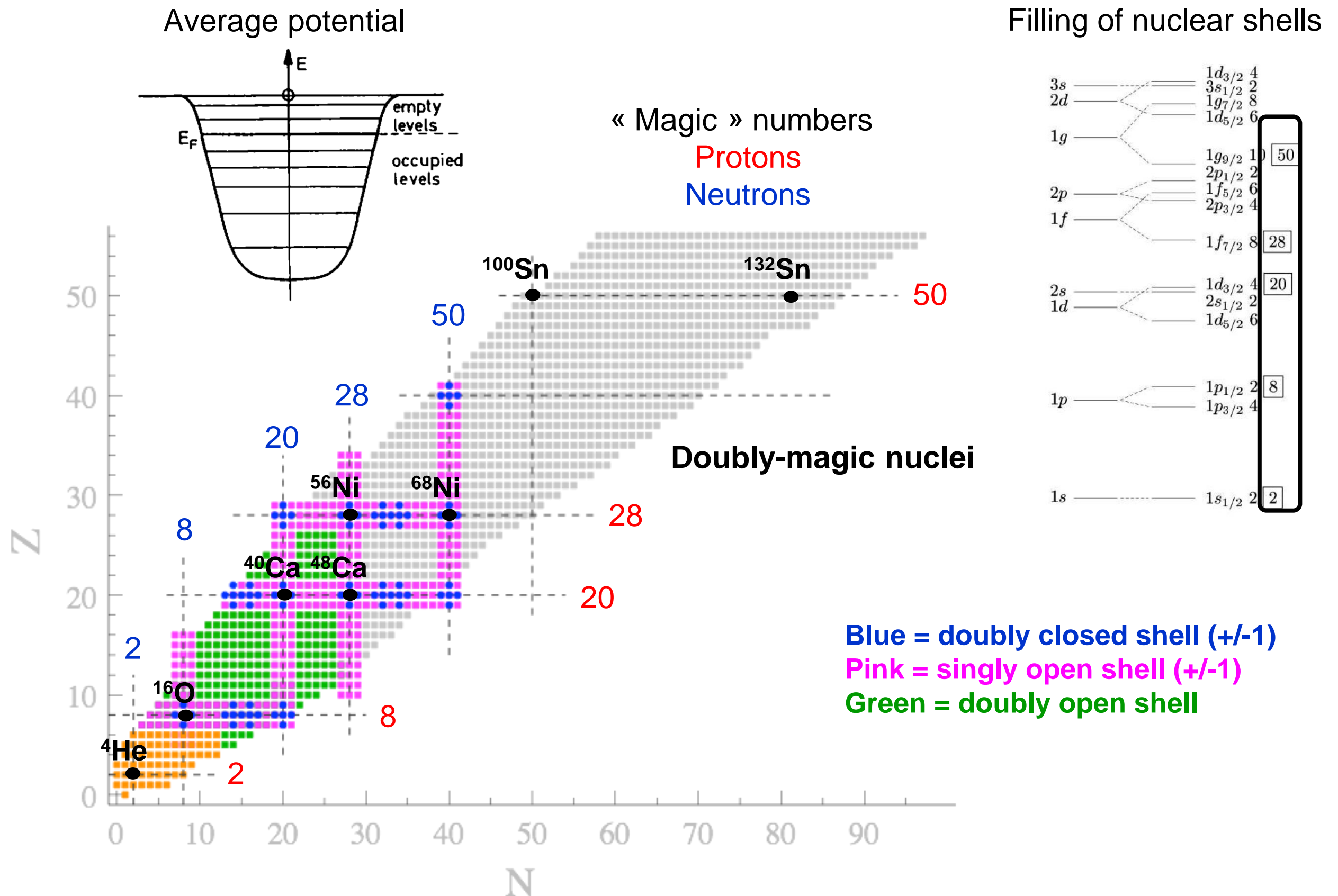
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(Non) closed-shell character of nuclear ground states



Ab initio nuclear chart

● Approximate methods for doubly closed-shells

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

● Approximate methods for singly open-shell

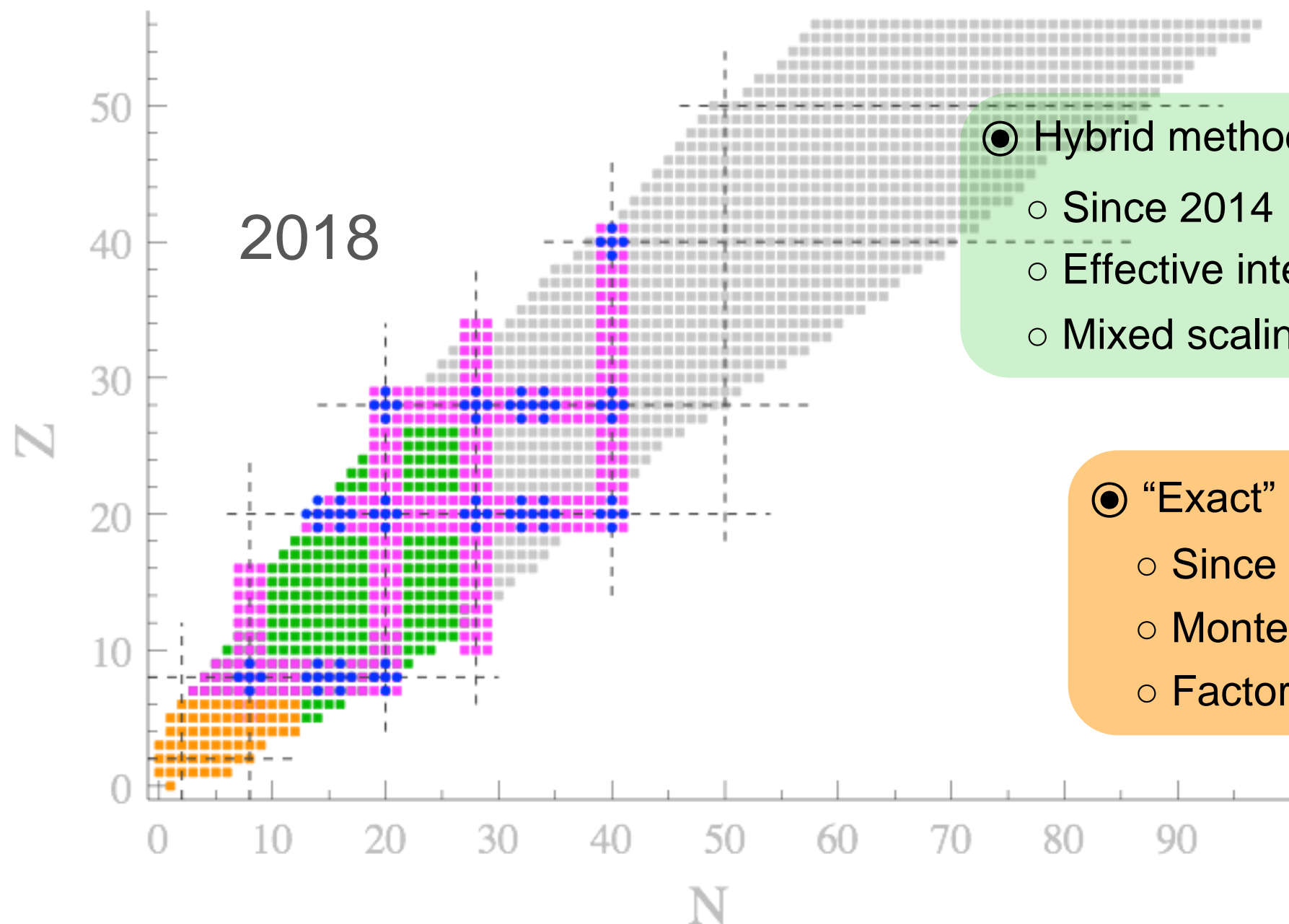
- Since 2010's
- **BMBPT, GGF, BCC**, MR-IMSRG, MCPT
- Polynomial scaling

● Hybrid methods (ab initio shell model)

- Since 2014
- Effective interaction via CC/IMSRG
- Mixed scaling

● “Exact” methods

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



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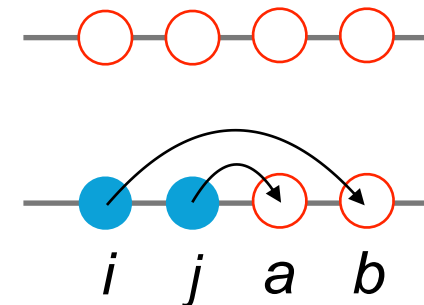
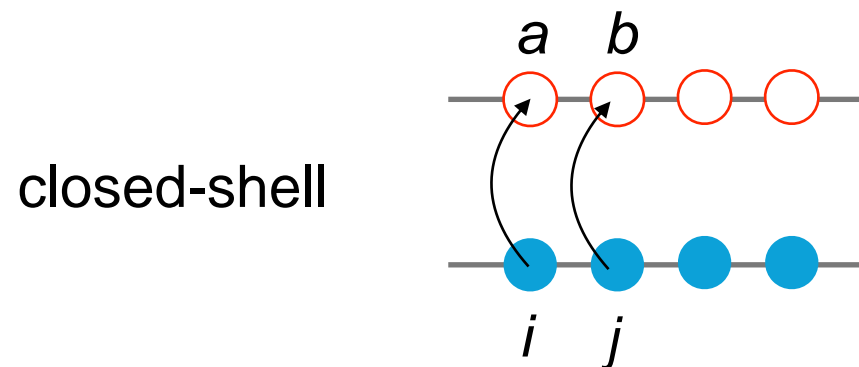
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(Near-)degenerate systems via expansion methods

- Expansions around **one** determinant capture **dynamical** correlations via sums of **ph excitations**
- Open-shell (sub-closed shell) nuclei are **(near-)degenerate** with respect to ph excitations



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

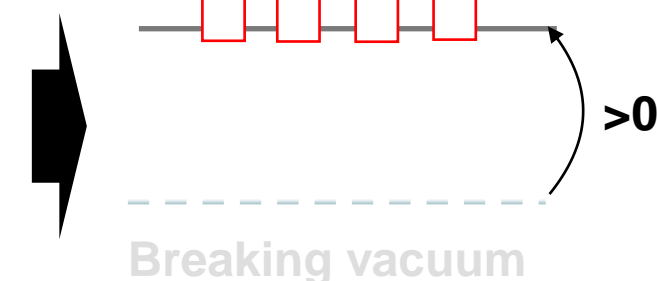
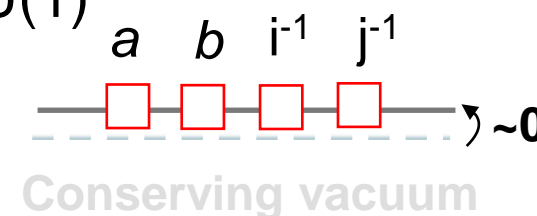
Expansion **breaks down** when $e_a + e_b \approx e_i + e_j$
 Signals important **non-dynamical** correlations

- 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, MCPT** To be compared
- Expand around a **symmetry-breaking** determinantal reference state (non-perturbative)

➔ **Lifts the degeneracy**, e.g. BMBPT(2) breaking U(1)

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



- Independent of the number of nucleons in open-shell
- Particularly beneficial in heavy nuclei/high-j shells

➔ **Symmetries must be eventually restored** in finite quantum systems
 1) Lowest reference energy 2) Expansion well behaved again

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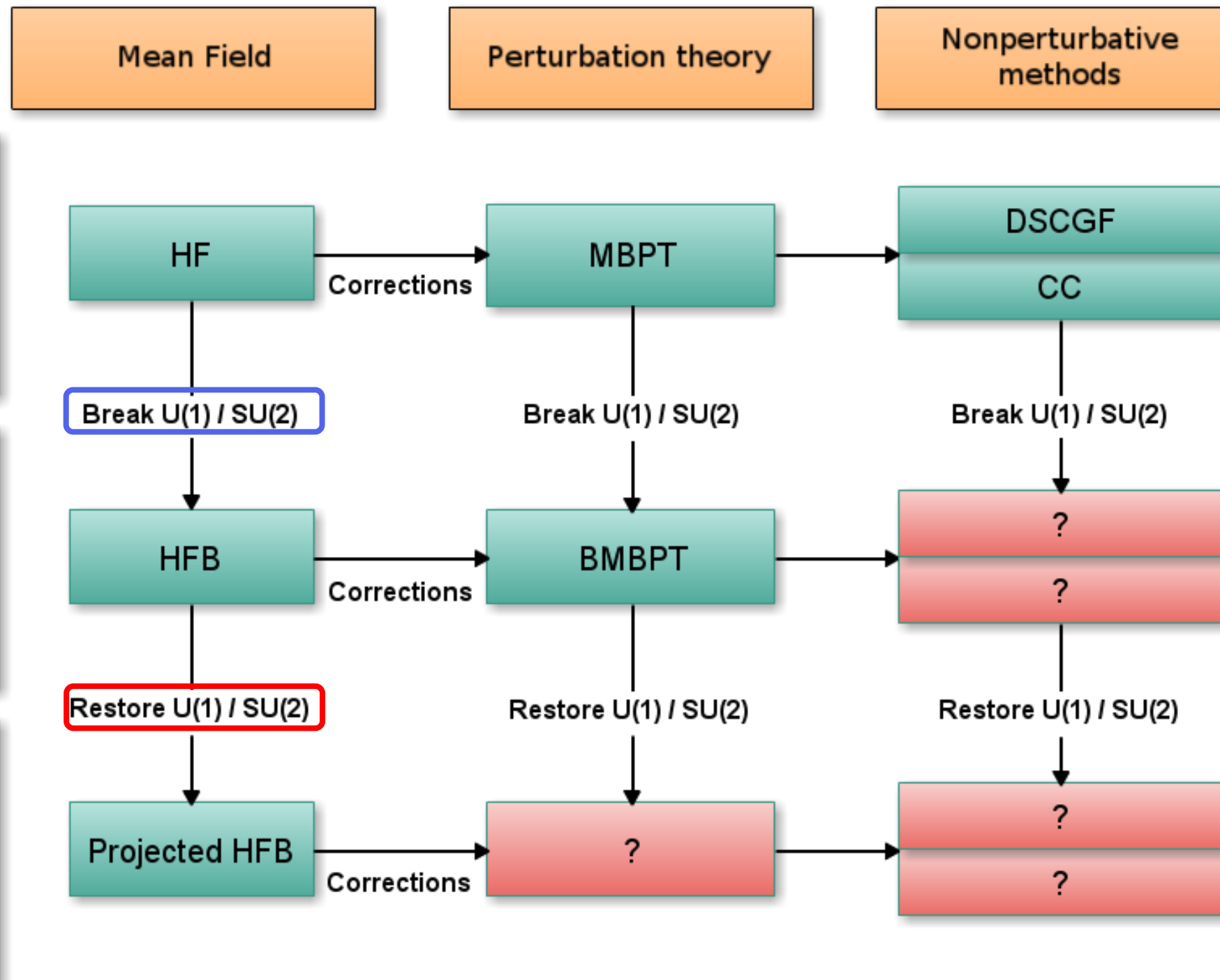
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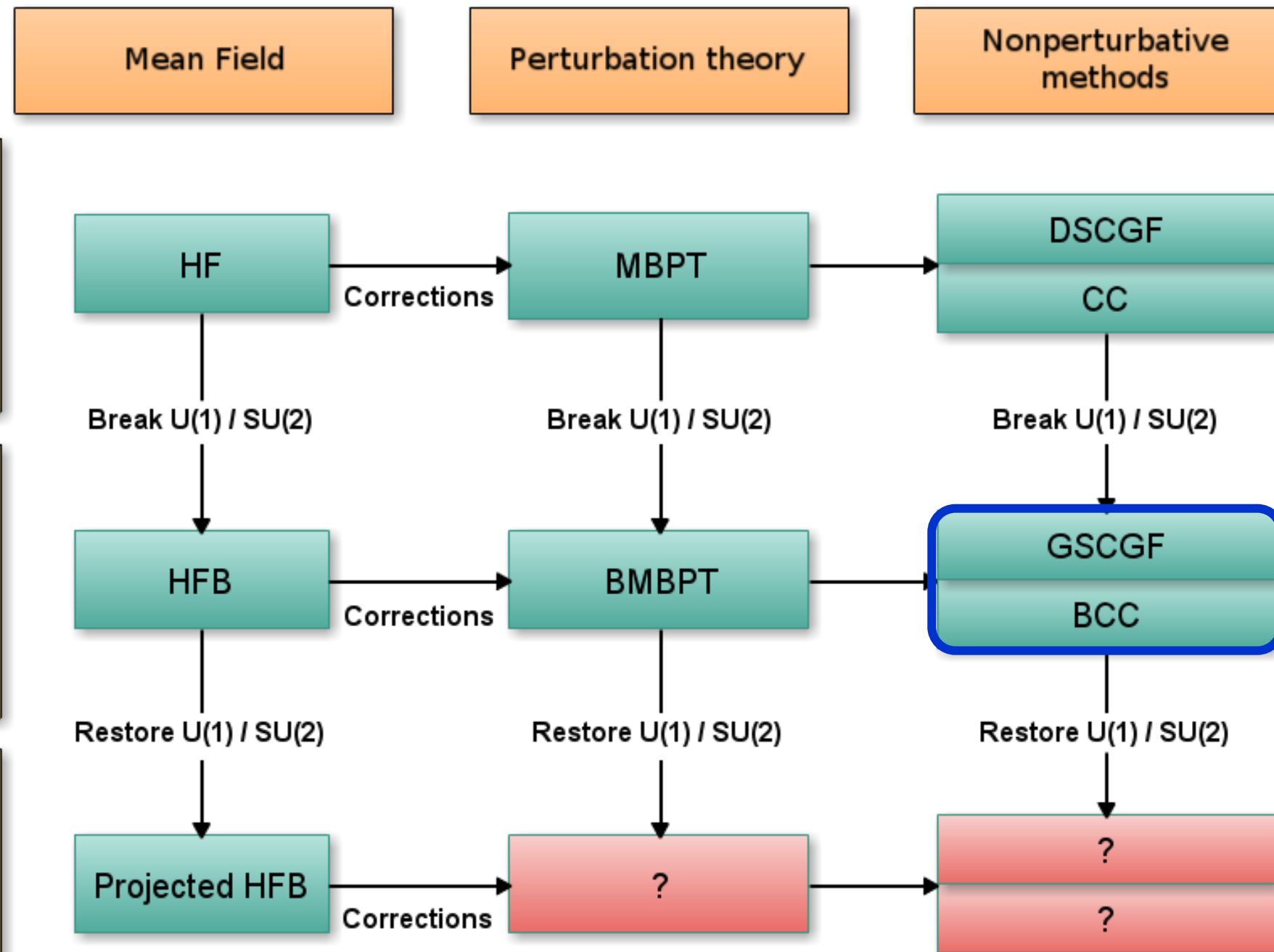
Single-determinantal many-body methods and symmetries

Nuclear Many-Body Methods



Single-determinantal many-body methods and symmetries

Nuclear Many-Body Methods



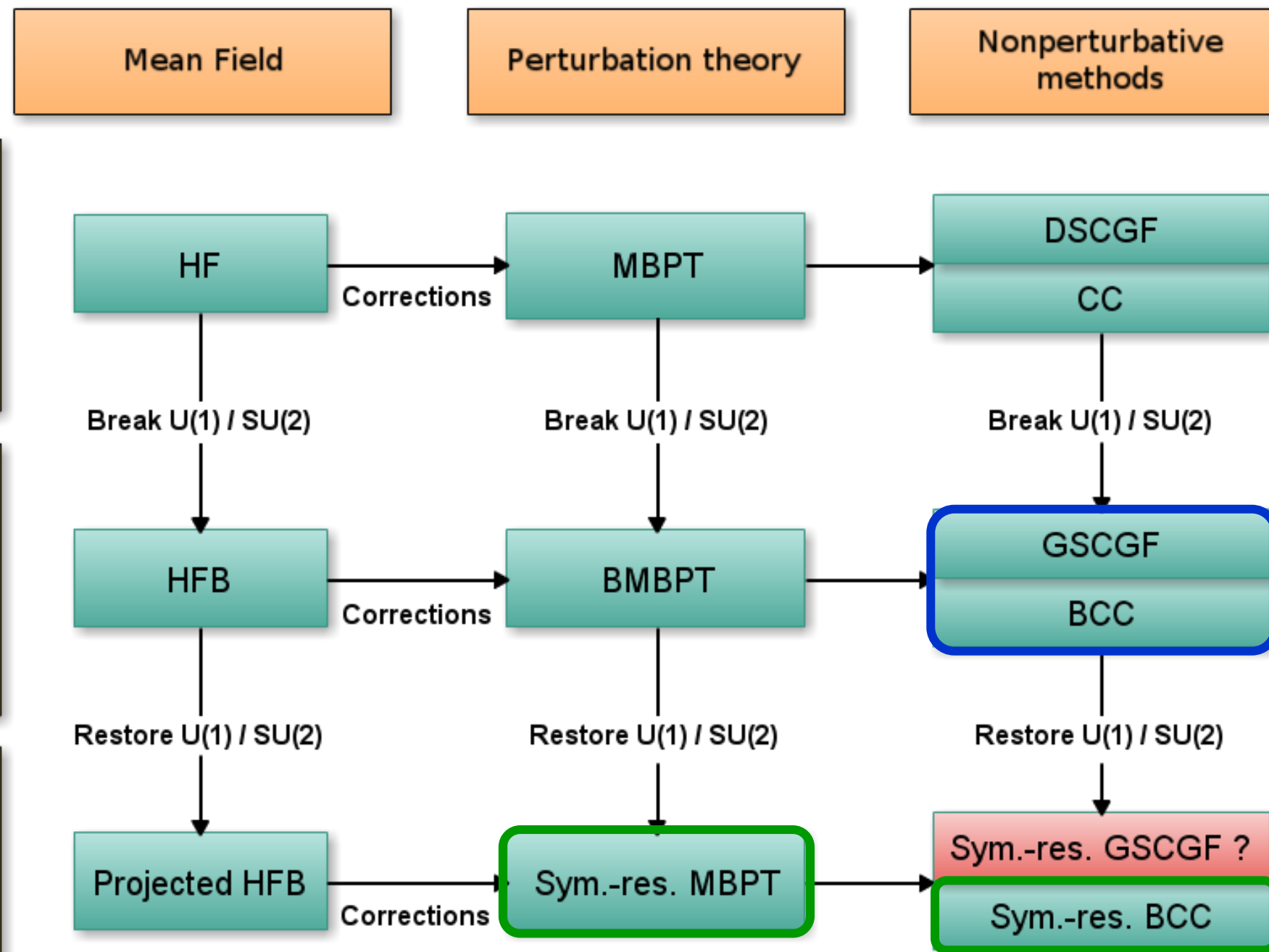
**Recently -implemented
-proposed**

[Somà *et al.* 2011]

[Signoracci *et al.* 2014]

Single-determinantal many-body methods and symmetries

Nuclear Many-Body Methods



**Recently -implemented
-proposed**

[Somà *et al.* 2011]

[Signoracci *et al.* 2014]

Recently proposed

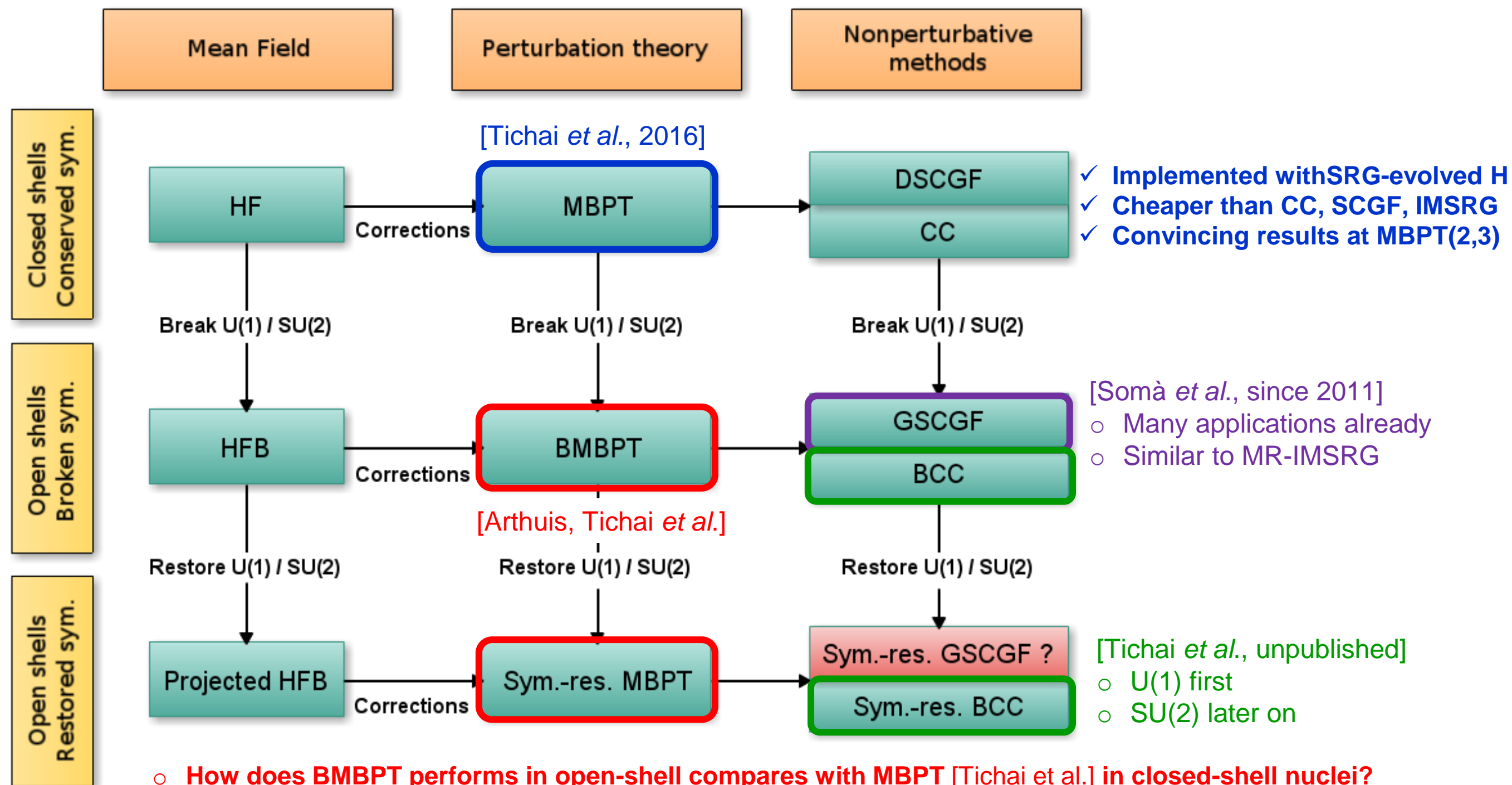
[Duguet 2015] for $SU(2)$

[Duguet, Signoracci 2016] for $U(1)$

[Qiu *et al.* 2017] for $SU(2)$

On-going projects: deal with U(1) symmetry in semi-magic nuclei

Nuclear Many-Body Methods



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Connection to Piotr's lecture – technical comments

MBPT within a (imaginary) time-dependent formalism

- ⦿ Equivalent for stationary states to **time-independent approach used by Piotr**
 - Time-dependence is fictitious and disappears through time-integration from 0 to ∞
 - Interesting technical variant towards genuine time-dependent method
- ⦿ **Use of Feynman diagrams**
 - Explicit time variable that is integrated over
 - Captures many time orderings at once corresponding to a whole set of Goldstone diagrams
 - See talk by P. Arthuis on Thursday for in-depth considerations about that**
- ⦿ Time flows from bottom to top (as opposed to left-to-right in Piotr's Goldstone diagrams)

Generalization of standard MBPT

- ⦿ Allows the reference state to break symmetry of H (**U(1) global gauge symmetry today**)
 - Symmetry-unrestricted algebra that cannot exploit symmetry degeneracy
- ⦿ **Further restores the broken symmetry at the same time**
 - Insertion of symmetry projection operator
 - Generalizes the diagrammatics
 - Provides a multi-reference character through N different single-reference calculations

U(1) global gauge symmetry

Unitary representation of Abelian compact Lie group on Fock space

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

A

Particle-number operator
Infinitesimal generator of the group

Symmetry of the physical system

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

Definition of irreducible representations

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

Orthogonality of irreducible representations

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-iA\varphi} e^{+iA'\varphi} = \delta_{AA'}$$

Stationary eigenstates

$$A |\Psi_{\mu}^A\rangle = A |\Psi_{\mu}^A\rangle$$

$$H |\Psi_{\mu}^A\rangle = E_{\mu}^A |\Psi_{\mu}^A\rangle$$

Tensor operators and eigenstates

$$S(\varphi) O S(\varphi)^{-1} = e^{iA\varphi} O$$

$$S(\varphi) |\Psi_{\mu}^A\rangle = e^{iA\varphi} |\Psi_{\mu}^A\rangle$$

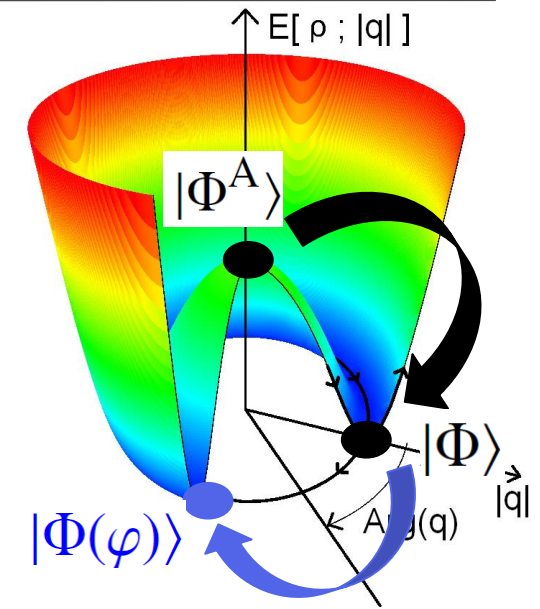
U(1) breaking and projection

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: $|\Phi\rangle \Rightarrow A|\Phi\rangle \neq A|\Phi\rangle \Rightarrow S(\varphi)|\Phi\rangle \equiv |\Phi(\varphi)\rangle \neq e^{iA\varphi}|\Phi\rangle$



Particle-number projection operator

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

$$P^{A\dagger} = P^A$$

$$(P^A)^2 = P^A$$

$$[H, P^A] = [A, P^A] = 0$$

Particle number projection

Extracts component in \mathcal{H}_A

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

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Bogoliubov reference state and rotated partner

Bogoliubov transformation

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

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

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \text{ unitary, i.e. } \begin{cases} \{\beta_k, \beta_{k'}\} = 0 \\ \{\beta_k^\dagger, \beta_{k'}^\dagger\} = 0 \\ \{\beta_k, \beta_{k'}^\dagger\} = \delta_{kk'} \end{cases}$$

Gauge-rotated partner

$$|\Phi(\varphi)\rangle \equiv \langle \Phi | \Phi(\varphi) \rangle \underbrace{e^{\left[\frac{1}{2} \sum_{k_1 k_2} Z_{k_1 k_2}^{20}(\varphi) \beta_{k_1}^\dagger \beta_{k_2}^\dagger \right]}}_{\text{Thouless transformation}} |\Phi\rangle$$

Thouless matrix $Z_{k_1 k_2}^{20}(\varphi)$ = known function of (U, V, φ)

Bogoliubov state

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

$$\underbrace{\beta_k |\Phi\rangle = 0 \quad \forall k}_{\text{Vacuum state}}$$

Reduces to SD in \mathcal{H}_A if V=0

Breaks U(1) symmetry

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

Quasi-particle excitations

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

Orthonormal basis of Fock space

Elementary off-diagonal contractions

Reduces to n-p-n excit. in \mathcal{H}_A if V=0

$$\begin{aligned} \mathbf{R}(\varphi) &= \begin{pmatrix} \frac{\langle \Phi | \beta^\dagger \beta | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} & \frac{\langle \Phi | \beta \beta | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} \\ \frac{\langle \Phi | \beta^\dagger \beta^\dagger | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} & \frac{\langle \Phi | \beta \beta^\dagger | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} \end{pmatrix} \\ &\equiv \begin{pmatrix} R^{+-}(\varphi) & R^{--}(\varphi) \\ R^{++}(\varphi) & R^{-+}(\varphi) \end{pmatrix} \\ &= \begin{pmatrix} 0 & -Z^{20}(\varphi) \\ 0 & 1 \end{pmatrix} \end{aligned}$$

$Z^{20}(0) = 0$, i.e. when $|\Phi(0)\rangle = |\Phi\rangle$

One non-zero diagonal contraction

Key operators

Nuclear Hamiltonian

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

Genuine three-body interaction / six-legs vertex
Makes diagrammatic more involved

Particle number

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

Grand potential

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

Chemical potential

As we work in Fock space

Controls the average particle number in the system

Normal-ordered operators

Normal ordering w.r.t. Bogoliubov vacuum

Each $\Omega_{k_1 \dots k_i k_{i+1} \dots k_{i+j}}^{ij}$ is a fully anti-symmetric

function of $\begin{bmatrix} t_{pq} \\ \bar{v}_{pqrs} \\ \bar{w}_{pqrst} \end{bmatrix} \begin{bmatrix} U_{pk} \\ V_{pk} \end{bmatrix}$

$$\Omega \equiv \Omega^{[0]} + \Omega^{[2]} + \Omega^{[4]} + \Omega^{[6]}$$

$$= \Omega^{00} + \frac{1}{1!} \sum_{k_1 k_2} \Omega_{k_1 k_2}^{11} \beta_{k_1}^\dagger \beta_{k_2}$$

$$+ \frac{1}{2!} \sum_{k_1 k_2} \left\{ \Omega_{k_1 k_2}^{20} \beta_{k_1}^\dagger \beta_{k_2}^\dagger + \Omega_{k_1 k_2}^{02} \beta_{k_2} \beta_{k_1} \right\}$$

$$+ \frac{1}{(2!)^2} \sum_{k_1 k_2 k_3 k_4} \Omega_{k_1 k_2 k_3 k_4}^{22} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_4} \beta_{k_3}$$

$$+ \frac{1}{3!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega_{k_1 k_2 k_3 k_4}^{31} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4} + \Omega_{k_1 k_2 k_3 k_4}^{13} \beta_{k_1}^\dagger \beta_{k_4} \beta_{k_3} \beta_{k_2} \right\}$$

$$+ \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega_{k_1 k_2 k_3 k_4}^{40} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4}^\dagger + \Omega_{k_1 k_2 k_3 k_4}^{04} \beta_{k_4} \beta_{k_3} \beta_{k_2} \beta_{k_1} \right\}$$

Similarly for H and A

+ $\Omega^{[6]}$



NO2B approximation

1-3% error in closed shell

[R. Roth *et al.*, PRL 109 (2012) 052501]



2-body like operators only

Captures essential of 3-body

Diagrammatics with 2-body

Symmetry-projected many-body method

Project g.s. eigenvalue equations onto $|\Theta\rangle \equiv P^A|\Phi\rangle$

Expanded projector

$$A = \frac{\langle \Psi_0^A | A P^A | \Phi \rangle}{\langle \Psi_0^A | P^A | \Phi \rangle}$$

$$E_0^A = \frac{\langle \Psi_0^A | H P^A | \Phi \rangle}{\underbrace{\langle \Psi_0^A |}_{\text{Bogoliubov state}} \underbrace{P^A | \Phi \rangle}_{\text{Bogoliubov state}}}$$

Exact known result to be obtained at any truncation order

Integral over the group extracts component with correct A even after truncation

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

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

To be expanded around the same Bogoliubov state

P^A superfluous in exact limit but not after expansion/truncation

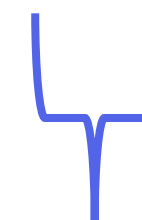
Standard many-body methods as sub-cases

Off-diagonal kernels

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

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

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



Rotated Bogoliubov state
= collective transformation

1) Reference Slater determinant = P^A altogether superfluous: MBPT, CC

$$E_0^A = \langle \Psi_0^A | H | \Phi^A \rangle$$

2) Only break but do not restore = P^A omitted: BMBPT, BCC

$$A = \langle \Psi_0^A | A | \Phi \rangle \quad \text{a) Diagonal kernels only}$$

$$E_0^A = \langle \Psi_0^A | H | \Phi \rangle \quad \text{b) Norm kernel easily dealt with (IN)}$$

(See BMBPT talk by P. Arthuis on Thursday)

Encode fingerprint of gauge transformation

Non-trivial norm kernel to be dealt with

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Time-dependent formalism

Imaginary-time evolution operator

$$\mathcal{U}(\tau) \equiv e^{-\tau\Omega}$$

Time-dependent state and ground state

$$|\Psi(\tau)\rangle \equiv \frac{\mathcal{U}(\tau)|\Phi\rangle}{\langle\Phi|\mathcal{U}(\tau)|\Phi\rangle} \quad \Rightarrow \quad |\Psi_0^A\rangle = \lim_{\tau \rightarrow \infty} |\Psi(\tau)\rangle$$

Intermediate normalization

Ground-state off-diagonal kernels

$$\mathcal{N}(\varphi) = \lim_{\tau \rightarrow \infty} \mathcal{N}(\tau, \varphi)$$

$$\mathcal{H}(\varphi) = \lim_{\tau \rightarrow \infty} \mathcal{H}(\tau, \varphi)$$

$$\mathcal{A}(\varphi) = \lim_{\tau \rightarrow \infty} \mathcal{A}(\tau, \varphi)$$

Time-dependent off-diagonal kernels

$$\mathcal{N}(\tau, \varphi) \equiv \langle\Psi(\tau)|\Phi(\varphi)\rangle = \frac{\langle\Phi|\mathcal{U}(\tau)|\Phi(\varphi)\rangle}{\langle\Phi|\mathcal{U}(\tau)|\Phi\rangle} \equiv \frac{N(\tau, \varphi)}{N(\tau, 0)}$$

$$\mathcal{H}(\tau, \varphi) \equiv \langle\Psi(\tau)|H|\Phi(\varphi)\rangle = \frac{\langle\Phi|\mathcal{U}(\tau)H|\Phi(\varphi)\rangle}{\langle\Phi|\mathcal{U}(\tau)|\Phi\rangle} \equiv \frac{H(\tau, \varphi)}{N(\tau, 0)}$$

$$\mathcal{A}(\tau, \varphi) \equiv \langle\Psi(\tau)|A|\Phi(\varphi)\rangle = \frac{\langle\Phi|\mathcal{U}(\tau)A|\Phi(\varphi)\rangle}{\langle\Phi|\mathcal{U}(\tau)|\Phi\rangle} \equiv \frac{A(\tau, \varphi)}{N(\tau, 0)}$$

Many-body expansion

$N(\tau, \varphi), H(\tau, \varphi), A(\tau, \varphi)$ in the numerators are the quantities to be expanded

$N(\tau, 0), H(\tau, 0), A(\tau, 0)$ in the denominators are particular cases of the above

Set up of perturbation theory

Partitioning of the grand potential

$$\Omega = \Omega_0 + \Omega_1 \quad \left\{ \begin{array}{l} \Omega_0 \equiv \Omega^{00} + \bar{\Omega}^{11} \\ \Omega_1 \equiv \Omega^{20} + \check{\Omega}^{11} + \Omega^{02} + \Omega^{22} + \Omega^{31} + \Omega^{13} + \Omega^{40} + \Omega^{04} \end{array} \right.$$

$\bar{\Omega}^{11} \equiv \sum E_k \beta_k^\dagger \beta_k$ with $E_k > 0$ for all k
 Unperturbed grand potential

$\check{\Omega}^{11} \equiv \Omega^{11} - \bar{\Omega}^{11}$

$$[\Omega_0, S(\varphi)] \neq 0$$

Particle-number breaking Bogoliubov unperturbed reference state

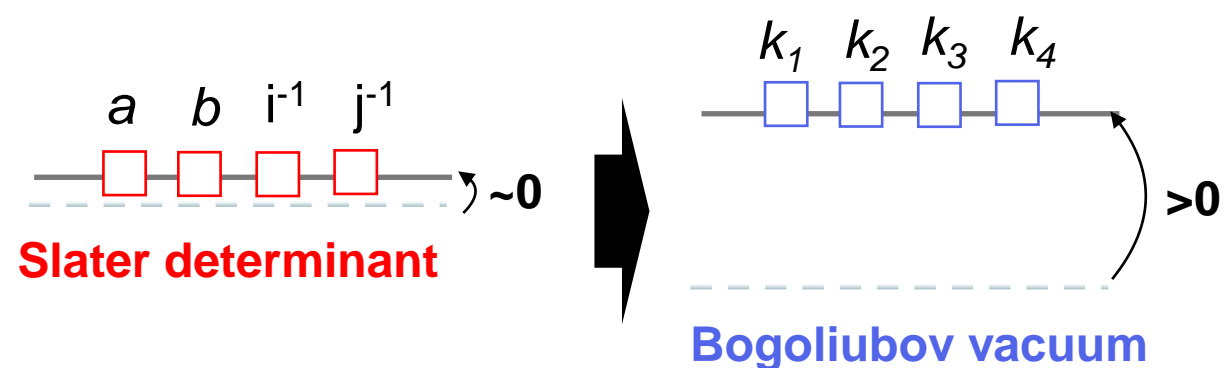
$$[\Omega_1, S(\varphi)] \neq 0$$

Unperturbed basis

$$\Omega_0 |\Phi\rangle = \Omega^{00} |\Phi\rangle$$

$$\Omega_0 |\Phi^{k_1 k_2 \dots}\rangle = \left[\Omega^{00} + \underbrace{E_{k_1} + E_{k_2} + \dots}_{>0} \right] |\Phi^{k_1 k_2 \dots}\rangle$$

>0 Non-degenerate reference state



How to pick

1) the E_k ?

2) the β_k ; i.e. $|\Phi\rangle$ or (U, V) ?

Hartree-Fock-Bogoliubov reference state

Ritz variational problem with a Bogoliubov ansatz (extension of Hartree-Fock)

Minimize $\frac{\langle \Phi | \Omega | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \Omega^{00}$ while keeping

- 1) the Bogoliubov transformation unitary
- 2) the particle number fixed on average

HFB eigenvalue equation

$$\Rightarrow \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \underbrace{\begin{pmatrix} U_k \\ V_k \end{pmatrix}}_{\text{Fully characterize } |\Phi\rangle} = \underbrace{E_k}_{\text{Quasi-particle energies } > 0} \begin{pmatrix} U_k \\ V_k \end{pmatrix} \quad \text{with} \quad \begin{aligned} h_{pq} &\equiv \langle \Phi | \{ [c_p, \Omega], c_q^\dagger \} | \Phi \rangle \\ \Delta_{pq} &\equiv \langle \Phi | \{ [c_p, \Omega], c_q \} | \Phi \rangle \end{aligned}$$

$$\Rightarrow \begin{pmatrix} \Omega^{11} & \Omega^{20} \\ -\Omega^{20*} & -\Omega^{11*} \end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \mathcal{W} = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

$$\Rightarrow \begin{aligned} \Omega^{11} &= \bar{\Omega}^{11} = \sum_k E_k \beta_k^\dagger \beta_k \\ \check{\Omega}^{11} &= \Omega^{20} = \Omega^{02} = 0 \end{aligned} \quad \Rightarrow \quad \boxed{\begin{aligned} \Omega_0 &\equiv \Omega^{00} + \Omega^{11} \\ \Omega_1 &\equiv \Omega^{22} + \Omega^{31} + \Omega^{13} + \Omega^{40} + \Omega^{04} \end{aligned}}$$

Canonical diagrams only (extension of Moller-Plesset to (symmetry-projected) BMBPT)

Unperturbed off-diagonal propagators

Quasi-particle operators in interaction representation

$$\beta_k(\tau) \equiv e^{+\tau\Omega_0} \beta_k e^{-\tau\Omega_0} = e^{-\tau E_k} \beta_k$$

$$\beta_k^\dagger(\tau) \equiv e^{+\tau\Omega_0} \beta_k^\dagger e^{-\tau\Omega_0} = e^{+\tau E_k} \beta_k^\dagger$$

Four propagators in quasi-particle space

Time-ordering operator

$$G_{k_1 k_2}^{+- (0)}(\tau_1, \tau_2; \varphi) \equiv \frac{\langle \Phi | T[\beta_{k_1}^\dagger(\tau_1) \beta_{k_2}(\tau_2)] | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} = -e^{-(\tau_2 - \tau_1) E_{k_1}} \theta(\tau_2 - \tau_1) \delta_{k_1 k_2} \quad \text{Normal propagator}$$

$$G_{k_1 k_2}^{-- (0)}(\tau_1, \tau_2; \varphi) \equiv \frac{\langle \Phi | T[\beta_{k_1}(\tau_1) \beta_{k_2}(\tau_2)] | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} = +e^{-\tau_1 E_{k_1}} e^{-\tau_2 E_{k_2}} R_{k_1 k_2}^{--}(\varphi) \quad \begin{array}{l} \text{Carries full } \varphi \text{ dependence} \\ \text{Anomalous propagator} \\ \text{Null for } \varphi=0 \end{array}$$

$$G_{k_1 k_2}^{++ (0)}(\tau_1, \tau_2; \varphi) \equiv \frac{\langle \Phi | T[\beta_{k_1}^\dagger(\tau_1) \beta_{k_2}^\dagger(\tau_2)] | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} = 0 \quad \begin{array}{l} \text{No two op-creation prop.} \\ \text{Anomalous propagator} \end{array}$$

$$G_{k_1 k_2}^{-+ (0)}(\tau_1, \tau_2; \varphi) \equiv \frac{\langle \Phi | T[\beta_{k_1}(\tau_1) \beta_{k_2}^\dagger(\tau_2)] | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle} = -G_{k_2 k_1}^{+- (0)}(\tau_2, \tau_1; \varphi) \quad \text{Normal propagator}$$

Equal-time propagators

$$G_{k_1 k_2}^{-- (0)}(\tau, \tau; \varphi) \equiv +e^{-\tau(E_{k_1} + E_{k_2})} R_{k_1 k_2}^{--}(\varphi)$$

- 1) Only non-zero equal-time propagator is anomalous
- 2) No self-contraction onto a given vertex for $\varphi=0$

Perturbative expansion of $N(\tau, \varphi) = \langle \Phi | \mathcal{U}(\tau) | \Phi(\varphi) \rangle$

Evolution operator $\mathcal{U}(\tau) = e^{-\tau\Omega_0} T e^{-\int_0^\tau dt \Omega_1(t)}$ with $\Omega_1(\tau) \equiv e^{\tau\Omega_0} \Omega_1 e^{-\tau\Omega_0}$

Off-diagonal norm kernel

$$N(\tau, \varphi) = \langle \Phi | e^{-\tau\Omega_0} T e^{-\int_0^\tau dt \Omega_1(t)} | \Phi(\varphi) \rangle \quad \text{Off-diagonal matrix elements of strings of quasi-particle operators}$$

$$= e^{-\tau\Omega^{00}} \left\{ \underbrace{\langle \Phi | \Phi(\varphi) \rangle}_{0^{\text{th}} \text{ order}} - \underbrace{\int_0^\tau d\tau_1 \langle \Phi | \Omega_1(\tau_1) | \Phi(\varphi) \rangle}_{1^{\text{st}} \text{ order}} + \frac{1}{2!} \underbrace{\int_0^\tau d\tau_1 d\tau_2 \langle \Phi | T[\Omega_1(\tau_1) \Omega_1(\tau_2)] | \Phi(\varphi) \rangle}_{2^{\text{nd}} \text{ order}} + \dots \right\}$$

Order-p matrix element

Ω_1 contains terms with 2/4 qp operators
(only with 4 if HFB reference state)

$$\propto \sum_{\substack{i_1 + j_1 = 2, 4 \\ \vdots \\ i_p + j_p = 2, 4}} \langle \Phi | T \left[\underbrace{\Omega^{i_1 j_1}(\tau_1)}_{\text{Normal-ordered operator with } i_1 (j_1) \beta^+ (\beta) \text{ operators}} \dots \Omega^{i_p j_p}(\tau_p) \right] | \Phi(\varphi) \rangle$$

Off-diagonal Wick's theorem [R. Balian and E. Brézin, Nuovo Cimento 64, 37 (1969)]

$$\langle \Phi | T \left[\dots \beta_{k_p}^{(\dagger)}(\tau_p) \dots \beta_{k_q}^{(\dagger)}(\tau_q) \dots \right] | \Phi(\varphi) \rangle = \pm \sum_{\text{all sets of contractions}} \dots G_{k_p k_q}^{\pm\pm(0)}(\tau_p, \tau_q; \varphi) \dots \times \langle \Phi | \Phi(\varphi) \rangle$$

Diagrammatic representation of building blocks

Canonical representation of normal-ordered operators

$$\Omega^{[0]} = \bullet$$

Ω^{00}

$$\Omega^{[2]} = \begin{array}{c} \uparrow \\ \bullet \\ \uparrow \end{array} + \begin{array}{c} \swarrow \quad \searrow \\ \bullet \end{array} + \begin{array}{c} \swarrow \quad \searrow \\ \bullet \end{array}$$

$\Omega^{11} \quad \Omega^{20} \quad \Omega^{02}$

$$\Omega^{[4]} = \begin{array}{c} \swarrow \quad \searrow \\ \bullet \\ \swarrow \quad \searrow \end{array} + \begin{array}{c} \swarrow \quad \searrow \\ \bullet \\ \uparrow \end{array} + \begin{array}{c} \uparrow \\ \bullet \\ \swarrow \quad \searrow \end{array} + \begin{array}{c} \swarrow \quad \searrow \\ \bullet \\ \swarrow \quad \searrow \end{array} + \begin{array}{c} \swarrow \quad \searrow \\ \bullet \\ \swarrow \quad \searrow \end{array}$$

$\Omega^{22} \quad \Omega^{31} \quad \Omega^{13} \quad \Omega^{40} \quad \Omega^{04}$

Example given for Ω

Similarly for other operators, e.g. H or A , with different vertices

Elementary propagators

$$\begin{array}{c} k_2 \uparrow \tau_2 \\ \uparrow \\ k_1 \uparrow \tau_1 \end{array} \quad \begin{array}{c} k_2 \uparrow \tau_2 \\ \uparrow \\ k_1 \uparrow \tau_1 \end{array}$$

$G_{k_1 k_2}^{+- (0)}(\tau_1, \tau_2; \varphi) \quad G_{k_1 k_2}^{-- (0)}(\tau_1, \tau_2; \varphi)$

How to depart from canonical representation

$$\begin{array}{c} k_1 \quad k_2 \\ \swarrow \quad \searrow \\ \bullet \\ \swarrow \quad \searrow \\ k_3 \quad k_4 \end{array} + \Omega_{k_1 k_2 k_3 k_4}^{22} = \begin{array}{c} \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \\ \bullet \\ k_3 \quad k_4 \quad k_2 \quad k_1 \end{array} = \begin{array}{c} \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \\ \bullet \\ k_3 \quad k_2 \quad k_4 \quad k_1 \end{array} = \begin{array}{c} \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \\ \bullet \\ k_2 \quad k_1 \quad k_3 \quad k_4 \end{array}$$

$$\begin{array}{c} k_2 \downarrow \tau_2 \\ \downarrow \\ k_1 \uparrow \tau_1 \end{array} \quad \begin{array}{c} k_2 \downarrow \tau_2 \\ \downarrow \\ k_1 \uparrow \tau_1 \end{array}$$

$G_{k_1 k_2}^{++ (0)}(\tau_1, \tau_2; \varphi) \quad G_{k_1 k_2}^{-+ (0)}(\tau_1, \tau_2; \varphi)$

Diagrammatic rules

Norm kernel at order p

- 1) All topologically distinct vacuum-to-vacuum Feynman diagrams with p operators $\Omega^{ijk}(\tau_k)$
- 2) Normal and anomalous contractions allowed (only anomalous ones closed onto a vertex)
- 3) Sign $(-1)^{p+n}$ with n = number of crossing lines in the diagram
- 4) Factor $1/n_e!$ for each group of n_e equivalent lines (same type of propagators!)
- 5) Factor $1/2$ for each anomalous line closed onto a vertex
- 6) Symmetry factor $1/n_s$ for exchanges of time labels giving topologically equivalent diagrams
- 7) Normal lines linking two vertices must propagate in the same direction
- 8) As $G^{++}(\varphi) = 0$, the number of anomalous contractions is $0 \leq n_a = \sum_{k=1}^p (j_k - i_k) \leq 2p$
- 9) Sum over all quasi-particle and all time labels from 0 to τ



$n_a = 0$ for diagonal kernels ($\varphi = 0$)

Diagrammatic expansion of $N(\tau, \varphi)$

Exponentiation of connected diagrams

Each diagram is decomposed into its connected parts

$$\begin{aligned}
 N(\tau, \varphi) &= e^{-\tau \Omega^{00}} \langle \Phi | \Phi(\varphi) \rangle \sum_{\Gamma} \Gamma(\tau, \varphi) \\
 &= e^{-\tau \Omega^{00}} \langle \Phi | \Phi(\varphi) \rangle \sum_{n_1 n_2 \dots} \frac{[\Gamma_1(\tau, \varphi)]^{n_1}}{n_1!} \frac{[\Gamma_2(\tau, \varphi)]^{n_2}}{n_2!} \dots \\
 &= e^{-\tau \Omega^{00}} \langle \Phi | \Phi(\varphi) \rangle e^{\Gamma_1(\tau, \varphi) + \Gamma_2(\tau, \varphi) + \dots} \\
 &= e^{-\tau \Omega^{00} + n(\tau, \varphi)} \langle \Phi | \Phi(\varphi) \rangle
 \end{aligned}$$

Symmetry factor

Diagrams with any number of all possible connected parts exhaust the sum

Gauge-angle dependence

with $n(\tau, \varphi) \equiv \sum_{p=1}^{\infty} n^{(p)}(\tau, \varphi)$ the connected diagrams

Diagrams with no anomalous contraction

$$n(\tau, \varphi) \equiv \overbrace{n(\tau; n_a = 0)} + n(\tau, \varphi; n_a > 0)$$

Finite when $\tau \rightarrow \infty$

Null for $\varphi = 0$ =1 for $\varphi = 0$

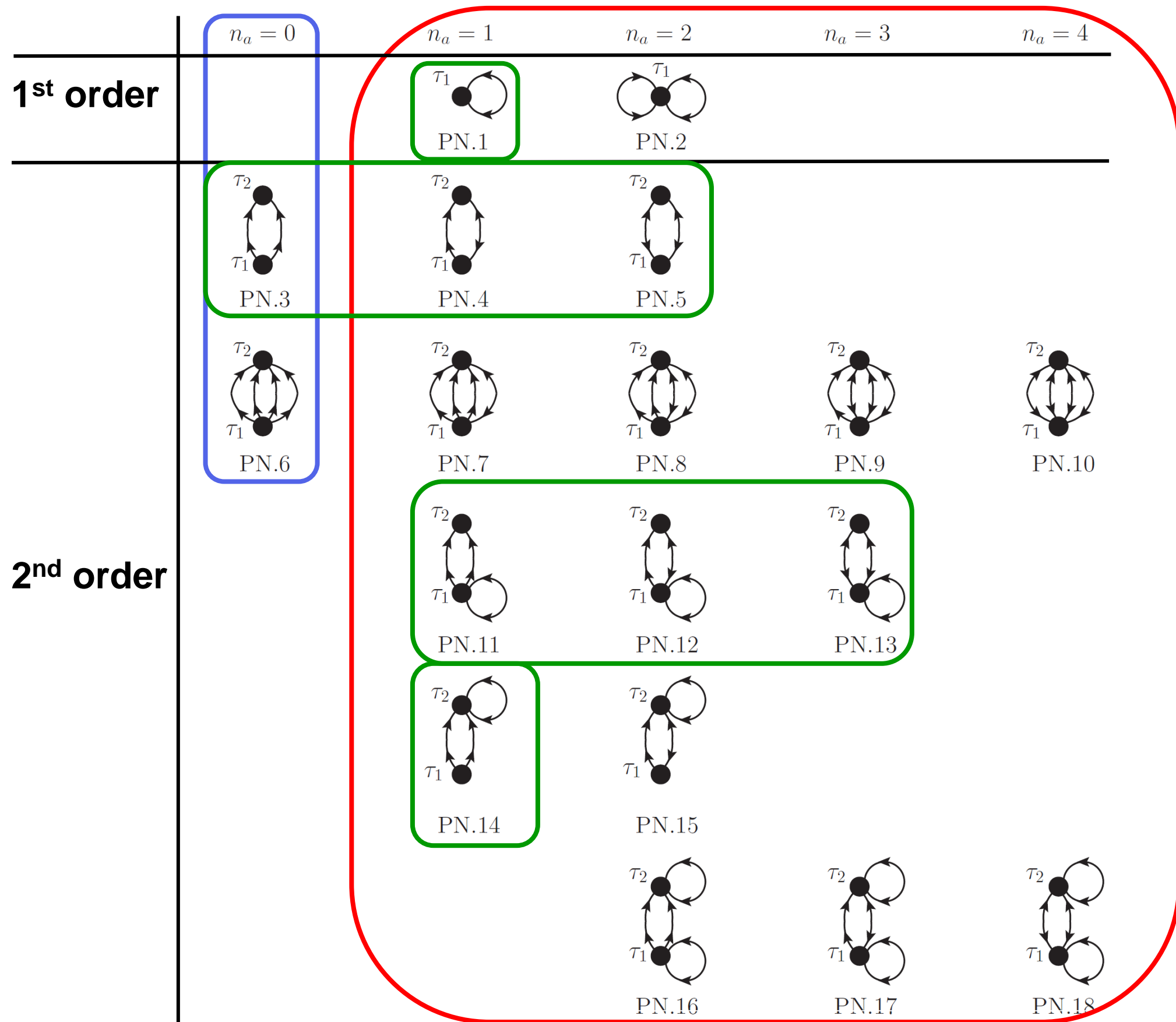
The only ones that need to be computed

The logarithm of the norm is size extensive

$$\Rightarrow \mathcal{N}(\tau, \varphi) = \frac{N(\tau, \varphi)}{N(\tau, 0)} = e^{\overbrace{n(\tau, \varphi; n_a > 0)}} \overbrace{\langle \Phi | \Phi(\varphi) \rangle}$$

Intermediate normalization for $\varphi = 0$

Diagrams of $n(\tau, \varphi)$ to second order



18 diagrams

2 diagrams

15 diagrams

8 diagrams

Only contributions to $\varphi = 0$

Carry the φ dependence

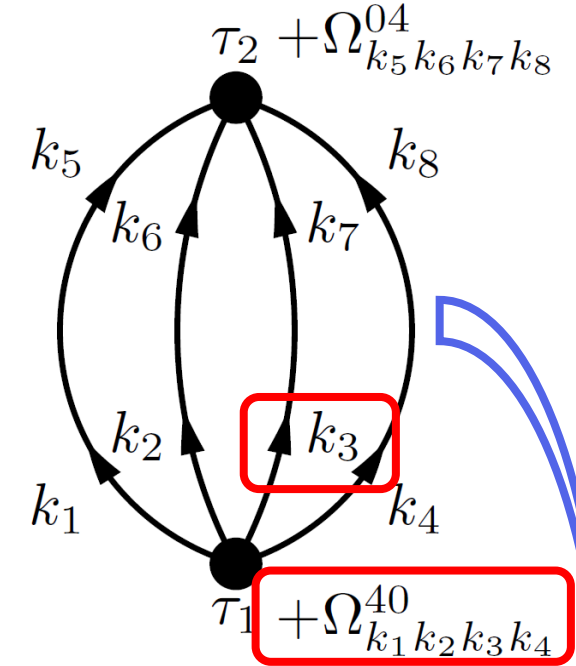
Null for HFB reference state

Algebraic expression of $n(\tau, \varphi)$ to second order

PN.6: example of diagram contributing to $n(\tau, 0)$

$$\text{PN.6} = \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega_{k_1 k_2 k_3 k_4}^{04} \Omega_{k_1 k_2 k_3 k_4}^{40}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \left[\tau - \frac{1 - e^{-\tau(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4})}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \right]$$

$$\stackrel{\tau \rightarrow \infty}{=} \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega_{k_1 k_2 k_3 k_4}^{04} \Omega_{k_1 k_2 k_3 k_4}^{40}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \left[\tau - \frac{1}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \right]$$



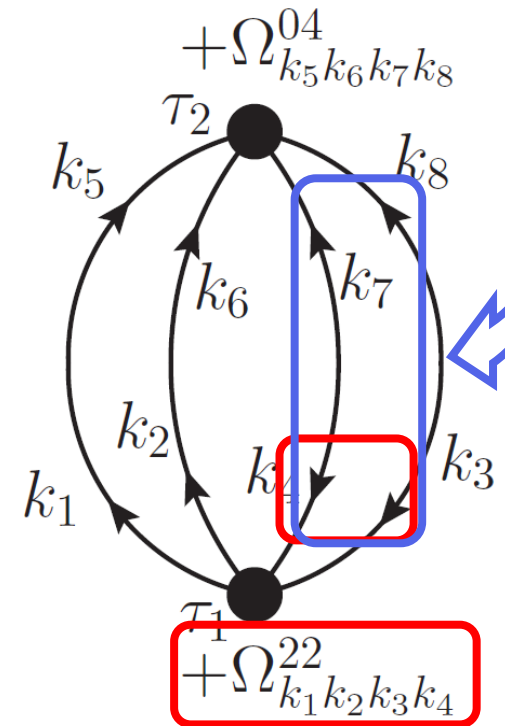
Two right lines are now anomalous ($n_a=2$)
The lowest vertex has changed accordingly

PN.8: example of diagram with genuine φ dependence

$$\text{PN.8} = \frac{1}{4} \sum_{\substack{k_1 k_2 k_3 k_4 \\ k_5 k_6}} \frac{\Omega_{k_1 k_2 k_3 k_4}^{22} \Omega_{k_5 k_6 k_1 k_2}^{04}}{E_{k_1} + E_{k_2} - E_{k_3} - E_{k_4}} \left[\frac{1 - e^{-\tau(E_{k_3} + E_{k_4} + E_{k_5} + E_{k_6})}}{E_{k_3} + E_{k_4} + E_{k_5} + E_{k_6}} \right. \\ \left. - \frac{1 - e^{-\tau(E_{k_1} + E_{k_2} + E_{k_5} + E_{k_6})}}{E_{k_1} + E_{k_2} + E_{k_5} + E_{k_6}} \right] R_{k_3 k_6}^{--}(\varphi) R_{k_4 k_5}^{--}(\varphi)$$

$$\stackrel{\tau \rightarrow \infty}{=} \frac{1}{4} \sum_{\substack{k_1 k_2 k_3 k_4 \\ k_5 k_6}} \frac{\Omega_{k_1 k_2 k_3 k_4}^{22} \Omega_{k_5 k_6 k_1 k_2}^{04}}{(E_{k_3} + E_{k_4} + E_{k_5} + E_{k_6})(E_{k_1} + E_{k_2} + E_{k_5} + E_{k_6})} R_{k_3 k_6}^{--}(\varphi) R_{k_4 k_5}^{--}(\varphi)$$

Null for $\varphi = 0$



Perturbative expansion of $\Omega(\tau, \varphi) = \langle \Phi | \mathcal{U}(\tau) \Omega | \Phi(\varphi) \rangle$

Off-diagonal operator kernel

Difference with norm kernel: presence of the (time-independent) operator

Put at **fixed** time 0 to be inserted in time-ordering at no cost

$$\begin{aligned}\Omega(\tau, \varphi) &= \langle \Phi | e^{-\tau \Omega_0} T e^{-\int_0^\tau dt \Omega_1(t)} \Omega | \Phi(\varphi) \rangle \\ &= e^{-\tau \Omega^{00}} \left\{ \underbrace{\langle \Phi | \Omega(0) | \Phi(\varphi) \rangle}_{0^{\text{th}} \text{ order}} - \underbrace{\int_0^\tau d\tau_1 \langle \Phi | T[\Omega_1(\tau_1) \Omega(0)] | \Phi(\varphi) \rangle}_{1^{\text{st}} \text{ order}} + \dots \right\}\end{aligned}$$

Factorization of disconnected pieces

All vacuum-to-vacuum diagrams of order n

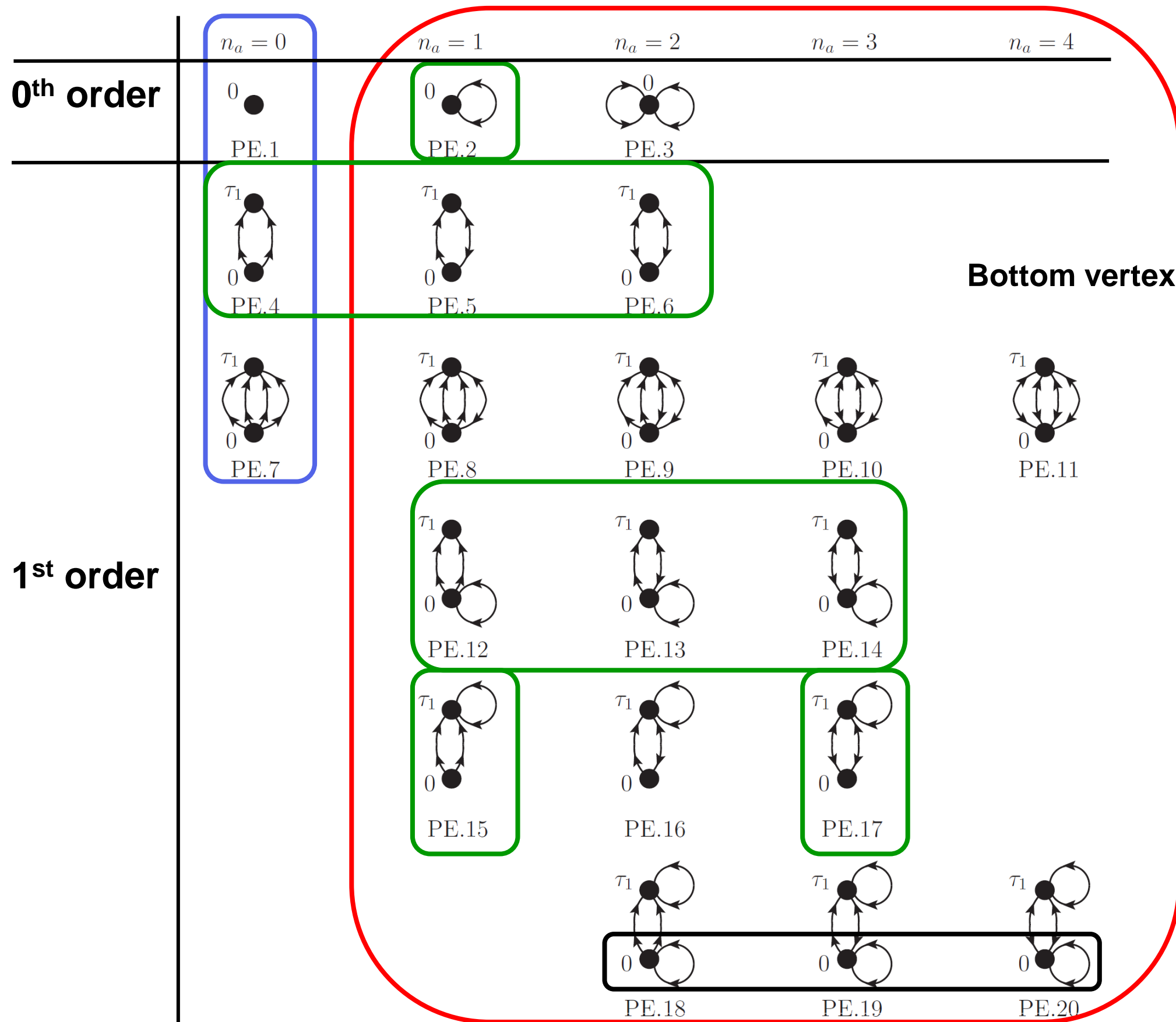
$$\Omega(\tau, \varphi) \equiv e^{-\tau \Omega^{00}} \sum_{n=0}^{\infty} \Omega^{(n)}(\tau, \varphi) \langle \Phi | \Phi(\varphi) \rangle$$

→ Only vacuum-to-vacuum diagrams of order n **linked to $\Omega(0)$**

$$\equiv \sum_{n=0}^{\infty} \omega^{(n)}(\tau, \varphi) N(\tau, \varphi)$$

Norm kernel factorizes in operator kernel

Diagrams of $\omega(\tau, \varphi)$ to first order



20 diagrams

3 diagrams

17 diagrams

9 diagrams

Bottom vertex is here at fixed time 0

Only contributions to $\varphi = 0$

Carry the φ dependence

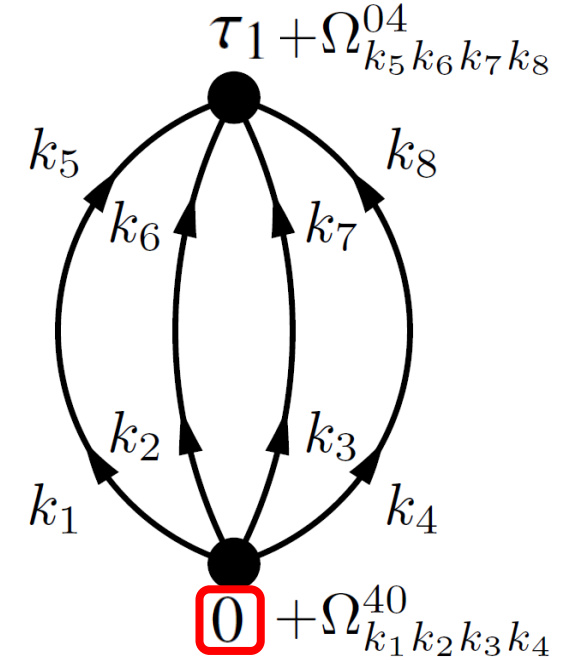
Null for HFB reference state

Algebraic expression of $\omega(\tau, \varphi)$ to first order

PE.7: example of diagram contributing to $\omega(\tau, 0)$

$$\text{PE.7} = -\frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega_{k_1 k_2 k_3 k_4}^{04} \Omega_{k_1 k_2 k_3 k_4}^{40}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \left[1 - e^{-\tau(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4})} \right]$$

$$\stackrel{\tau \rightarrow \infty}{=} -\frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega_{k_1 k_2 k_3 k_4}^{04} \Omega_{k_1 k_2 k_3 k_4}^{40}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$



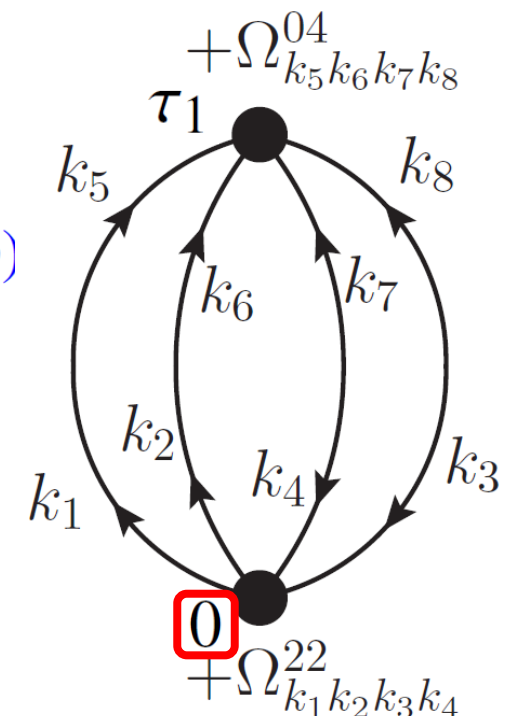
Standard « second »-order MBPT correction based on a **Bogoliubov** reference state

Lowest vertex at fixed time 0

PE.9: example of diagram with genuine φ dependence

$$\text{PE.9} = -\frac{1}{4} \sum_{\substack{k_1 k_2 k_3 k_4 \\ k_5 k_6}} \frac{\Omega_{k_1 k_2 k_3 k_4}^{04} \Omega_{k_1 k_2 k_5 k_6}^{22}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \left[1 - e^{-\tau(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4})} \right] R_{k_3 k_6}^{--}(\varphi) R_{k_4 k_5}^{--}(\varphi)$$

$$\stackrel{\tau \rightarrow \infty}{=} -\frac{1}{4} \sum_{\substack{k_1 k_2 k_3 k_4 \\ k_5 k_6}} \frac{\Omega_{k_1 k_2 k_3 k_4}^{04} \Omega_{k_1 k_2 k_5 k_6}^{22}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \frac{R_{k_3 k_6}^{--}(\varphi) R_{k_4 k_5}^{--}(\varphi)}{\text{Null for } \varphi = 0}$$



Relation between $N(\tau, \varphi)$ and $A(\tau, \varphi)$

First-order differential equation for $\mathcal{N}(\tau, \varphi)$

$$\begin{aligned} \mathcal{N}(\tau, \varphi) &\equiv \langle \Psi(\tau) | \Phi(\varphi) \rangle & | \Phi(\varphi) \rangle &= e^{iA\varphi} | \Phi(\varphi) \rangle \\ \mathcal{A}(\tau, \varphi) &\equiv \langle \Psi(\tau) | A | \Phi(\varphi) \rangle & \mathcal{A}(\tau, \varphi) &= \underbrace{a(\tau, \varphi)}_{\text{linked to operator A}} \mathcal{N}(\tau, \varphi) \end{aligned} \quad \oplus \quad \Rightarrow \quad \boxed{\frac{d}{d\varphi} \mathcal{N}(\tau, \varphi) - i a(\tau, \varphi) \mathcal{N}(\tau, \varphi) = 0}$$

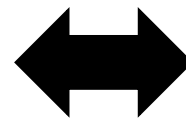
Vacuum-to-vacuum diagrams linked to operator A

Closed-form solution

Direct expansion

$$\begin{aligned} \mathcal{N}(\tau, \varphi) &= e^{i \int_0^\varphi d\phi a(\tau, \phi)} \\ &= e^{i \int_0^\varphi d\phi [a(\tau, \phi) - a^{(0)}(\tau, \phi)]} \langle \Phi | \Phi(\varphi) \rangle \end{aligned}$$

$$\mathcal{N}(\tau, \varphi) = e^{\boxed{n(\tau, \varphi; n_a > 0)}} \langle \Phi | \Phi(\varphi) \rangle$$



Connected vacuum-to-vacuum diagrams of the norm

Ensures exact restoration of good particle number

Perturbation theory

$$n^{(p)}(\tau, \varphi; n_a > 0) = i \int_0^\varphi d\phi a^{(p)}(\tau, \phi)$$

Indeed valid order by order

$$\begin{aligned} \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{A}(\tau, \varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\tau, \varphi)} &= -i \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} \frac{d}{d\varphi} \mathcal{N}(\tau, \varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\tau, \varphi)} \\ &= +i \frac{\int_0^{2\pi} d\varphi \frac{d}{d\varphi} [e^{-iA\varphi}] \mathcal{N}(\tau, \varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\tau, \varphi)} \end{aligned}$$

= A Independently of truncation of $a(\tau, \varphi)$!

Summing up

Particle-number restored quantities

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

$$E_0^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} h(\varphi) \mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)}$$

- 1) Compute at order p via off-diagonal BMBPT at each angle φ
- 2) Compute from $a(\varphi)$ at order p (first equation valid by construction)
- 3) Integrate over (discretized) φ

Projected HFB recovered at lowest order

$$h^{(0)}(\tau, \varphi) = \frac{\langle \Phi | H | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle}$$

$$\mathcal{N}^{(0)}(\tau, \varphi) = \langle \Phi | \Phi(\varphi) \rangle$$

Symmetry-broken BMBPT at $\varphi = 0$

$$E_0^A = h(0)$$

Subset of diagrams at $\varphi = 0$



$$E_0^{A(0)} = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} \langle \Phi | H | \Phi(\varphi) \rangle}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \langle \Phi | \Phi(\varphi) \rangle}$$

$$= \frac{\langle \Phi | H P^A | \Phi \rangle}{\langle \Phi | P^A | \Phi \rangle}$$

$$= \frac{\langle \Theta^A | H | \Theta^A \rangle}{\langle \Theta^A | \Theta^A \rangle}$$

PHFB

where $|\Theta^A\rangle \equiv P^A |\Phi\rangle$

(See BMBPT talk by P. Arthuis on Thursday)

Summing up

Particle-number restored quantities

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

$$E_0^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} h(\varphi) \mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)}$$

CC expansion of operator kernels

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

$$a(\varphi) \equiv \frac{\mathcal{A}(\varphi)}{\mathcal{N}(\varphi)} = \langle \Phi | \tilde{A}(\varphi) e^{\mathcal{T}(\varphi)} | \Phi \rangle$$

- 1) Compute at order p via off-diagonal BMBPT at each angle φ
- 2) Compute from $a(\varphi)$ at order p (first equation valid by construction)
- 3) Integrate over (discretized) φ

Coupled-cluster formulation also available

$$|\Psi_0^A\rangle \equiv e^U |\Phi\rangle$$



$$\begin{aligned} \mathcal{N}(\varphi) &\equiv \langle \Phi(\varphi) | e^U | \Phi \rangle, \\ \mathcal{H}(\varphi) &\equiv \langle \Phi(\varphi) | H e^U | \Phi \rangle \\ \mathcal{A}(\varphi) &\equiv \langle \Phi(\varphi) | A e^U | \Phi \rangle \end{aligned}$$

with

$$\tilde{H}(\varphi) \equiv e^{Z^\dagger(\varphi)} H e^{-Z^\dagger(\varphi)}$$

$$\tilde{A}(\varphi) \equiv e^{Z^\dagger(\varphi)} A e^{-Z^\dagger(\varphi)}$$

ODE for φ dependence of amplitudes

$$\frac{d}{d\varphi} \mathcal{T}_{k_1 \dots k_{2n}}(\varphi) = -i a_{k_1 \dots k_{2n}}^{02}(\varphi) \text{ with } \mathcal{T}(0) = U$$

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

[T. Duguet, A. Signoracci, J. Phys. G: Nucl. Part. Phys. 44 (2016) 015103]

[Y. Qiu, T. M. Henderson, J. Zhao, G. E. Scuseria, J. Chem. Phys. 147, 064111 (2017)]

[T. Duguet, Y. Qiu, T. M. Henderson, J. Zhao, G. E. Scuseria, unpublished]

where $a_{k_1 \dots k_{2n}}^{02}(\varphi) \equiv \langle \Phi^{k_1 \dots k_{2n}} | \tilde{A}^{02}(\varphi) e^{\mathcal{T}(\varphi)} | \Phi \rangle_C$

Contents

● Introduction

- Nuclear chart and ab initio methods
- Why breaking symmetries?
- On-going developments and projects in this direction

● Symmetry broken&restored Bogoliubov many-body perturbation theory

- Generalities
- Set up of the formalism
- Perturbation theory and diagrammatic representations

● Conclusions

Collaborators on ab initio many-body calculations



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D. Lacroix



C. Barbieri



P. Navrátil



**G. Hagen
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R. Roth

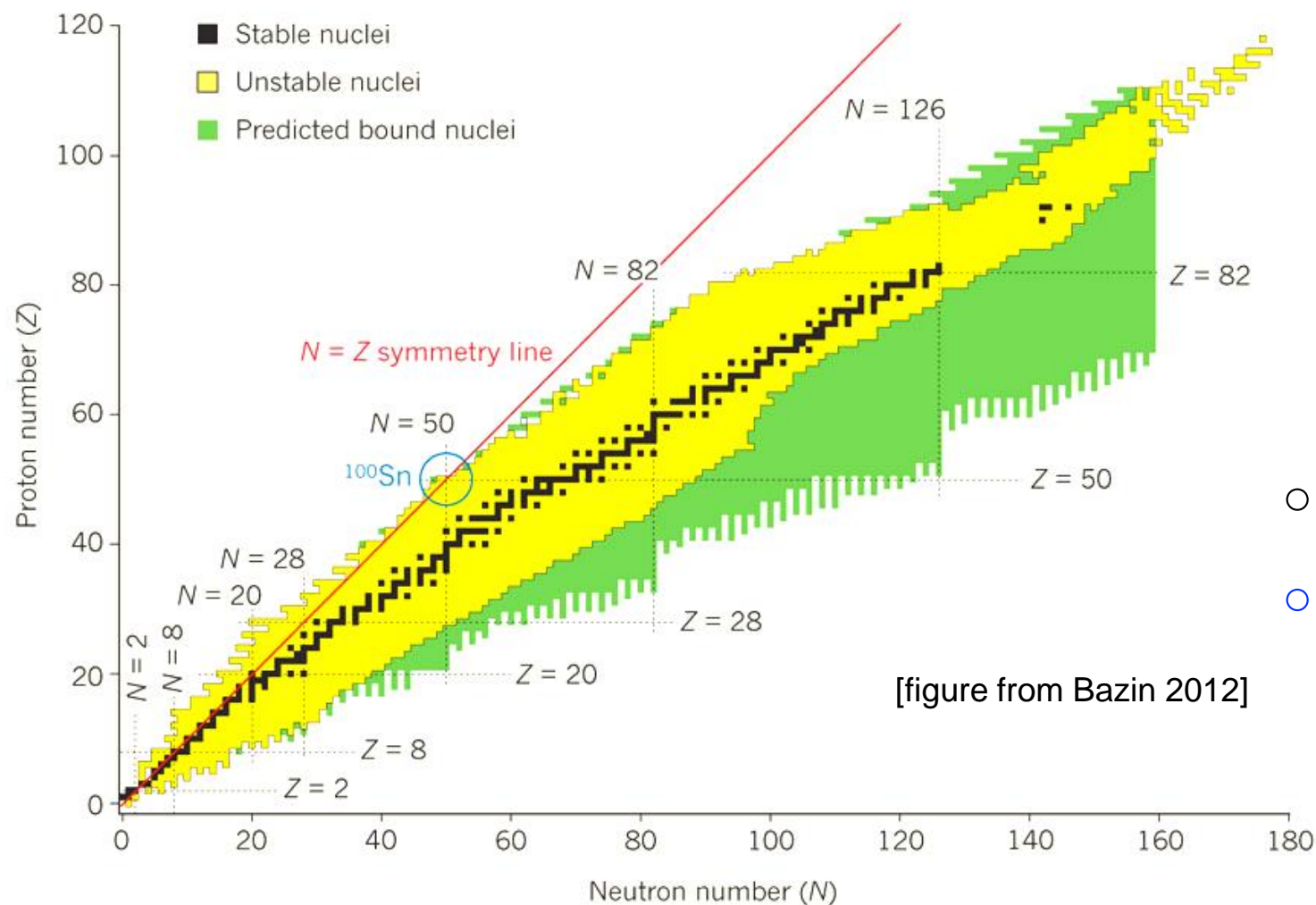
Appendix

Elementary facts and questions about nuclei

- 254 **stable** isotopes, ~3100 synthesised in the lab
- **How many** bound (w.r.t strong force) nuclei exist; 9000?

- **Heaviest** synthesized element $Z=118$

- **Heaviest possible** element?
- Enhanced stability near $Z=120$?



- Modes of **instability** (α , β , γ decays, fission)
- Are there more exotic decay modes?

- Elements **up to Fe** produced in stellar fusion
- How have heavier elements been produced?

- Neutron **drip-line** known up to $Z=8$ (16 neutrons)

- Where is the neutron drip-line beyond $Z=8$?

- Over-stable "magic" nuclei (2, 8, 20, 28, 50, 82, ...)

- Are **magic numbers** the same for unstable nuclei?

Ab initio many-body problem

Ab initio (= “from scratch”) many-body scheme

A-body Hamiltonian

$$H = T + V^{2N} + V^{3N} + V^{4N} + \dots + V^{AN}$$

A-body wave-function
5 variables x A nucleons

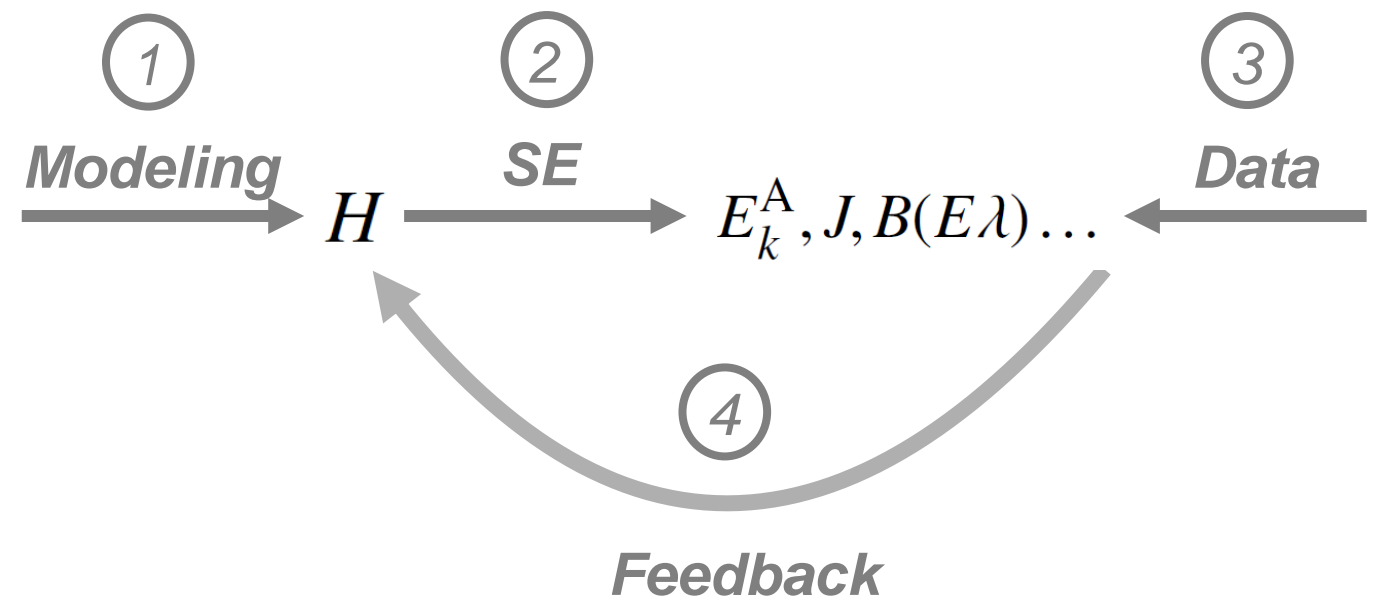
$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

Definition

- A structure-less nucleons
- All nucleons active in full Hilbert space \mathcal{H}_A
- Elementary interactions between them
- Solve A-body Schroedinger equation (SE)
- Thorough estimate of error

Hamiltonian

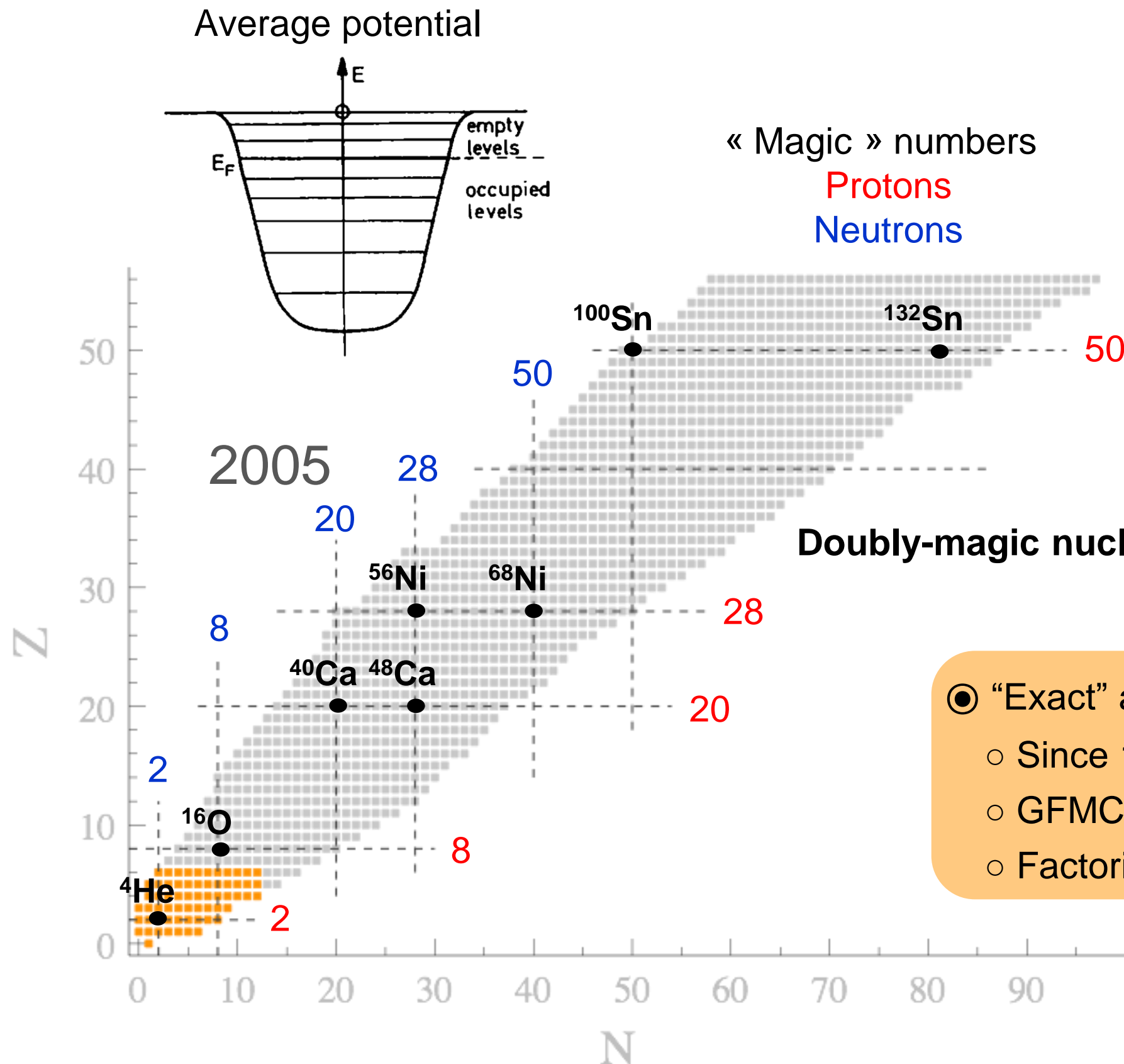
Do we know the form of V^{2N} , V^{3N} etc
Do we know how to derive them from QCD?
Why would there be forces beyond pairwise?
Do we need all the terms up to AN forces?



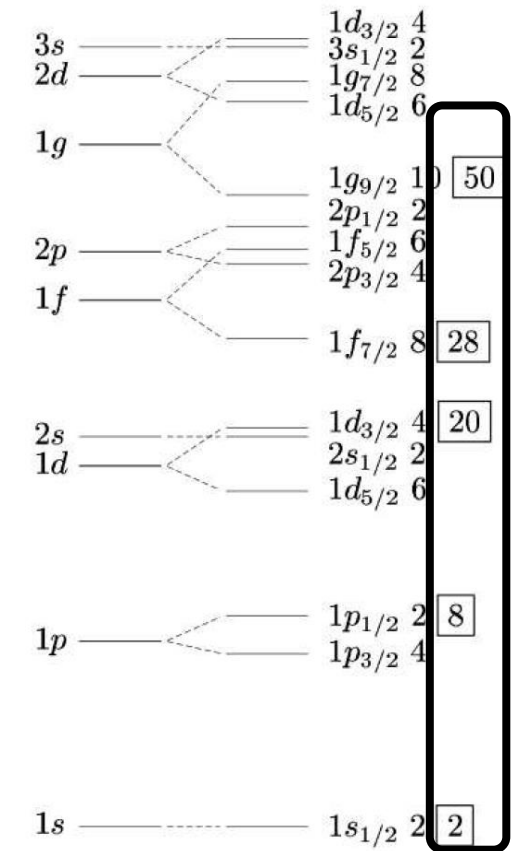
Schroedinger equation

Can we solve the SE with relevant accuracy?
Can we do it for any $A=N+Z$?
Is it even reasonable for $A=200$ to proceed this way?
More effective approaches needed?

Evolution of ab initio nuclear chart



Filling of nuclear shells

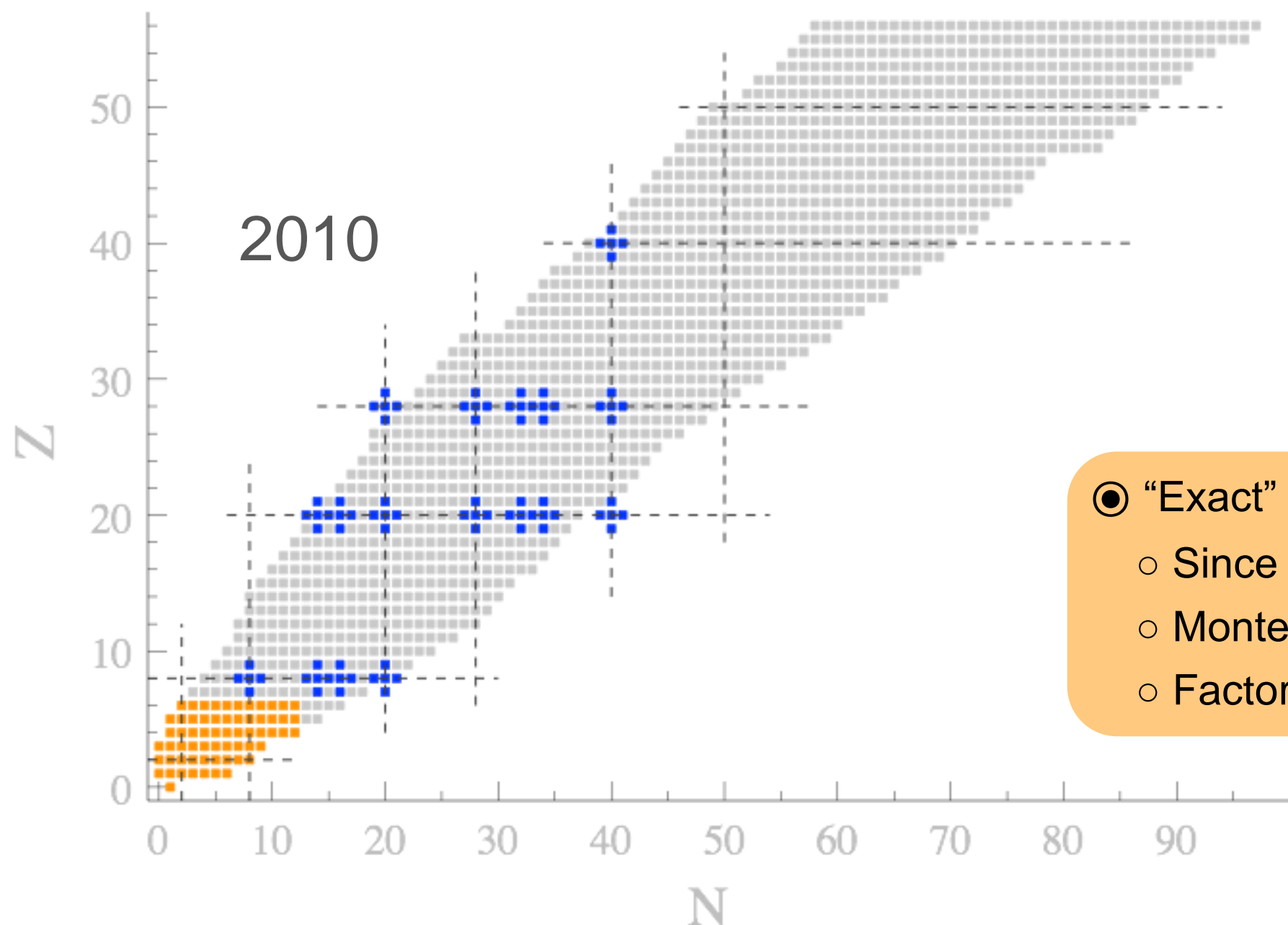


- “Exact” ab initio approaches
 - Since 1980’s
 - GFMC, NCSM, ...
 - Factorial scaling

Evolution of ab initio nuclear chart

● Approximate methods for doubly closed-shells

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



● “Exact” methods

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

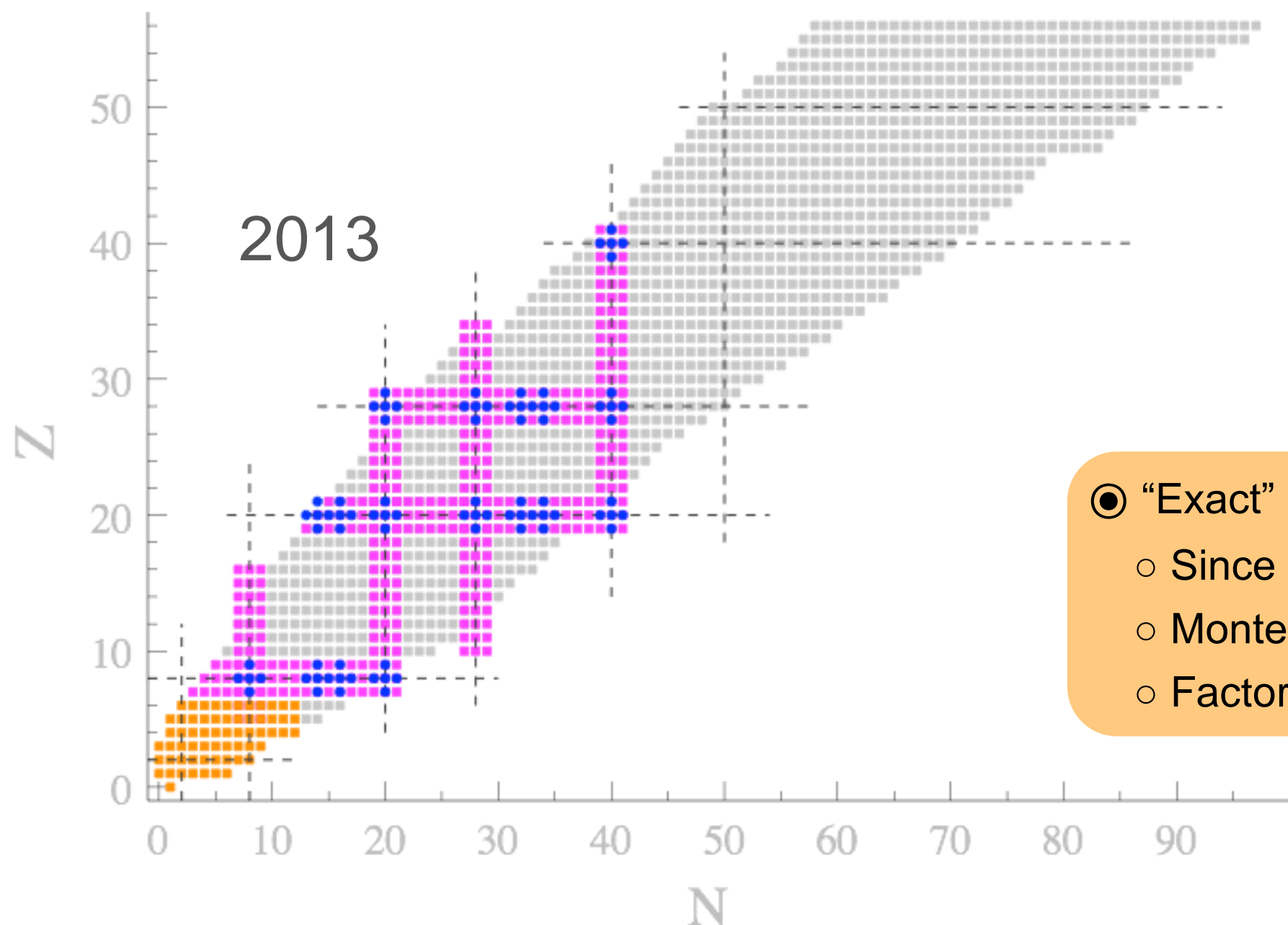
Evolution of ab initio nuclear chart

● Approximate methods for doubly closed-shells

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

● Approximate methods for singly open-shell

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



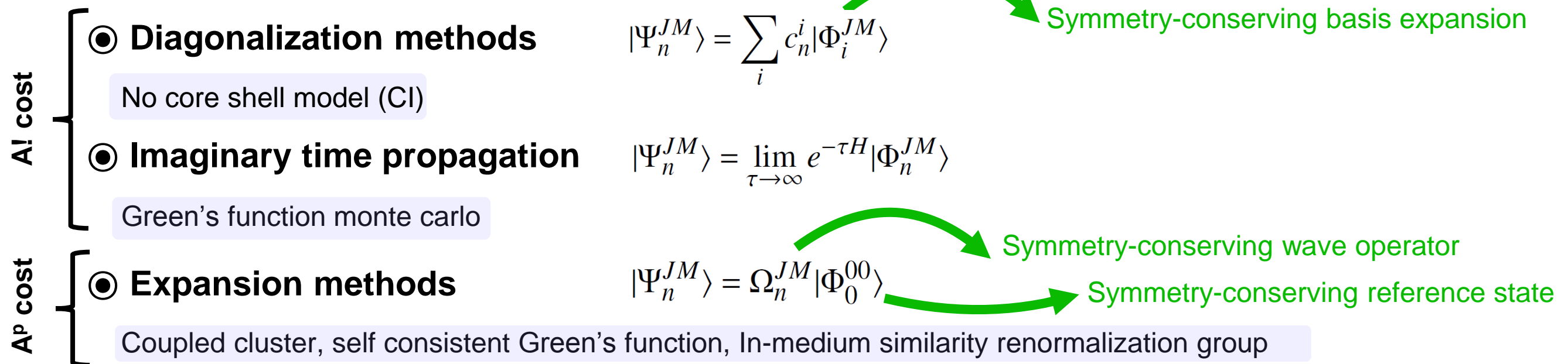
● “Exact” methods

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

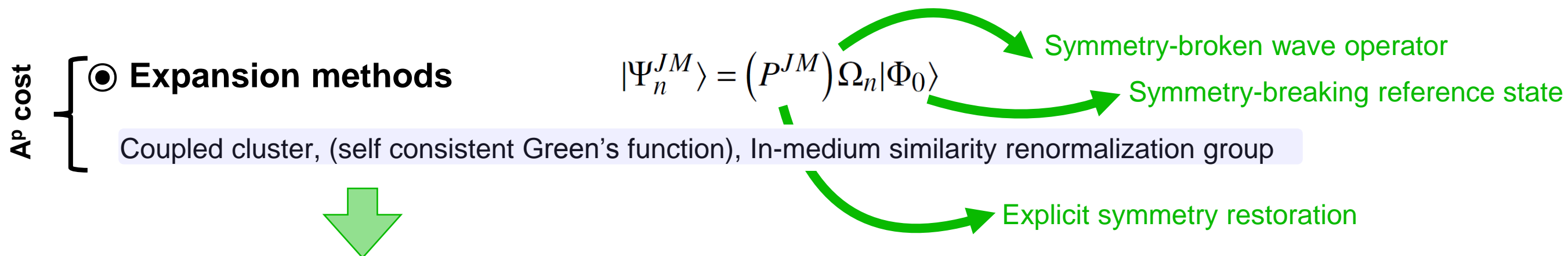
Two strategies to deal with symmetries of H (e.g. $SU(2)$)

$$H|\Psi_n^{JM}\rangle = E_n^J |\Psi_n^{JM}\rangle$$

A. Enforced throughout = **symmetry-conserving methods**



B. Allowed to break at low order before being restored = **symmetry-broken and -restored methods**



But why breaking (+ restoring) symmetries, e.g. $SU(2)$ and/or $U(1)$? (focus on $U(1)$, i.e. singly open shell, today)

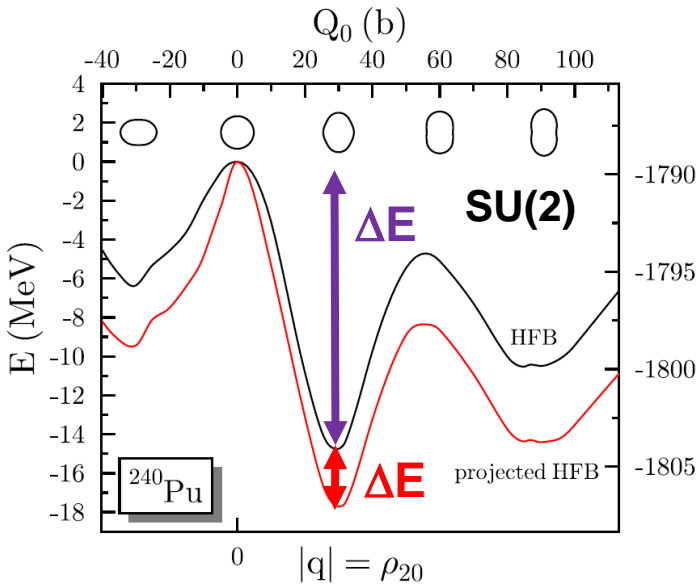
Emergent symmetry breaking in quantum finite systems

Symmetries of H

Invariance	Group	$ \Psi^X\rangle$
Gauge rotation	U(1)	N,Z
Spatial rotation	SU(2)	J,M

Symmetry breaking mean-field (HFB)

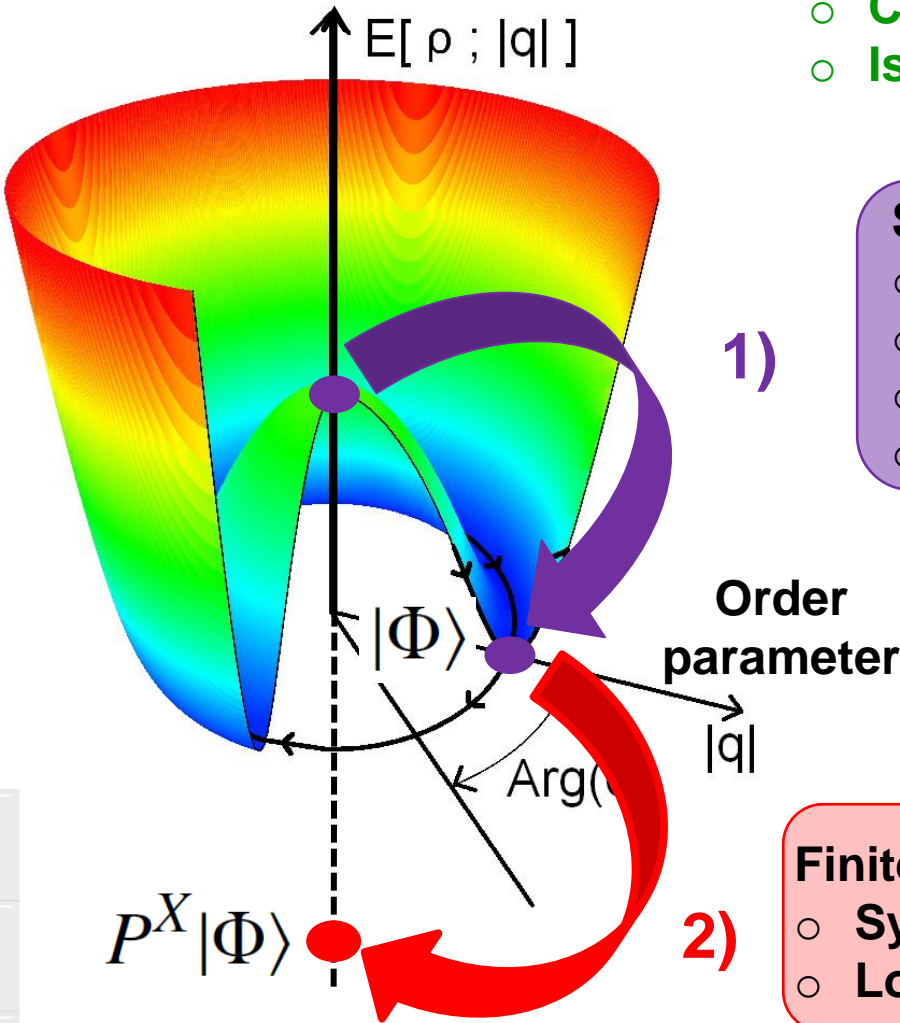
Correlations	ΔE	Excitation	All nuclei...
Pairing	<2MeV	Gap	...but doubly magic
Angular local.	<20MeV	Rot. band	...but singly magic



[M. Bender, private communication]

Symmetry-restored mean-field (HFB)

$ \Psi^X\rangle$	ΔE	Excitations
N,Z	~1MeV	Pair rot.
J,M	~2MeV	Rot. band



- Emergent**
- Cannot be anticipated from dof + H
 - Is not fully realized

- Spontaneous breaking**
- GS has lower symmetry than H
 - GS = wave packet mixing IRREPs
 - Goldstone boson = rotations
 - Higgs modes = vibrations

- Finite system = breaking only emergent**
- Symmetry is actually enforced
 - Lower symmetry imprints excitations

But missing correlations beyond mean field here, i.e. from wave operator Ω

Projective and symmetric many-body methods

Time-independent eigenvalue equations

$$A|\Psi_\mu^A\rangle = A|\Psi_\mu^A\rangle$$

$$H|\Psi_\mu^A\rangle = E_\mu^A |\Psi_\mu^A\rangle$$

Projective method

$$\langle \Theta | A | \Psi_\mu^A \rangle = A \langle \Theta | \Psi_\mu^A \rangle$$

$$\underbrace{\langle \Theta | H | \Psi_\mu^A \rangle}_{\text{Simple, e.g. uncorrelated, state}} = E_\mu^A \langle \Theta | \Psi_\mu^A \rangle$$

Simple, e.g. uncorrelated, state

Expectation-value method

$$\langle \Psi_\mu^A | A | \Psi_\mu^A \rangle = A \langle \Psi_\mu^A | \Psi_\mu^A \rangle$$

$$\underbrace{\langle \Psi_\mu^A | H | \Psi_\mu^A \rangle}_{\text{Fully correlated state itself}} = E_\mu^A \langle \Psi_\mu^A | \Psi_\mu^A \rangle$$

Fully correlated state itself

Equivalent in exact limit

Not after truncation

Real for E at each MBPT order
Not (necessarily) true for A

Can be symmetrized prior to expansion

$$A = \frac{\langle \Theta | A | \Psi_\mu^A \rangle}{\langle \Theta | \Psi_\mu^A \rangle}$$

$$E_\mu^A = \frac{\langle \Theta | H | \Psi_\mu^A \rangle}{\langle \Theta | \Psi_\mu^A \rangle}$$

Ex: MBPT, CC...

$$A = \frac{\langle \Psi_\mu^A | A | \Psi_\mu^A \rangle}{\langle \Psi_\mu^A | \Psi_\mu^A \rangle}$$

$$E_\mu^A = \frac{\langle \Psi_\mu^A | H | \Psi_\mu^A \rangle}{\langle \Psi_\mu^A | \Psi_\mu^A \rangle}$$

Ex: SCGF, Λ CC...

Asymmetric form

symmetric form

... and for SU(2)

Correspondence table

Group	$U(1)$	$SU(2)$
Infinitesimal generator	A	S_y (J_y)
Rotation angle	φ	β
Measure	$d\varphi$	$\sin \beta d\beta$
Rotation operator	$e^{iA\varphi}$	$e^{-iS_y\beta}$ ($e^{-iJ_y\beta}$)
Quantum number	A	S (J)
IRREP	$e^{iA\varphi}$	$d^S(\beta)_{00}$ ($d^J(\beta)_{00}$)
QP creation operator	β_k^\dagger	a_a^\dagger or a_i
QP annihilation operator	β_k	a_a or a_i^\dagger
Vacuum $ \Phi\rangle$	Bogoliubov state	SU-HF state