Symmetry-restored coupled cluster formalism

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

I. Let the reference state break symmetry(ies)
II. Safely expand the many-body state around it
III. Restore the symmetry(ies) exactly

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Outline

I. Introduction

II. Angular-momentum-restored coupled cluster formalism

T. D., J. Phys. G42, 025107 (2015)

III. Preliminary results in the doubly-open shell ^{24}Mg nucleus

S. Binder, T. D., G. Hagen, T. Papenbrock, unpublished

Introduction

Breaking and restoring symmetries

Expansion around a single reference state

Target state → $|\Psi_0\rangle = \Xi_0 |\Phi\rangle$ ← Reference state

Wave operator ↓ (Ξ_0)

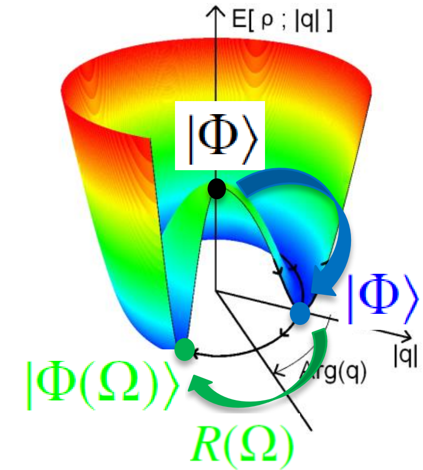
A-body ground state

Expand Ξ_0 →

Size extensive

$$E_0 = \frac{\langle \Psi_0 | H | \Phi \rangle}{\langle \Psi_0 | \Phi \rangle}$$

Ground-state energy



Closed shell	Singly/doubly open shell	Singly/doubly open shell
RHF reference	UHF(B) reference	UHF(B) manifold
conserves A, J^2, M	*breaks A / J^2 and M*	*restores A / J^2 and M*
Dy-SCGF CC	*Go*-SCGF BCC ***First implementation***	PNR-BCC/AMR-CC ***New formalism*** SCGF: to be done
Breaks down for open-shell nuclei	***Symmetry contaminants***	***Multi-reference character***
	ph degeneracy <-> Zero mode	Finite inertia <-> *Resolve zero mode*

Symmetry-restored coupled-cluster theory

Angular-momentum-restored coupled-cluster formalism

T. D., J. Phys. G42, 025107 (2015)

Particle-number-restored Bogoliubov coupled-cluster formalism

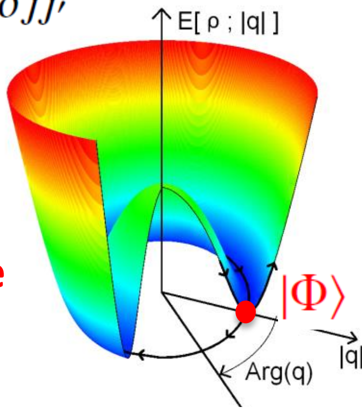
T. D., A. Signoracci, in preparation (2015)

....can be extended to essentially any symmetry group

Single-reference CC based on UHF (GHF)

Symmetry group of H includes SU(2) = non abelian compact Lie group – Lie algebra $\{J_x, J_y, J_z\}$

$$R(\alpha,\beta,\gamma) = e^{-\frac{i}{\hbar}\alpha J_z} e^{-\frac{i}{\hbar}\beta J_y} e^{-\frac{i}{\hbar}\gamma J_z} \equiv R(\Omega)$$ **IRREPs** $D^J_{MK}(\Omega) \equiv \langle \Psi^{JM} | R(\Omega) | \Psi^{J'K} \rangle \delta_{JJ'}$



Eigenstates of H $[H, R(\Omega)] = 0$ **leads to** $H|\Psi^{JM}_\mu\rangle = E^J_\mu |\Psi^{JM}_\mu\rangle$

Symmetry-breaking unperturbed system

U(G)HF reference state

➡ **Degeneracy lifted**

$H \equiv H_0 + H_1$ **where** $H_0 \equiv T + U = \sum_\alpha e_\alpha a^\dagger_\alpha a_\alpha$ **Such that** $[H_0, R(\Omega)] \neq 0$ **and** $[H_1, R(\Omega)] \neq 0$

$$H_0 |\Phi\rangle = \varepsilon_0 |\Phi\rangle$$
$$H_0 |\Phi^{ab\dots}_{ij\dots}\rangle = (\varepsilon_0 + \varepsilon^{ab\dots}_{ij\dots}) |\Phi^{ab\dots}_{ij\dots}\rangle$$

with

$$|\Phi\rangle = \prod_{i=1}^{N} a^\dagger_i |0\rangle$$
$$|\Phi^{ab\dots}_{ij\dots}\rangle \equiv a^\dagger_a a_i a^\dagger_b a_j \dots |\Phi\rangle$$

➡ **Mixes various IRREPs**

CC wave-function ansatz $|\Psi_0\rangle \equiv e^T |\Phi\rangle$

with

$$T \equiv T_1 + T_2 + T_3 + \dots$$
$$T_n \equiv \frac{1}{(n!)^2} \sum_{ijk\dots abc\dots} t^{abc\dots}_{ijk\dots} a^\dagger_a a^\dagger_b a^\dagger_c \dots a_k a_j a_i$$

Single-reference CC based on UHF (GHF)

Time-independent G.S. Schrödinger equation

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

xe^{-T}

$$\bar{H}|\Phi\rangle = E_0|\Phi\rangle$$

$$(He^T)_c|\Phi\rangle = E_0|\Phi\rangle$$

Similarity-transformed Hamiltonian

$$\bar{H} \equiv e^{-T} H e^{T}$$

Baker-Campbell-Hausdorff + Wick theorem

$$\bar{H} = H + (HT)_c + \frac{1}{2!}(HTT)_c + \frac{1}{3!}(HTTT)_c + \frac{1}{4!}(HTTTT)_c$$

Exponential naturally terminates

Energy equation

$$\langle\Phi|(He^T)_c|\Phi\rangle = E_0$$

Disconnected parts canceled out a posteriori

Amplitude equation to determine T_n

$$\langle\Phi^{a\dots}_{i\dots}|(He^T)_c|\Phi\rangle = 0$$

Obtain algebraic expressions via Wick theorem

Variant without xe^{-T} first

$$\langle\Phi|He^T|\Phi\rangle = E_0\langle\Phi|e^T|\Phi\rangle$$

$$\langle\Phi^{a\dots}_{i\dots}|He^T|\Phi\rangle = E_0\langle\Phi^{a\dots}_{i\dots}|e^T|\Phi\rangle$$

Define energy and norm kernels

$$H(\infty,0) = E_0 N(\infty,0)$$

$$H^{a\dots}_{i\dots}(\infty,0) = E_0 N^{a\dots}_{i\dots}(\infty,0)$$

Intermediate normalization $N(\infty,0) \equiv \langle\Phi|\Psi_0\rangle = 1$

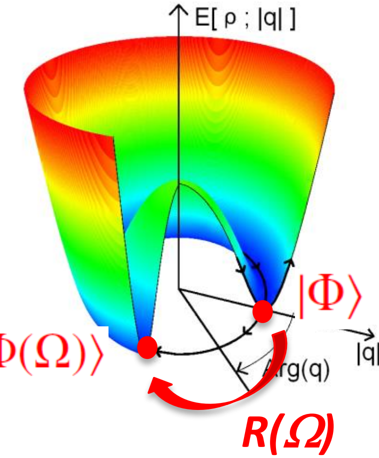
Master equations (1)

Rotated UHF reference states and overlap

$$|\Phi(\Omega)\rangle = \prod_{i=1}^{N} a_{\bar{i}}^{\dagger} |0\rangle \quad \textbf{with} \quad a_{\bar{\alpha}}^{\dagger} = \sum_{\beta} R_{\beta\alpha}(\Omega) a_{\beta}^{\dagger} \quad \textbf{and} \quad R_{\alpha\beta}(\Omega) \equiv \langle\alpha|R(\Omega)|\beta\rangle$$

$$|\Phi_{ij\ldots}^{ab\ldots}(\Omega)\rangle \equiv a_a^{\dagger} a_i a_b^{\dagger} a_j \ldots |\Phi(\Omega)\rangle$$

$$\langle\Phi|\Phi(\Omega)\rangle = \det M(\Omega) \quad \textbf{where} \quad M_{\alpha\beta}(\Omega) \equiv R_{\alpha\beta}(\Omega)\,\delta_{\alpha i}\delta_{\beta j}$$



Imaginary-time dependent scheme

Rotated U(G)HF reference state $|\Phi(\Omega)\rangle$

Time-evolved state $|\Psi(\tau)\rangle \equiv e^{-\tau H}|\Phi\rangle$ **and** $H|\Psi(\tau)\rangle = -\partial_\tau|\Psi(\tau)\rangle$

Off-diagonal kernels

$$\begin{aligned} N(\tau,\Omega) &\equiv \langle\Psi(\tau)|\mathbb{1}|\Phi(\Omega)\rangle \\ H(\tau,\Omega) &\equiv \langle\Psi(\tau)|H|\Phi(\Omega)\rangle \\ J_i(\tau,\Omega) &\equiv \langle\Psi(\tau)|J_i|\Phi(\Omega)\rangle \\ J^2(\tau,\Omega) &\equiv \langle\Psi(\tau)|J^2|\Phi(\Omega)\rangle \end{aligned}$$

1) **Standard kernels at $\Omega = 0$ and $\tau = \infty$**
2) **Same for n-tuply excited kernels**

$$N_{ij\ldots}^{ab\ldots}(\tau,\Omega) \equiv \langle\Psi(\tau)|\mathbb{1}|\Phi_{ij\ldots}^{ab\ldots}(\Omega)\rangle$$

$$H_{ij\ldots}^{ab\ldots}(\tau,\Omega) \equiv \langle\Psi(\tau)|H|\Phi_{ij\ldots}^{ab\ldots}(\Omega)\rangle$$

$$H_{ij\ldots}^{ab\ldots}(\tau,\Omega) = -\partial_\tau N_{ij\ldots}^{ab\ldots}(\tau,\Omega)$$

Schrödinger equation $H(\tau,\Omega) = -\partial_\tau N(\tau,\Omega)$

Reduced kernels $\mathcal{O}(\tau,\Omega) \equiv O(\tau,\Omega)/N(\tau,0)$

➡ ***Intermediate normalization at $\Omega = 0$***

Master equations (2)

Expansion of off-diagonal kernels over IRREPs of SU(2)

$$N(\infty,\Omega) = e^{-\tau E_0^{J_0}} \sum_{MK} \langle \Phi | \Psi_0^{J_0 M} \rangle \langle \Psi_0^{J_0 K} | \Phi \rangle D^{J_0}_{MK}(\Omega)$$

$$H(\infty,\Omega) = e^{-\tau E_0^{J_0}} E_0^{J_0} \sum_{MK} \langle \Phi | \Psi_0^{J_0 M} \rangle \langle \Psi_0^{J_0 K} | \Phi \rangle D^{J_0}_{MK}(\Omega)$$

Time propagation selects the proper IRREP

Straight ratio

$$\mathcal{H}(\infty,\Omega) = E_0^{J_0} \mathcal{N}(\infty,\Omega)$$

Schrödinger equation for G.S.

Truncating kernels expanded around a symmetry-breaking reference $|\Phi\rangle$

$$\mathcal{N}_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathrm{N}^J_{MK}\, D^J_{MK}(\Omega)$$

$$\mathcal{H}_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathrm{E}^J_{MK}\, \mathrm{N}^J_{MK}\, D^J_{MK}(\Omega)$$

IRREPs still mixed as $\tau \rightarrow \infty$

<=>

The good symmetry is lost

Extract good IRREP

Orthogonality of IRREPs

Symmetry-restored energy

$$E_0^{J_0} = \frac{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega\, D^{J_0 *}_{MK}(\Omega)\, \mathcal{H}(\infty,\Omega)}{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega D^{J_0 *}_{MK}(\Omega)\, \mathcal{N}(\infty,\Omega)}$$

Superfluous in exact limit but not after truncation

Standard many-body methods at $\Omega = 0$

$$\mathcal{N}_{\text{approx}}(\infty,0) \equiv \sum_J \sum_M \mathrm{N}^J_{MM}$$

$$\mathcal{H}_{\text{approx}}(\infty,0) \equiv \sum_J \sum_M \mathrm{E}^J_{MM}\, \mathrm{N}^J_{MM}$$

$$D^J_{MK}(0) = \delta_{MK}$$

No fingerprint of mixing left to be used

Benefit of inserting rotation operator in kernels

Angular-momentum-restored CC theory

Goal: extend exact symmetry restoration techniques beyond PHF to any order in CC such that

1. **It keeps the simplicity of a single-reference-like CC theory (and includes it)**
2. **It is valid for any symmetry (spontaneously) broken by the reference state**
3. **It is valid for any system, i.e. closed shell, near degenerate and open shell**
4. **It accesses not only the ground state but also the lowest state of each IRREP**

1) Static correlations from "horizontal" expansion, i.e. from integral over SU(2)
2) Dynamic correlations from "vertical" expansion, i.e. from MBPT/CC expansions of kernels

+ their consistent interference!

Technical points of importance

- **Wick Theorem for off-diagonal matrix element $\langle \Phi | \ldots | \Phi(\Omega) \rangle$ of strings of operators**
  [R. Balian, E. Brezin, NC 64, 37 (1969)]
- **Care must be taken of both the *rotated* energy $\mathcal{H}(\tau, \Omega)$ *and* norm $\mathcal{N}(\tau, \Omega)$ kernels**

Expansion and truncation must be consistent

Has no naturally terminating expansion

Does not stay normalized when Ω varies

Expansion of the operator kernels

Possess generalized expansions
1. MBPT expansion
2. Naturally terminating CC expansion

All kernels are reduced ones at t = ∞

$J_z|\Phi\rangle = 0$ → only one Euler angle β

Expanding the kernel of an operator O

$$\mathcal{O}(\beta) = o(\beta)\, \mathcal{N}(\beta)$$

The norm kernel factorizes exactly for any β

This is proved via the MBPT expansions of $\mathcal{O}(\beta)$ **and** $\mathcal{N}(\beta)$

$o(\beta)$ = connected/linked diagrams to operator O

$\mathcal{N}(\beta)$ = disconnected (exponential of connected) diagrams

$$\mathcal{H}(\beta) \equiv h(\beta)\, \mathcal{N}(\beta)$$
$$\mathcal{J}_i(\beta) \equiv j_i(\beta)\, \mathcal{N}(\beta)$$
$$\mathcal{J}^2(\beta) \equiv j^2(\beta)\, \mathcal{N}(\beta)$$

Extends [J. Goldstone, PRSL A239 (1957) 267 ; N.M. Hugenholtz, Phys. 23 (1957) 481; C. Bloch, NP7 (1958) 451]

Final CC expansion (via time-dependent MBPT…)

β-dependent cluster amplitudes

$$o(\beta) = \frac{\langle \Phi | e^{\mathcal{T}^\dagger(\beta)} O | \Phi(\beta) \rangle_c}{\langle \Phi | \Phi(\beta) \rangle}$$

Off-diagonal connected matrix element

Signals the symmetry breaking

In the exact limit $\frac{d}{d\beta} o(\beta) = 0$

After truncation $\frac{d}{d\beta} o(\beta) \neq 0$

Algebraic expressions

β-dependent elementary contractions

$$\rho_{\alpha\beta}(\beta) \equiv \frac{\langle \Phi | a^+_\beta a_\alpha | \Phi(\beta) \rangle}{\langle \Phi | \Phi(\beta) \rangle} \longrightarrow \rho(\beta) \equiv \rho(0) + \rho^{ph}(\beta)$$

β-dependent part connects holes and particles

$\beta_\alpha \beta_\beta$ in quasi-particle language

Diagonal density matrix of UHF reference state

Standard MBPT/CC expansions recovered at β = 0

Algebraic expressions

Kinetic and potential energy kernels

Natural termination of the exponential
Expand with off-diagonal Wick theorem

$$t(\beta) = \langle \Phi | T + \mathcal{T}_1^\dagger(\beta)\, T | \Phi(\beta) \rangle_c \, \langle \Phi | \Phi(\beta) \rangle^{-1}$$

$$= \sum_i t_{\tilde{i}\tilde{i}}(\beta) + \sum_{ia} \mathcal{T}^\dagger_{ia}(\beta)\, t_{\tilde{a}\tilde{i}}(\beta)$$

Cumbersome expressions
Very rich content in β

$$v(\beta) = \langle \Phi | V + \mathcal{T}_1^\dagger(\beta)\, V + \mathcal{T}_2^\dagger(\beta)\, V + \tfrac{1}{2} \mathcal{T}_1^{\dagger\,2}(\beta)\, V | \Phi(\beta) \rangle_c \, \langle \Phi | \Phi(\beta) \rangle^{-1}$$

$$= \frac{1}{2} \sum_{ij} \bar{v}_{\tilde{i}\tilde{j}\tilde{i}\tilde{j}}(\beta) + \sum_{ija} \mathcal{T}^\dagger_{ia}(\beta)\, \bar{v}_{\tilde{a}\tilde{j}\tilde{i}\tilde{j}}(\beta) + \frac{1}{4} \sum_{ijab} \mathcal{T}^\dagger_{ijab}(\beta)\, \bar{v}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}(\beta) + \sum_{ijab} \mathcal{T}^\dagger_{ia}(\beta)\, \mathcal{T}^\dagger_{jb}(\beta)\, \bar{v}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}(\beta)$$

Transformed operators

Same formal expressions as in standard CC
Same diagrammatic with transformed operators

Bi-orthogonal bases

$$|\tilde{\alpha}\rangle \equiv B(\beta)\, |\alpha\rangle$$
$$\langle\tilde{\alpha}| \equiv \langle \alpha | B^{-1}(\beta)$$
$$B(\beta) \equiv 1 + \rho^{ph}(\beta)$$

$$\tilde{O}(\beta) \equiv \left(\frac{1}{n!}\right)^2 \sum_{\alpha\ldots\beta\gamma\ldots\delta} O_{\tilde{\alpha}\ldots\tilde{\beta}\tilde{\gamma}\ldots\tilde{\delta}}(\beta)\, a^\dagger_\alpha \ldots a^\dagger_\beta\, a_\delta \ldots a_\gamma$$

n-body operator

Similarly for CC amplitudes $0 = \langle \Phi | e^{\mathcal{T}^\dagger(\beta)}\, \tilde{H}(\beta) | \Phi^{ab\ldots}_{ij\ldots} \rangle_c$

CC expansion of the off-diagonal energy kernel

$$h(\beta) = \frac{\langle \Phi | e^{\mathcal{T}^\dagger(\beta)} H | \Phi(\beta) \rangle_c}{\langle \Phi | \Phi(\beta) \rangle} = \langle \Phi | e^{\mathcal{T}^\dagger(\beta)}\, \tilde{H}(\beta) | \Phi \rangle_c$$

Norm kernel

Two key questions about $\mathcal{N}(\beta)$

1. No naturally terminating expansion
2. Consistent expansion with operator kernels $\mathcal{O}(\beta)$?

Energy of the yrast states

$$E_0^J = \frac{\int_0^\pi d\beta \sin\beta \, d_{00}^{J\,*}(\beta) \, h(\beta) \, \mathcal{N}(\beta)}{\int_0^\pi d\beta \sin\beta \, d_{00}^{J\,*}(\beta) \, \mathcal{N}(\beta)}$$

Solution: apply the symmetry-restored scheme to J^2 operator and require exact symmetry restoration

$$\frac{\int_0^\pi d\beta \sin\beta \, d_{00}^{J\,*}(\beta) \, \mathcal{J}^2(\beta)}{\int_0^\pi d\beta \sin\beta \, d_{00}^{J\,*}(\beta) \, \mathcal{N}(\beta)} = J(J+1)\hbar^2$$

This leads to the ODE satisfied by $\mathcal{N}(\beta)$

Displays a naturally terminating CC expansion

$$\frac{d^2}{d\beta^2}\mathcal{N}(\beta) + \cot\beta \frac{d}{d\beta}\mathcal{N}(\beta) + \frac{j^2(\beta)}{\hbar^2}\mathcal{N}(\beta) = 0$$

Initial conditions

$$\mathcal{N}(0) = 1$$

$$\frac{d}{d\beta}\mathcal{N}(\beta)\Big|_{\beta=0} = -\frac{i}{\hbar} j_y(0)$$

This ensures that the symmetry is exactly/consistently restored *at any truncation order* of $\mathcal{O}(\beta)$

Alternatively one can solve a first-order ODE invoking $j_y(\beta)$

Note: Extends to any CC order a known result of projected HF

e.g. [K. Enami et al., PRC59 (1999) 135]

Limits of interest

1. Standard SR-CC theory recovered at β = 0 or if $|\Phi\rangle$ does not break the symmetry $E_0^{J_0} = h(0)$

2. First order = Projected Hartree-Fock approximation

$$
\begin{aligned}
h^{(1)}(\beta) &= \frac{\langle\Phi|H|\Phi(\beta)\rangle}{\langle\Phi|\Phi(\beta)\rangle} \\
j_y^{(1)}(\beta) &= \frac{\langle\Phi|J_y|\Phi(\beta)\rangle}{\langle\Phi|\Phi(\beta)\rangle} \\
\mathcal{N}^{(1)}(\beta) &= \langle\Phi|\Phi(\beta)\rangle
\end{aligned}
$$

ODE

$$\Rightarrow \quad E_0^J = \frac{\langle\Phi_0^{J0}|H|\Phi_0^{J0}\rangle}{\langle\Phi_0^{J0}|\Phi_0^{J0}\rangle}$$

where

$$|\Phi_0^{J0}\rangle = P_{00}^J|\Phi\rangle \equiv \frac{2J+1}{2}\int_0^{\pi} d\beta \sin\beta \, d_{00}^{J\,*}(\beta)\,|\Phi(\beta)\rangle$$

3. Second-order MBPT

$$
\begin{aligned}
h^{(2)}(\beta) &= \frac{\langle\Phi|\left[1+\mathcal{T}_1^{\dagger(2)}(\beta)+\mathcal{T}_2^{\dagger(2)}(\beta)\right]H|\Phi(\beta)\rangle_c}{\langle\Phi|\Phi(\beta)\rangle} \\
j_y^{(2)}(\beta) &= \frac{\langle\Phi|\left[1+\mathcal{T}_1^{\dagger(2)}(\beta)\right]J_y|\Phi(\beta)\rangle_c}{\langle\Phi|\Phi(\beta)\rangle} \\
\mathcal{N}^{(2)}(\beta) &\equiv \aleph^{(2)}(\beta)\,\langle\Phi|\Phi(\beta)\rangle
\end{aligned}
$$

ODE

Recover standard MBPT2 at β = 0

Perturbative cluster amplitudes

$$
\begin{aligned}
\mathcal{T}_{ia}^{\dagger(2)}(\beta) &\equiv -\sum_{jb} \frac{\bar{v}_{ijab}}{e_a+e_b-e_i-e_j}\,\rho_{bj}^{ph}(\beta) \\
\mathcal{T}_{ijab}^{\dagger(2)}(\beta) &\equiv -\frac{\bar{v}_{ijab}}{e_a+e_b-e_i-e_j}
\end{aligned}
$$

E^0_J cannot be factorized in terms of a projected state

AMR-CC scheme in one slide

1. Off-diagonal operator kernels

$$O(\beta) = o(\beta)\mathcal{N}(\beta) \qquad \text{with } O \equiv J, J^2, j_k$$

2. Off-diagonal connected/linked kernels

$$o(\beta) = \langle \Phi | e^{\mathcal{T}^\dagger(\beta)} \tilde{O}(\beta) | \Phi \rangle_c$$

3. Transformed matrix elements

$$O_{\tilde{\alpha}\ldots\tilde{\beta}\tilde{\gamma}\ldots\tilde{\delta}}(\beta)$$

where

$$|\tilde{\alpha}\rangle \equiv B(\beta)\,|\alpha\rangle$$
$$\langle\tilde{\alpha}| \equiv \langle\alpha|B^{-1}(\beta)$$

Bi-orthogonal bases

4. Amplitude CC equations

$$0 = \langle \Phi | e^{\mathcal{T}^\dagger(\beta)} \tilde{H}(\beta) | \Phi^{ab\ldots}_{ij\ldots} \rangle_c$$

5. Norm kernel

$$\frac{d}{d\beta}\mathcal{N}(\beta) + \frac{i}{\hbar} j_y(\beta)\,\mathcal{N}(\beta) = 0$$

6. Symmetry-restored energy

$$E_0^J = \frac{\int_0^\pi d\beta \sin\beta\, d^{J\,*}_{00}(\beta)\, h(\beta)\, \mathcal{N}(\beta)}{\int_0^\pi d\beta \sin\beta\, d^{J\,*}_{00}(\beta)\, \mathcal{N}(\beta)}$$

Set of SR-CC calculations for N_{sym}~(10) values of β

Recovers single-reference CC at β = 0
Recovers Projected HF at lowest order

Part III

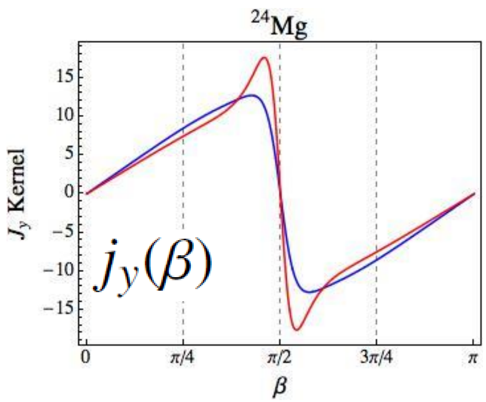
Preliminary results for ^{24}Mg

Set up

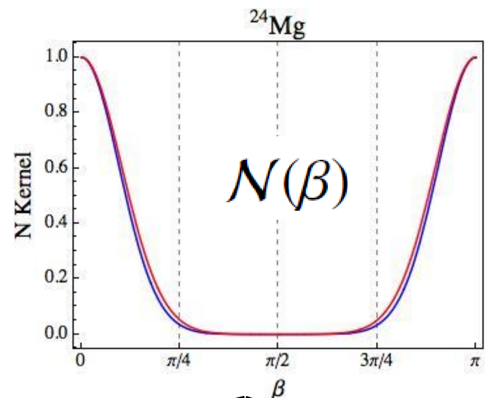
- NNLO$_{opt}$ 2NF (Λ = 500 MeV/c)
  [A. Ekstrom *et al.*, PRL110, 192502 (2013)]
- No 3NF yet
- Spherical HO basis
  - e$_{max}$ = 3,4,5,6,7
  - hw = 22 MeV
- m-scheme code

S. Binder, T. D., G. Hagen, T. Papenbrock, unpublished

Off-diagonal kernels



ODE



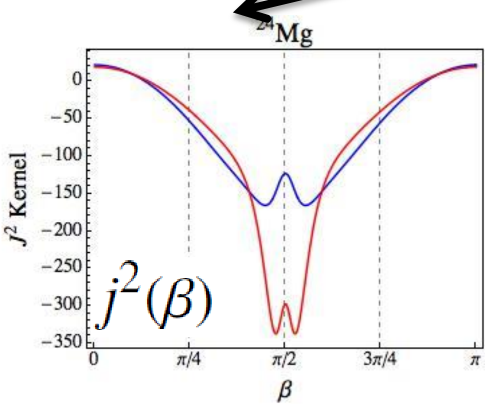
Hartree Fock (n=1)

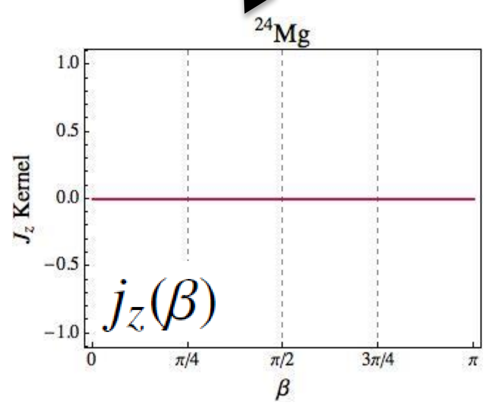
MBPT2 (n=2)

e_{max}=7 (not converged yet)

combined with

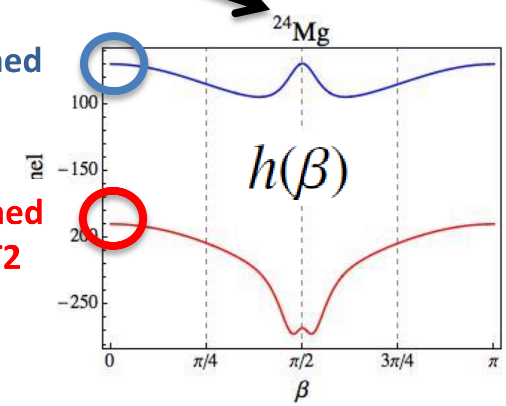
Scalar/vector operator's kernel is symmetric/antisymmetric with respect to π/2





Deformed HF

Deformed MBPT2



Integrate over β

Integrate over β

$$J(J+1)\hbar^2$$

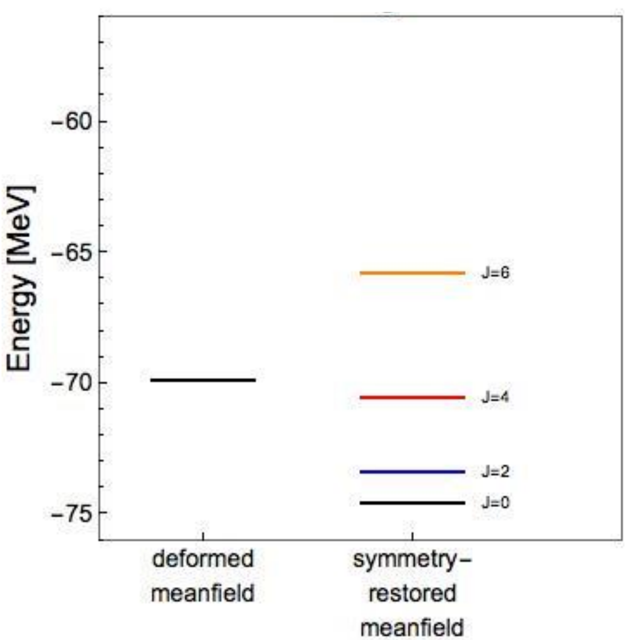
$$M\hbar = 0$$

$$E_0^J$$

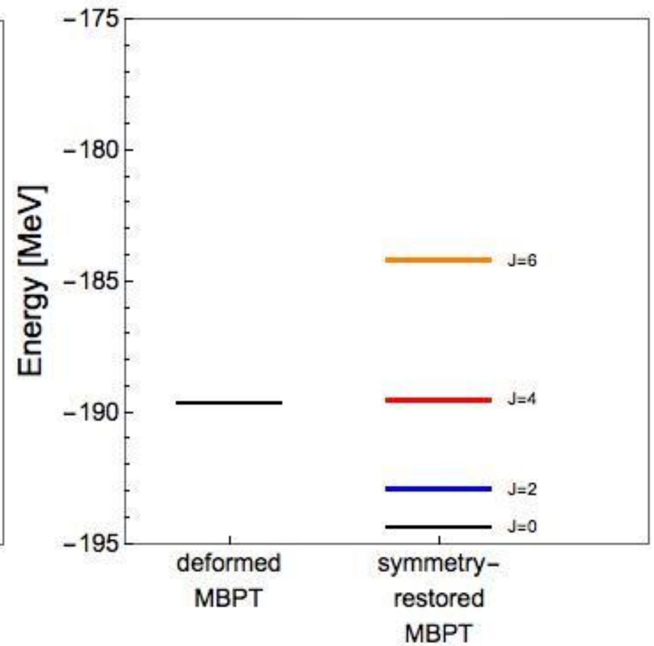
First (1) ab initio (2) beyond PHF such calculations

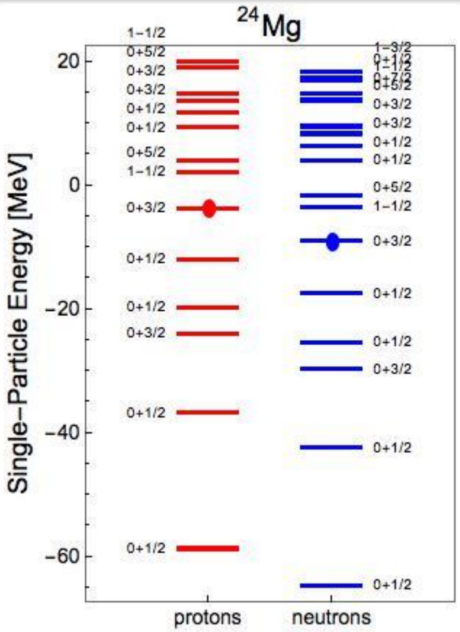
Angular momentum restoration

Hartree Fock



MBPT2





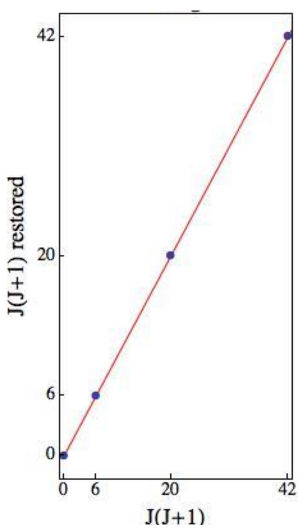
GS E (MeV)	Sym. Unr.	Sym. Rest.	ΔE (Sym. Rest.)
HF	-69.9	-74.6	4.7
MBPT2	-189.6	-194.4	4.8

Static correlations naturally captured: ~5MeV (vs 120MeV via MBPT)

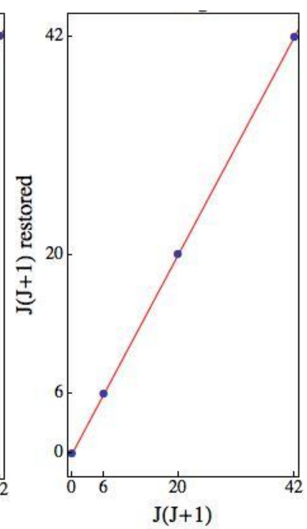
Dynamic & static correlations weakly interfere (^{24}Mg is well deformed)

N2LO$_{opt}$: MBPT & e$_{max}$ = 7 not enough yet

Hartree Fock



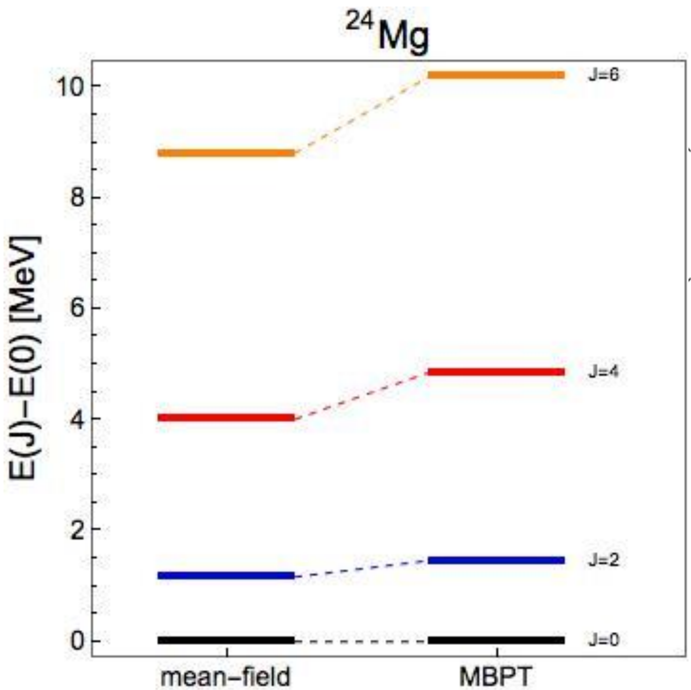
MBPT2

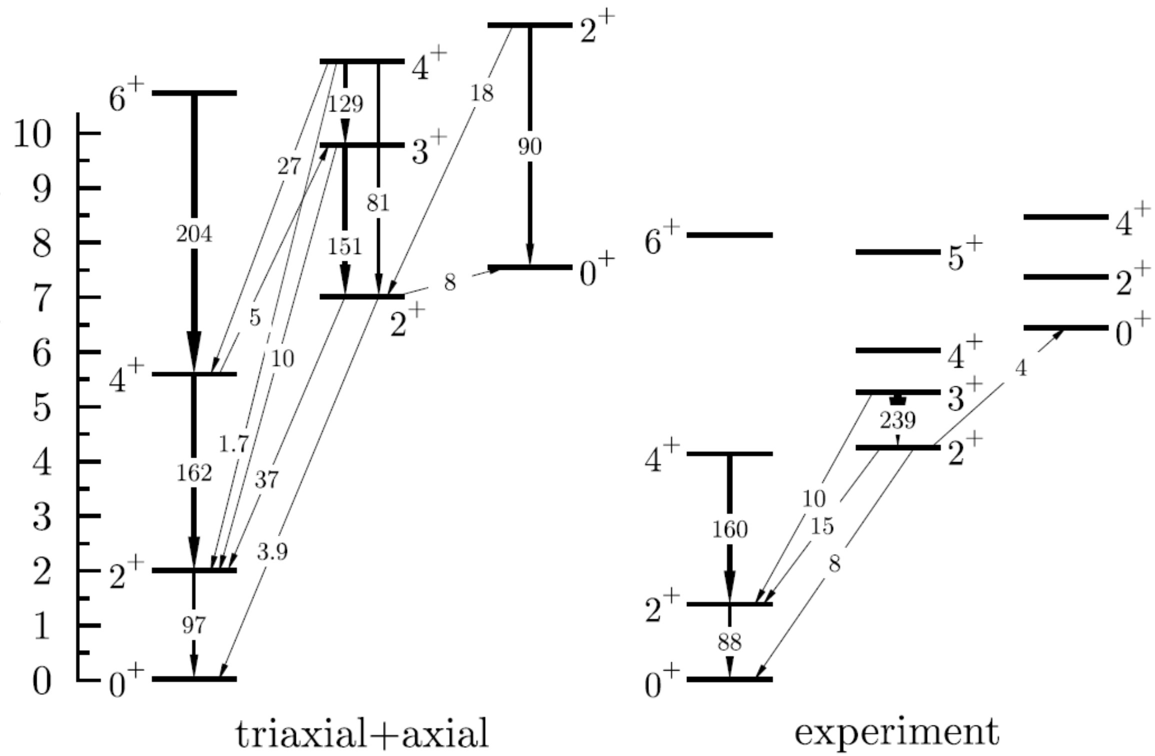


Perfect restoration of J^2

Ground-state rotational band

State-of-the-art MR-EDF: PNR & AMR + GCM (SLy4 + DDDI)





[M. Bender, P.-H. Heenen, PRC78 (2008) 024309]

J=6 excitation energy not yet converged with respect to e_{max}

Moment of inertia significantly impacted by dynamic correlations (have to look at PES)

Certainly look very reasonable and encouraging

No 3N interaction yet + non-perturbative CC needed for realistic Hamiltonians (in progress)

Future

Angular-momentum-restored potential energy surfaces,
EOM-like extension for non-yrast states,
Use of triaxial/cranked reference states…

Conclusions and perspectives

Conclusions

- First consistent symmetry-restoration MBPT/CC theory beyond PHF
- Main features
  - Applies to any symmetry and any system
  - Includes standard single-reference CC theory as a particular case
  - Reduces to Projected Hartree-Fock theory at lowest order
  - Accesses yrast spectroscopy
  - Denotes a multi-reference scheme amenable to parallelization
- Ab initio calculations of doubly open-shell nuclei in progress (encouraging)

Future

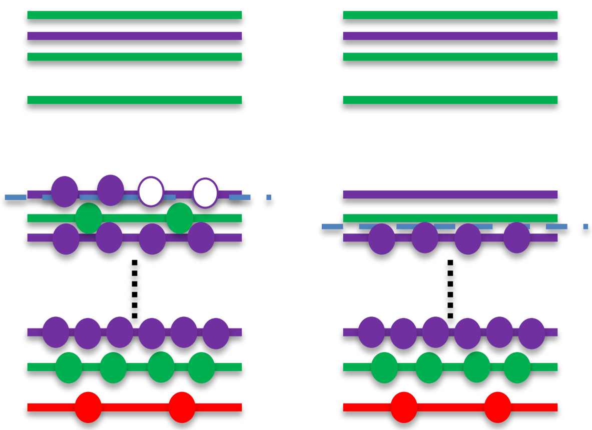
- Particle-number Bogoliubov CC formalism
  [T. D., A. Signoracci, in preparation]
- Apply PNR-BCC to solvable case for strongly interacting system?
  [T. M. Henderson *et al*.]
- Develop a similar formalism to extend *Go*-SCGF
  [T. D. V. Somà, C. Barbieri, to be done]

Appendix

Complementary slides

Issues with near degenerate systems

Problematic reference states



Open shell ***Near degenerate***

Single reference → Perturbative

MBPT fails because of $e_a - e_i \rightarrow 0$

Single reference → Non perturbative

High-order CC based on RHF or ROHF

-CCSDT or CR-CC(2,3) for single bond breaking

[J. Noga, R.J. Bartlett, JCP 86, 7041 (1987)]

[P. Piecuch, M. Wloch, JCP 123, 224105 (2005)]

-CCSDTQ or CR-CC(2,4) for double bond breaking

[J. Olsen *et al.*, JCP 104, 8007 (1996)]

-EOM-CC for states near closed shell reference

[J.F. Stanton, R. J. Bartlett, JCP 98, 7029 (1993)]

[G. Jansen *et al.*, PRC 83, 054306 (2011)]

-Spin-adapted CC theory for high spin states

[M. Heckert *et al.*, JCP 124, 124105 (2006)]

Single reference → Breaking symmetry

MBPT and CC based on UHF

[R. J. Bartlett, ARPC 32, 359 (1981)]

CC and SCGF based on HFB

[V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, arXiv:1412.2696]

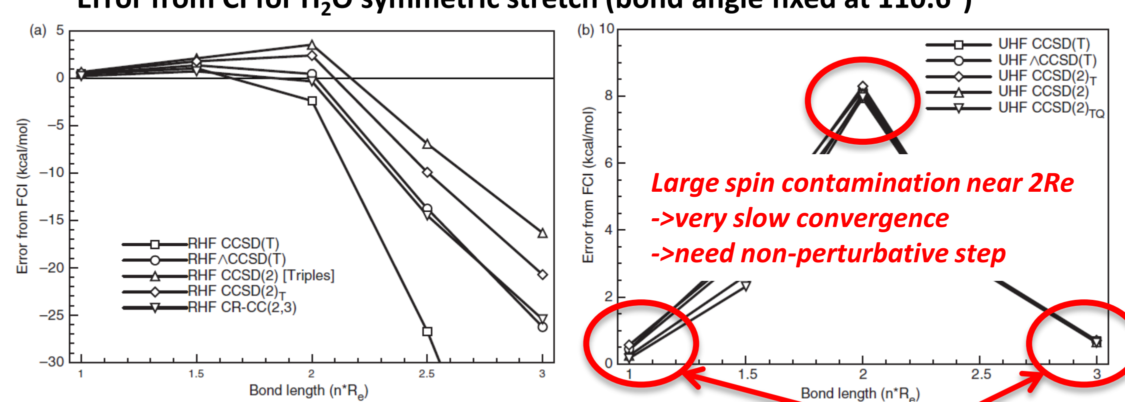
Multi reference ↓

MR-MBPT

MR-CC

MR-IMSRG

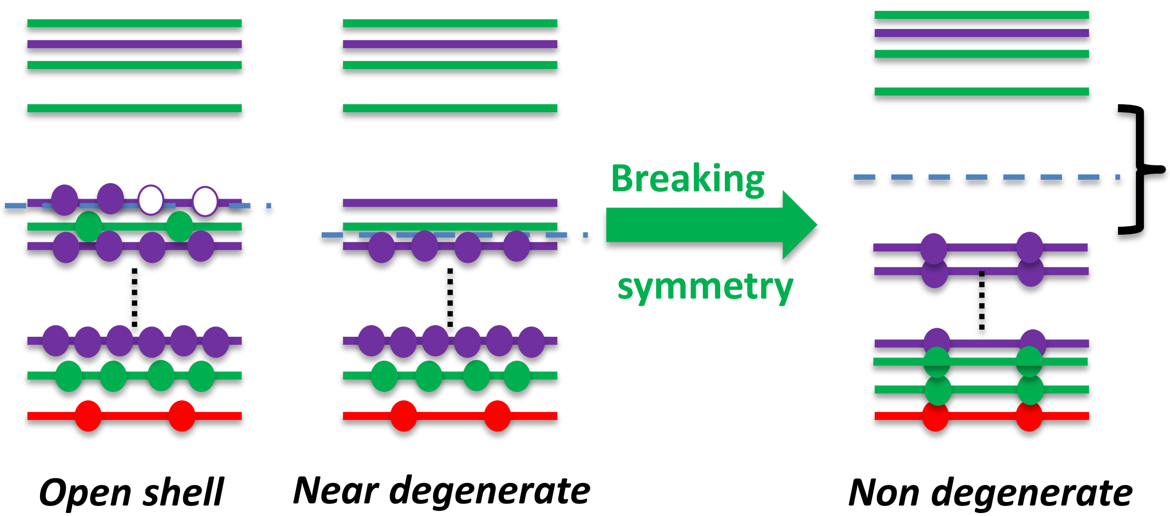
Error from CI for H_2O symmetric stretch (bond angle fixed at 110.6°)



[A.G. Taube, MP 108, 2951 (2010)]

Symmetry breaking reference state

Purpose of symmetry breaking reference state $|\Phi\rangle$



- Opens the gap at ε_F
- Non degenerate reference
- Diagrammatic methods well behaved
- Incorporates non-perturbative physics

Need to restore the symmetry

Lowdin operator in low-order MBPT based on UHF

[P.-O. Lowdin, PR 97, 1509 (1955)]
[H.B. Schlegel, JCP 92, 3075 (1988)]
[P.J. Knowles, N.C. Hardy, JCP 88, 6991 (1988)]

No generic and consistent symmetry broken & restored CC theory…

Non-perturbative *ab-initio* many-body theories

Ab-initio **many-body theories**
- Effective structure-less nucleons
- 2N + 3N + … inter-nucleon interactions
- Solve A-body Schrödinger equation
- Thorough assessment of errors needed

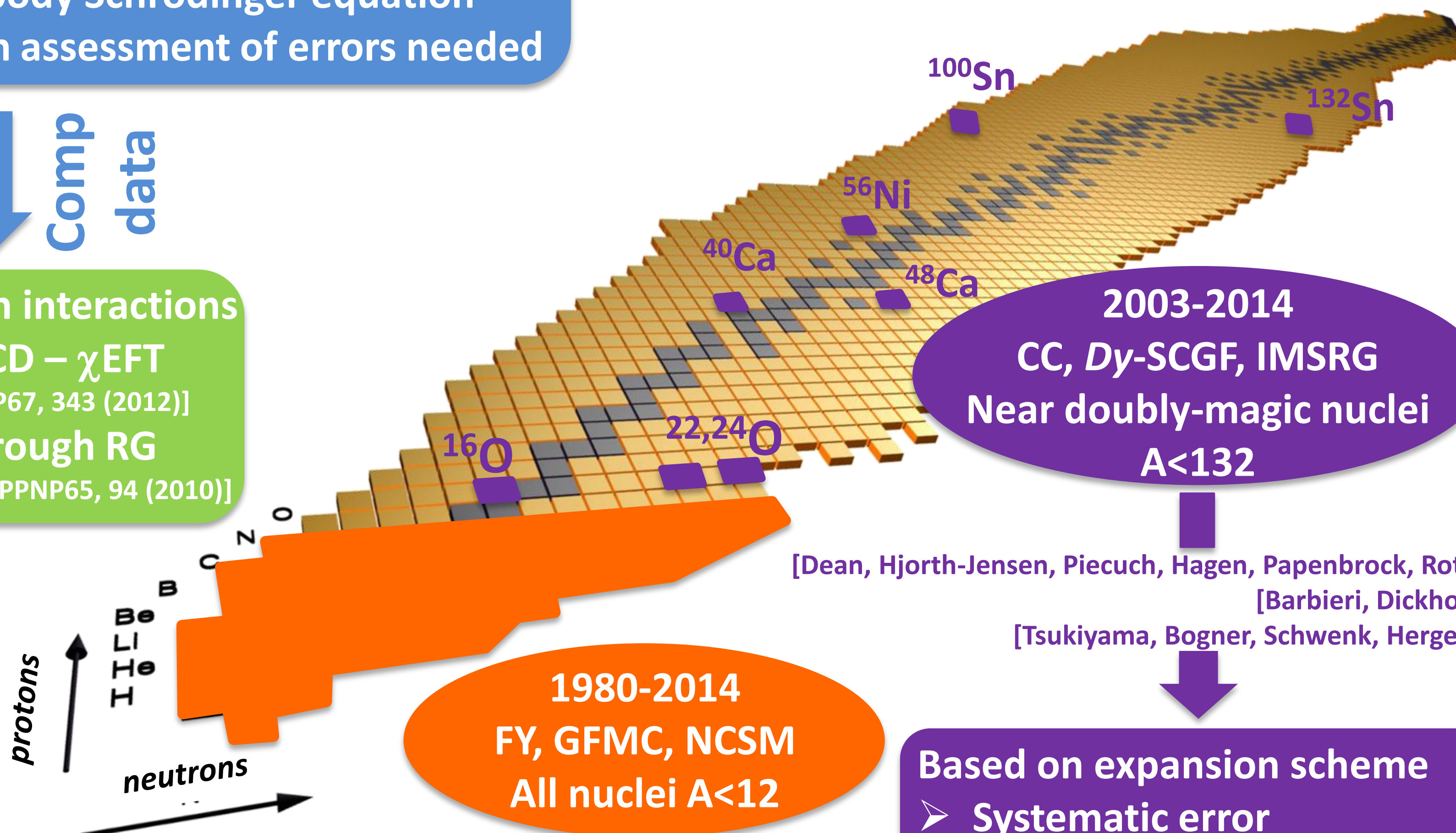
→ **High predictive power**
Limited applicability domain

↑ Input ↓ Comp data

Inter-nucleon interactions
- Link to QCD – χEFT

[E. Epelbaum, PPNP67, 343 (2012)]
- Soften through RG

[S.K. Bogner *et al.*, PPNP65, 94 (2010)]



2003-2014
CC, *Dy*-SCGF, IMSRG
Near doubly-magic nuclei
A<132

[Dean, Hjorth-Jensen, Piecuch, Hagen, Papenbrock, Roth]
[Barbieri, Dickhoff]
[Tsukiyama, Bogner, Schwenk, Hergert]

1980-2014
FY, GFMC, NCSM
All nuclei A<12

[Carlson, Pieper, Wiringa]
[Barrett, Vary, Navratil, Ormand]

Based on expansion scheme
- Systematic error
- Cross-benchmarks needed

Towards ab-initio methods for open-shell nuclei

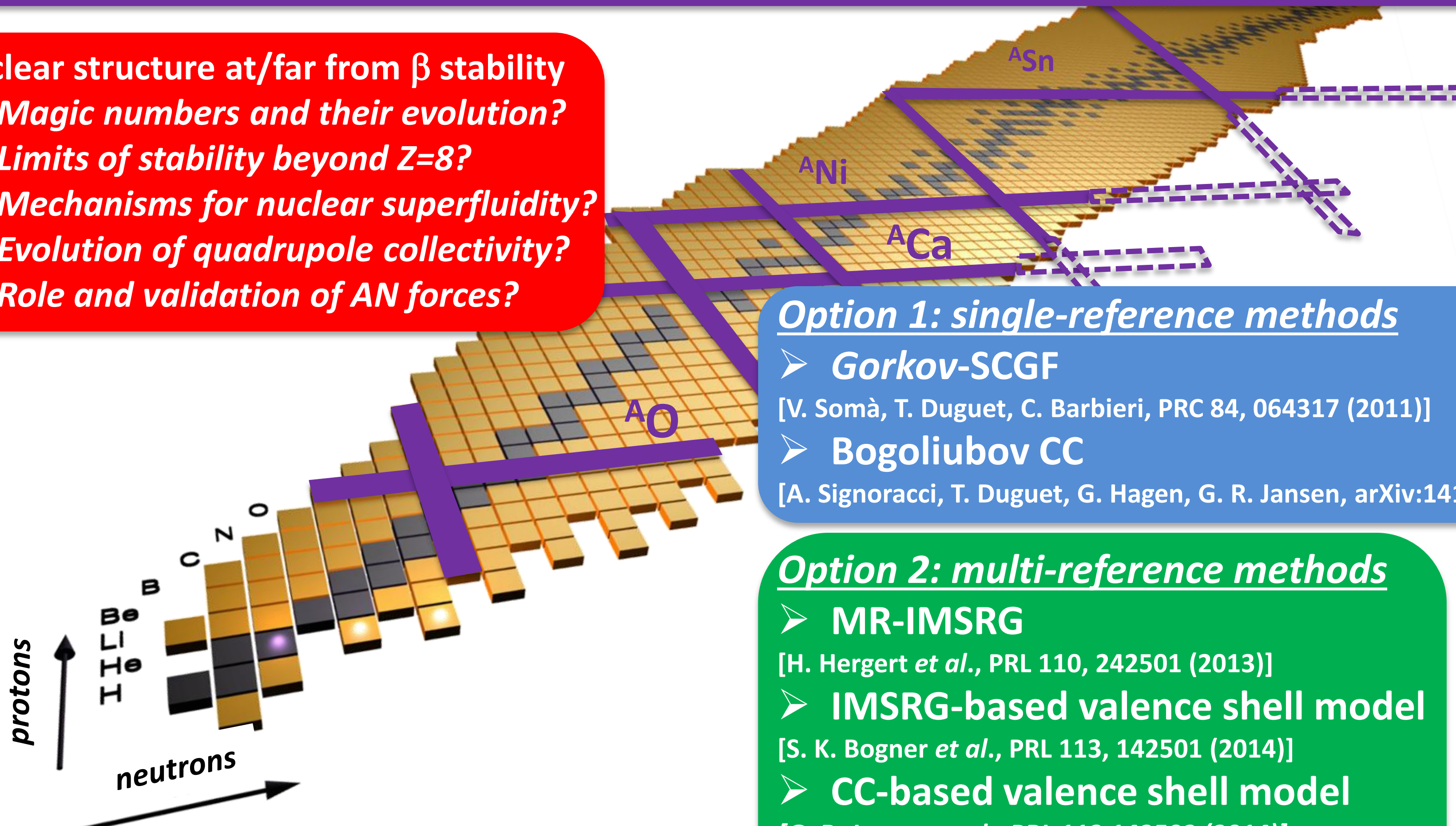
1. Design methods to study complete isotopic/isotonic chains, i.e. singly open-shell nuclei

2. Further extend methods to tackle doubly open-shell nuclei

- **Many 100s of nuclei eventually**

Nuclear structure at/far from β stability

- ***Magic numbers and their evolution?***
- ***Limits of stability beyond Z=8?***
- ***Mechanisms for nuclear superfluidity?***
- ***Evolution of quadrupole collectivity?***
- ***Role and validation of AN forces?***



Option 1: single-reference methods

- ***Gorkov*-SCGF**

[V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]

- **Bogoliubov CC**

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, arXiv:1412.2696]

Option 2: multi-reference methods

- **MR-IMSRG**

[H. Hergert *et al.*, PRL 110, 242501 (2013)]

- **IMSRG-based valence shell model**

[S. K. Bogner *et al.*, PRL 113, 142501 (2014)]

- **CC-based valence shell model**

[G. R. Jansen et al., PRL 113 142502 (2014)]

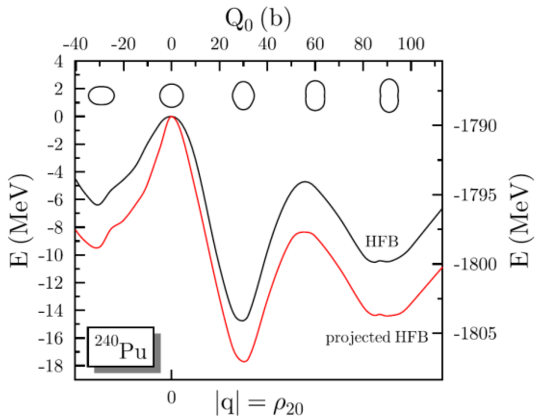
- **NCSM-based valence shell model**

[E. Dikmen et al., arXiv:1502.00700]

Symmetry and symmetry breaking (HF level)

Some symmetries of H

Invariance	Group	$\mid \Psi^X >$
Spatial trans.	T(1)	***P***
Gauge rot.	U(1)	N,Z
Spatial rot.	SO(3)	J,M



[M. Bender, private communication]

ΔE from projected HF

$\mid \Psi^X >$	ΔE	Spectro
N,Z	~1MeV	Pairing rot.
J,M	~2MeV	Rot. band

ΔE from symmetry breaking HF and associated physics

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

First way is to enforce the symmetry throughout the description

Second way is to let symmetry break in low order description

$$|\Psi_0\rangle = \Omega_0 |\Phi\rangle$$

Symmetry restricted

particle-hole (quasi)degeneracy

Good symmetry ☺
Hard to get ΔE ☹

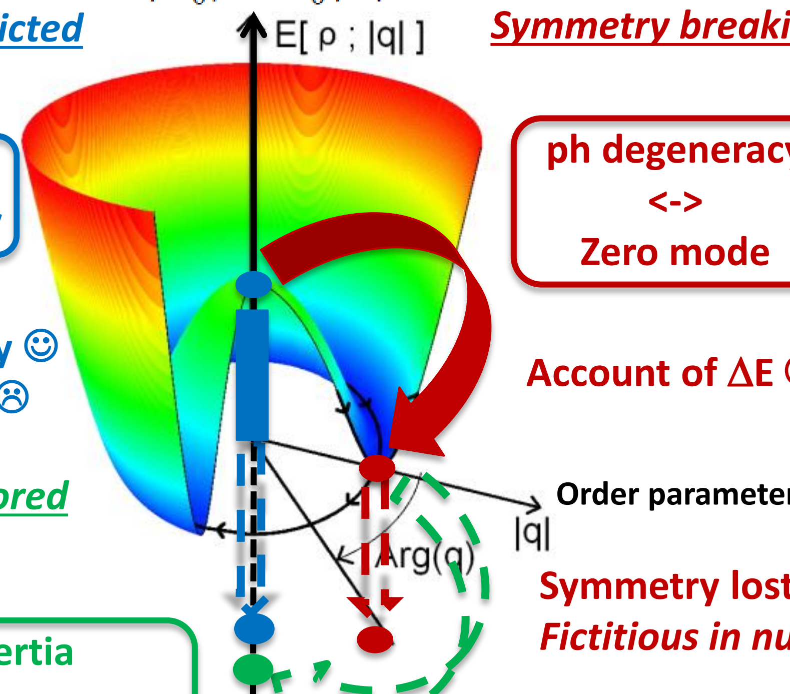
Symmetry restored description

Finite inertia
<->
Resolve Goldstone mode

Symmetry breaking

ph degeneracy
<->
Zero mode

Account of ΔE ☺



Symmetry lost ☹
Fictitious in nuclei!

Extra ΔE ☺
Good symmetry ☺

AMR-CC scheme in one slide

Recovers single-reference CC at $\Omega = 0$
Recovers Projected HF at lowest order

1. Off-diagonal operator kernels

$$\mathcal{O}(\Omega) = o(\Omega)\mathcal{N}(\Omega) \quad \text{with } O = H, J^2, J_z$$

2. Off-diagonal connected kernels

$$o(\Omega) = \langle \Phi | e^{\mathcal{T}^{\dagger}(\Omega)} \tilde{O}(\Omega) | \Phi \rangle_c$$

3. Transformed matrix elements

$$O_{\tilde{\alpha}\ldots\tilde{\beta}\tilde{\gamma}\ldots\tilde{\delta}}(\Omega) \quad \text{where} \quad \begin{cases} |\tilde{\alpha}\rangle & \equiv & B(\Omega)|\alpha\rangle \\ \langle\tilde{\alpha}| & \equiv & \langle\alpha|B^{-1}(\Omega) \end{cases}$$

Bi-orthogonal system

4. Amplitude CC equations

$$0 = \langle \Phi | e^{\mathcal{T}^{\dagger}(\Omega)} \tilde{H}(\Omega) | \Phi^{ab\ldots}_{ij\ldots} \rangle_c$$

5. Norm kernel

$$\begin{aligned}
\frac{\partial}{\partial\alpha}\mathcal{N}(\Omega) + \frac{i}{\hbar} j_z(\Omega)\mathcal{N}(\Omega) &= 0 \\
\frac{\partial}{\partial\beta}\mathcal{N}(\Omega) - \frac{i}{\hbar}\Big[\sin\alpha\, j_x(\Omega) - \cos\alpha\, j_y(\Omega)\Big]\mathcal{N}(\Omega) &= 0 \\
\frac{\partial}{\partial\gamma}\mathcal{N}(\Omega) + \frac{i}{\hbar}\Big[\sin\beta\cos\alpha\, j_x(\Omega) + \sin\beta\sin\alpha\, j_y(\Omega) + \cos\beta\, j_z(\Omega)\Big]\mathcal{N}(\Omega) &= 0
\end{aligned}$$

6. Symmetry-restored energy

$$E_0^J = \frac{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D^{J*}_{MK}(\Omega)\, h(\Omega)\, \mathcal{N}(\Omega)}{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D^{J*}_{MK}(\Omega)\, \mathcal{N}(\Omega)}$$

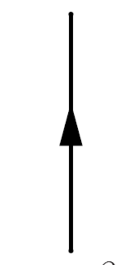
Set of SR-CC calculations for $N_{sym} \sim (10)^{\text{angles}}$ values of Ω

Many-body perturbation theory (2)

Off-diagonal unperturbed propagator = basic contraction for Wick Theorem

$$G^0_{\alpha\beta}(\tau_1,\tau_2;\Omega) \equiv \frac{\langle\Phi|T[a_\alpha(\tau_1)a^\dagger_\beta(\tau_2)]|\Phi(\Omega)\rangle}{\langle\Phi|\Phi(\Omega)\rangle} = G^0_{\alpha\alpha}(\tau_1-\tau_2)\delta_{\alpha\beta} + \underbrace{G^{ph}_{\alpha\beta}(\tau_1,\tau_2)\rho^{ph}_{\alpha\beta}(\Omega)}_{\text{Couples p and h}}$$

Couples p and h



Off-diagonal operator kernel (e.g. O=H)

Evolution operator $\mathcal{U}(\tau)$

Off-diagonal Wick theorem
[R. Balian, E. Brezin, NC 64, 37 (1969)]

$$O(\tau,\Omega) = \langle\Phi|\underbrace{e^{-\tau H_0}\, T e^{-\int_0^\tau d\tau_1 H_1(\tau_1)}}_{\mathcal{U}(\tau)} O|\Phi(\Omega)\rangle = \underbrace{o(\tau,\Omega)\, N(\tau,\Omega)}$$

Factorization of the norm kernel

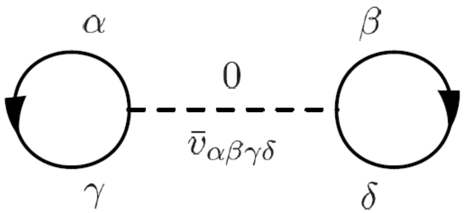
$$o(\tau,\Omega) \equiv \sum_{n=0}^{\infty} o^{(n)}(\tau,\Omega)$$ = connected vacuum-to-vacuum diagrams *linked* to O at time 0

Expansion in Feynman diagrams
Usual rules but off-diagonal propagators

Many-body perturbation theory (3)

Potential energy diagrams – example at zero order

$$v^{(0)}(\tau,\Omega) = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, G^{0}_{\gamma\alpha}(0,0;\Omega)\, G^{0}_{\delta\beta}(0,0;\Omega)$$



$$= +\frac{1}{2}\sum_{ij} \bar{v}_{ijij}$$

$v^{(0)}(\tau,0)$ ***= standard symmetry unrestricted MBPT-0 contribution***

$$+\sum_{ijc} \bar{v}_{ijcj}\,\rho^{ph}_{ci}(\Omega)$$

$$+\frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\,\rho^{ph}_{ai}(\Omega)\,\rho^{ph}_{bj}(\Omega)$$

Genuinely Ω-dependent part

Signals the symmetry breaking

Large τ limit $\quad h(\tau,\Omega) \underset{\tau\to\infty}{\longrightarrow} h(\Omega)$ $\quad \mathcal{H}(\infty,\Omega) = h(\Omega)\,\mathcal{N}(\Omega)$

In the exact limit $\quad \frac{\partial}{\partial\Omega} h(\Omega) = 0$

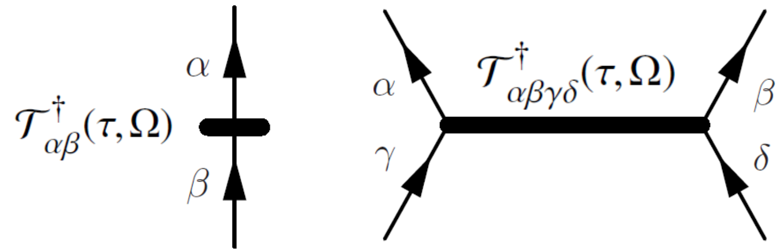
After truncation $\quad \frac{\partial}{\partial\Omega} h(\Omega) \neq 0$

Coupled cluster energy kernel

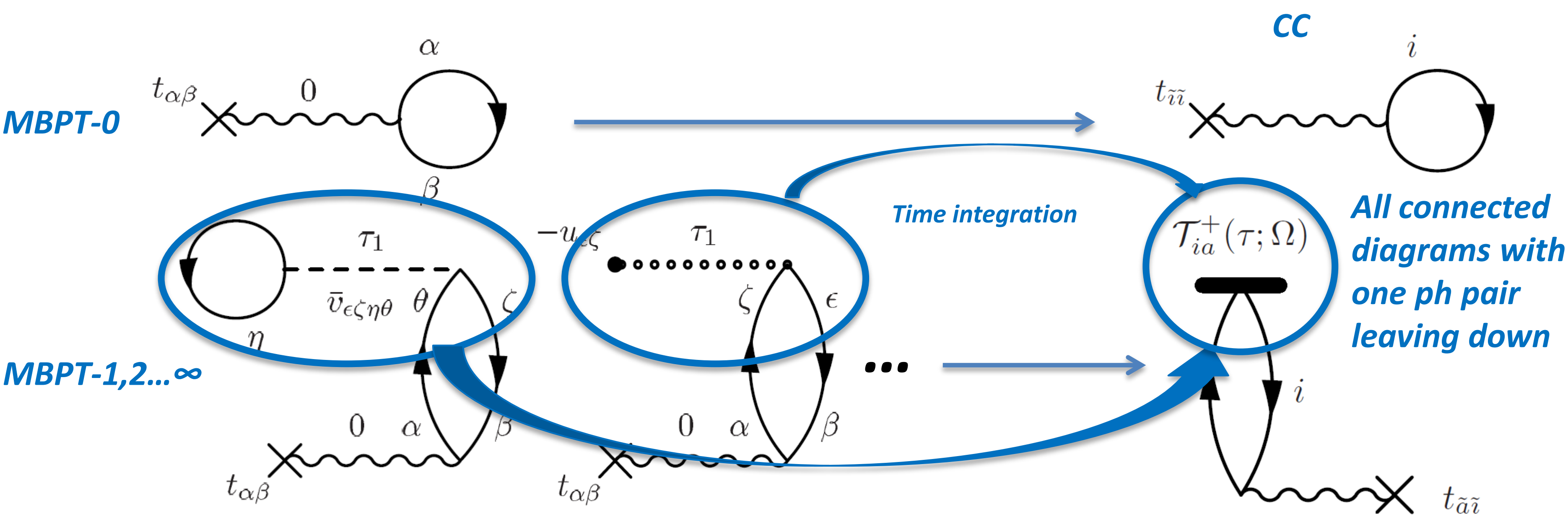
τ- and Ω-dependent cluster operators (or rather their hermitian conjuguate…)

$$\mathcal{T}_1^\dagger(\tau,\Omega) \equiv \frac{1}{(1!)^2}\sum_{ia}\mathcal{T}_{ia}^\dagger(\tau,\Omega)\, a_i^\dagger\, a_a$$

$$\mathcal{T}_2^\dagger(\tau,\Omega) \equiv \frac{1}{(2!)^2}\sum_{ijab}\mathcal{T}_{ijab}^\dagger(\tau,\Omega)\, a_i^\dagger\, a_j^\dagger\, a_b\, a_a$$



Kinetic energy kernel = connected diagrams linked to *T*



Similar for the potential energy kernel

Account of single-reference CC method (1)

Nuclear Hamiltonian

$$H = \sum_{\alpha\beta} t_{\alpha\beta}\, c^\dagger_\alpha c_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$$

Anti-symmetrized matrix elements

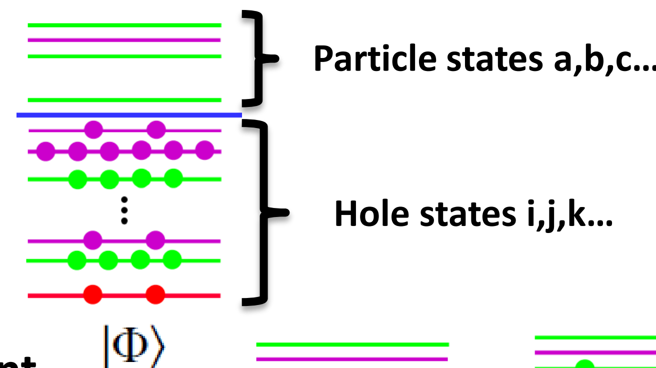
$$\bar{v}_{\alpha\beta\gamma\delta} \equiv v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$$

Wave-function ansatz

$$|\Psi_0\rangle \equiv e^T |\Phi\rangle$$

Product state of reference

$$|\Phi\rangle \equiv \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

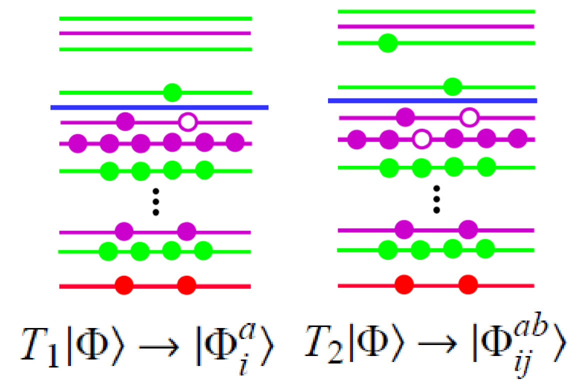


Cluster operator

$$T \equiv T_1 + T_2 + T_3 + \ldots$$

N-tuple connected component

$$T_n \equiv \frac{1}{(n!)^2} \sum_{ijk\ldots abc\ldots} t^{abc\ldots}_{ijk\ldots}\, a^\dagger_a a^\dagger_b a^\dagger_c \ldots a_k a_j a_i$$



Norm kernel in intermediate normalization

Only non-zero ph matrix elements

$$N(\infty,0) \equiv \langle\Phi|\Psi_0\rangle = 1 \quad \text{as} \quad \langle\Phi|T_n = 0$$

Exponential generates connected + disconnected n-tuple excitations

Size extensive

Set up

All kernels are reduced ones at t = ∞
$J_z|\Phi\rangle = 0$ ➡ **only one Euler angle β**

Symmetry-breaking unperturbed system

$$H \equiv H_0 + H_1 \quad \text{where } H_0 \equiv T + U = \sum_\alpha e_\alpha a^\dagger_\alpha a_\alpha$$

Such that $[H_0, R(\beta)] \neq 0$ **and** $[H_1, R(\beta)] \neq 0$

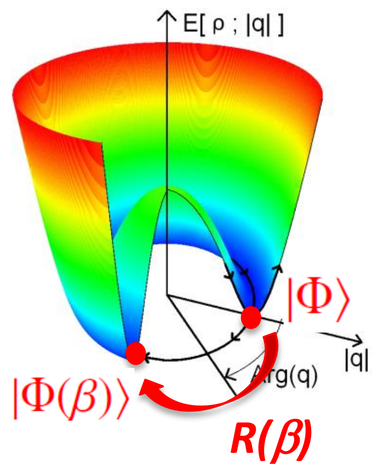
$$H_0\,|\Phi\rangle = \varepsilon_0\,|\Phi\rangle$$

$$H_0\,|\Phi^{ab\ldots}_{ij\ldots}\rangle = (\varepsilon_0 + \varepsilon^{ab\ldots}_{ij\ldots})\,|\Phi^{ab\ldots}_{ij\ldots}\rangle$$

with

$$\varepsilon_0 = \sum_{i=1}^{N} e_i$$

$$\varepsilon^{ab\ldots}_{ij\ldots} = e_a + e_b + \ldots - e_i - e_j - \ldots$$



where $|\Phi\rangle = \prod_{i=1}^{N} a^\dagger_i\,|0\rangle$ **and** $|\Phi^{ab\ldots}_{ij\ldots}\rangle \equiv a^\dagger_a a_i a^\dagger_b a_j \ldots |\Phi\rangle$

Rotated reference state and overlap

$$|\Phi(\beta)\rangle = \prod_{i=1}^{N} a^\dagger_{\bar{i}}\,|0\rangle \quad \text{with} \quad a^\dagger_{\bar{\alpha}} = \sum_\beta R_{\beta\alpha}(\beta)\, a^\dagger_\beta \quad \text{and} \quad R_{\gamma\delta}(\beta) \equiv \langle\gamma|R(\beta)|\delta\rangle$$

$$\langle\Phi|\Phi(\beta)\rangle = \det M(\beta) \quad \text{where} \quad M_{\alpha\beta}(\beta) \equiv R_{\alpha\beta}(\beta)\,\delta_{\alpha i}\delta_{\beta j}$$

and $|\Phi^{ab\ldots}_{ij\ldots}(\beta)\rangle \equiv a^\dagger_a a_i a^\dagger_b a_j \ldots |\Phi(\beta)\rangle$