Ab-initio coupled-cluster method for open-shell nuclei

I. Breaking symmetries

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Computational Challenges in Nuclear and Many-Body Physics

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Outline

I. Introduction: how does this fit with the rest?

II. Breaking U(1) symmetry *("trivial" for SU(2))* **(today)**

Bogoliubov coupled-cluster method

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, in preparation (2014)]

[T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, T. Duguet, PRC89, 054305 (2014)]

III. Restoring SU(2) or U(1) symmetries **(next thursday)**

Angular-momentum-restored coupled-cluster formalism

[T. Duguet, to be published in J. Phys. G: Nucl. Part. Phys (2014) ; arXiv:1406.7183]

Particle-number-restored Bogoliubov coupled-cluster formalism

[T. Duguet, in preparation (2014)]

Introduction

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

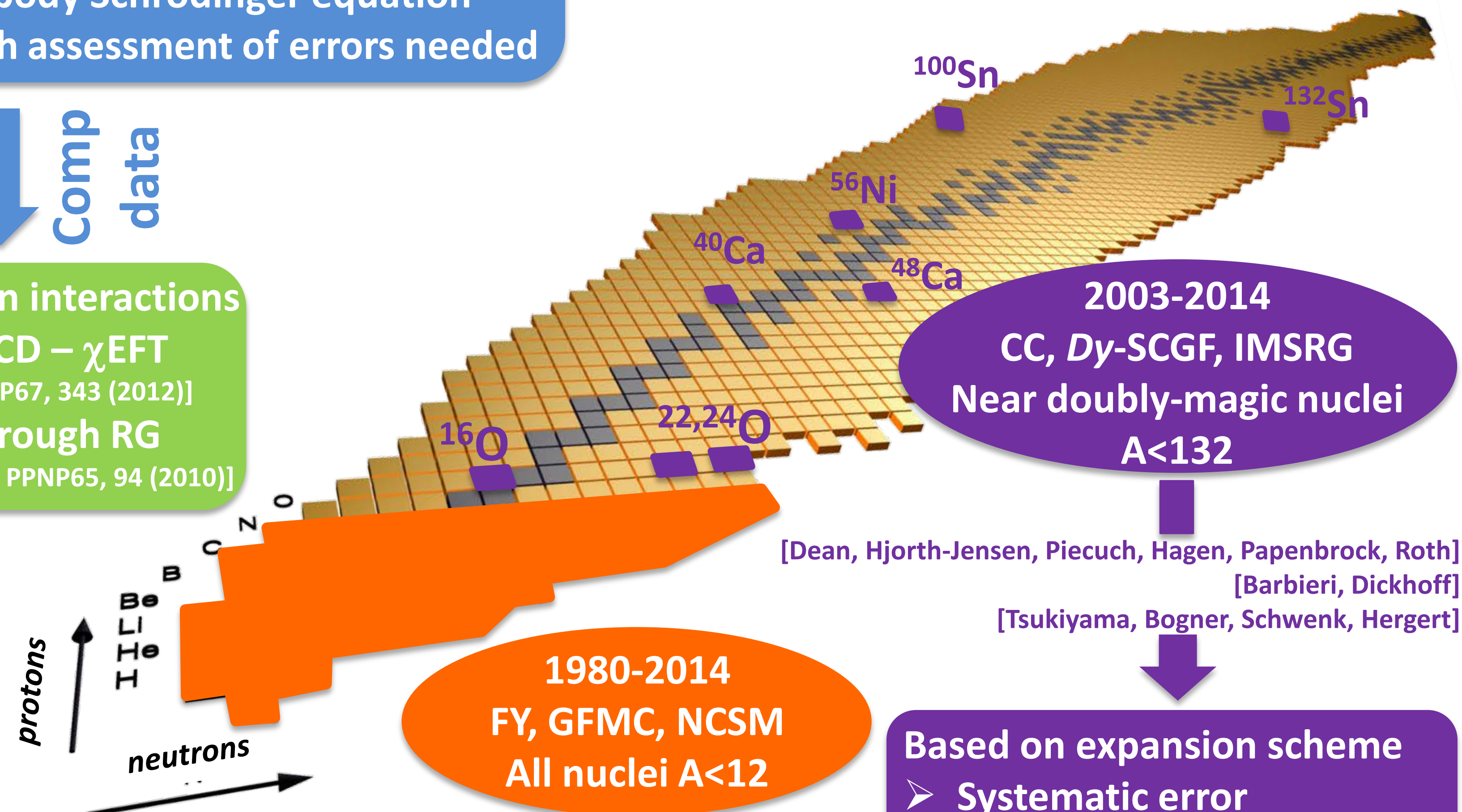
Input

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)]



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

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

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]

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

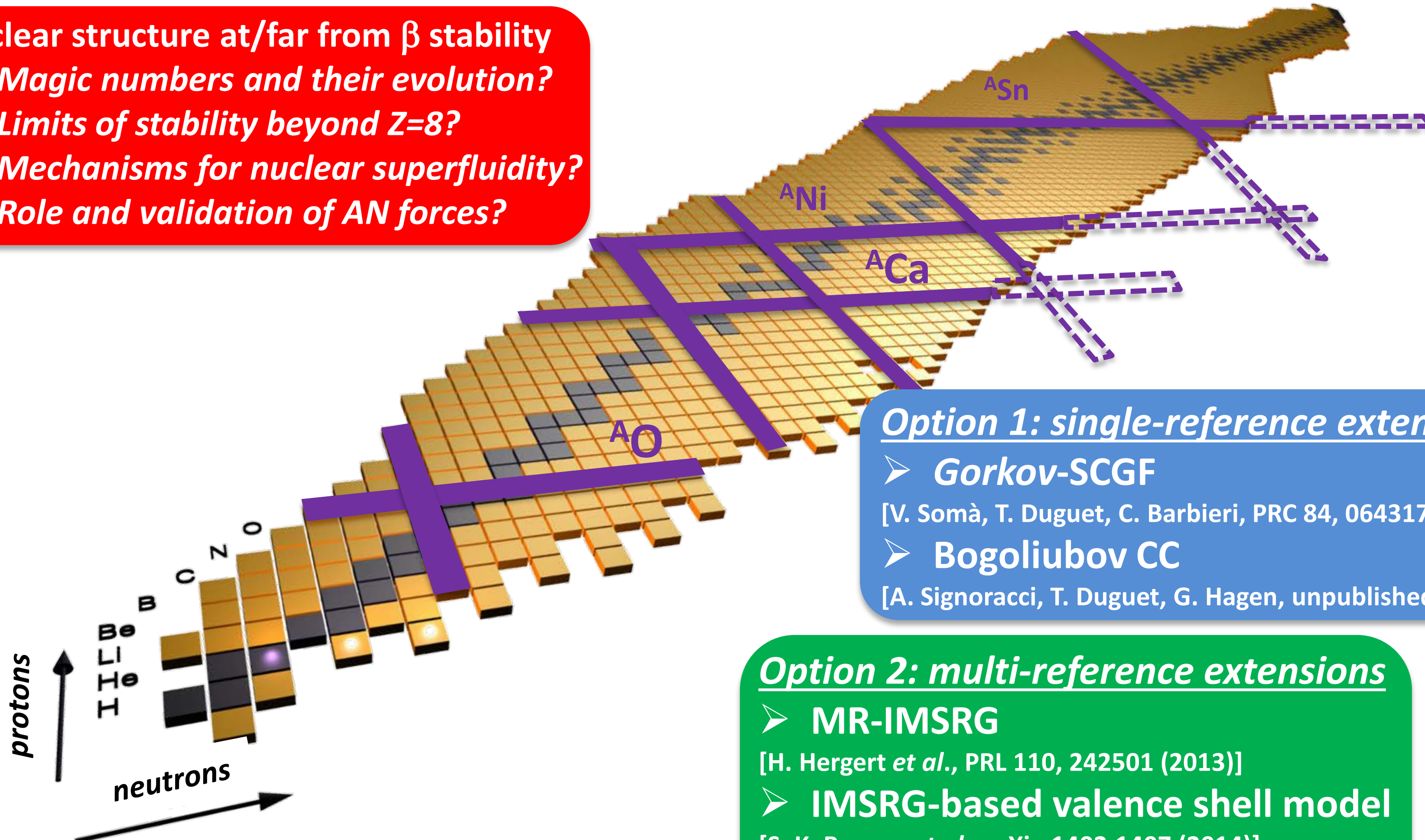
Towards ab-initio methods for open-shell nuclei

First objective: generalize many-body methods to study complete isotopic/isotonic chains

- Go from a few 10s of nuclei to several 100s of nuclei

Nuclear structure at/far from β stability

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



Option 1: single-reference extensions

- ***Gorkov**-SCGF*

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

- **Bogoliubov CC**

[A. Signoracci, T. Duguet, G. Hagen, unpublished (2014)]

Option 2: multi-reference extensions

- **MR-IMSRG**

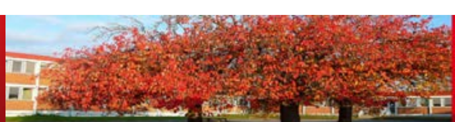
[H. Hergert *et al.*, PRL 110, 242501 (2013)]

- **IMSRG-based valence shell model**

[S. K. Bogner *et al.*, arXiv:1402.1407 (2014)]

- **CC-based valence shell model**

[G. R. Jansen *et al.*, arXiv:1402.2563 (2014)]



Breaking and restoring symmetries

Expansion around a single reference state

Target state → $|\Psi_0\rangle = \Omega_0 \, |\Phi_0\rangle$ ← Reference state; Wave operator ↓ Ω_0

A-body ground state

Expand Ω_0 such that

E_0 is size extensive

$$E_0 = \frac{\langle \Phi_0 | \hat{H} | \Psi_0 \rangle}{\langle \Phi_0 | \Psi_0 \rangle}$$

Ground-state energy

Closed shell

- RHF reference
- *conserves A, J^2, M*
- *Dy-SCGF*, CC

Breaks down for open-shell nuclei

⇒

Singly/doubly open shell

- UHF(B) reference
- *breaks A / J^2 and M*
- *Go-SCGF*, Today: BCC

Contamination from other A / J^2 and M

ph degeneracy <-> Goldstone mode

⇒

Singly/doubly open shell

- UHF(B) manyfold
- *restores A / J^2 and M*
- AMR-CC & PNR-BCC

Next thursday

Multi-reference character

Finite inertia <-> *Resolve Goldstone mode*

Part II

Bogoliubov coupled-cluster formalism for singly open-shell nuclei

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, in preparation (2014)]

[T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, T. Duguet, PRC89, 054305 (2014)]

Hartree-Fock-Bogoliubov reference

Nuclear Hamiltonian

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

Bogoliubov transformation

$$\beta^\dagger_\alpha = \sum_p U_{p\alpha}\, c^\dagger_p + V_{p\alpha}\, c_p$$

$$\beta_\alpha = \sum_p U^*_{p\alpha}\, c_p + V^*_{p\alpha}\, c^\dagger_p$$

Bogoliubov vacuum

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

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

Breaks U(1) symmetry associated with good A

Density matrices

$$\rho_{qp} \equiv \frac{\langle\Phi| c^\dagger_p c_q |\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

$$\kappa_{qp} \equiv \frac{\langle\Phi| c_p c_q |\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

Grand potential

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

Minimization under constraint

$$\delta \frac{\langle\Phi|\Omega|\Phi\rangle}{\langle\Phi|\Phi\rangle} = 0 \;/\; \langle\Phi|A|\Phi\rangle = \mathrm{A}$$

HFB equation

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

Quasi-particle excitations

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

Spectroscopic factors

$$\mathfrak{F}^-_\alpha = \sum_l |V_{l\alpha}|^2$$

Binding energy

$$\mathcal{E}_0 = +\frac{1}{2}\Big[\sum_{pq} t_{pq}\rho_{qp} - \sum_\alpha (E_\alpha - \lambda)\,\mathfrak{F}^-_\alpha\Big] - \frac{1}{6}\Big[\sum_{pq} \Gamma^{3N}_{pq}\rho_{qp} + \Delta^{3N}_{pq}\kappa^*_{qp}\Big]$$

*m-scheme code

*Benchmarked against J-coupled [V. Somà et al.]

Bogoliubov CC ansatz

Wave-function ansatz

$$|\Psi\rangle \equiv e^{\mathcal{T}}|\Phi\rangle$$

Quasi-particle cluster operator

$$\mathcal{T} \equiv \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \ldots$$

$$[\mathcal{T}_n, \mathcal{T}_m] = 0$$

Connected n-tuple excitation

$$\mathcal{T}_1 \equiv \frac{1}{2!}\sum_{k_1 k_2} \mathbf{t}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2}$$

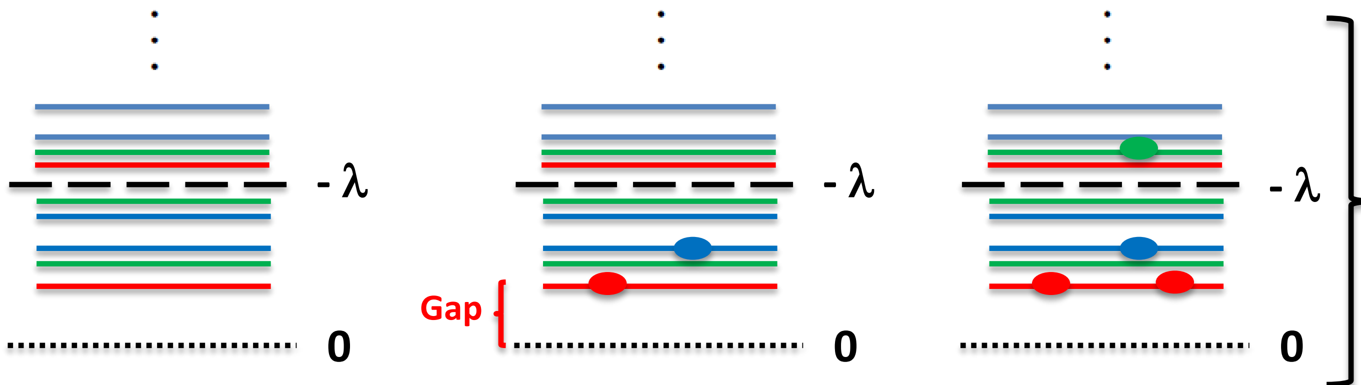
$$\mathcal{T}_2 \equiv \frac{1}{4!}\sum_{k_1 k_2 k_3 k_4} \mathbf{t}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$

⋮

Unknowns

Fully anti-symmetric

Action of n-tuple excitation on the HFB vacuum



$|\Phi\rangle$ $\quad$ $\mathcal{T}_1|\Phi\rangle \rightarrow |\Phi^{\alpha\beta}\rangle$ $\quad$ $\mathcal{T}_2|\Phi\rangle \rightarrow |\Phi^{\alpha\beta\gamma\delta}\rangle$

No distinction between particles and holes

Exponential generates connected + disconnected n-tuple excitations

HFB vacuum
1) Handles Cooper instability = grasps key static correlations
2) Opens gap in excitations = makes dynamic correlations safe

- **CC theory in qp basis with no breaking of U(1)**
  [L. Stolarczyk, H. Monkhorst, MP108, 3067 (2010)]
- **BCC theory restricted to BCS and simple geometry**
  [K. Emrich, J. G. Zabolitzky, PRB30, 2049 (1984)]
  [W. A. Lahoz, R. F. Bishop, ZPB73, 363 (1988)]

Normal-ordered grand potential

Bogoliubov transformation + Wick's theorem

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

$$= \Omega^{00} + \frac{1}{1!}\sum_{k_1k_2} \Omega^{11}_{k_1k_2}\beta^\dagger_{k_1}\beta_{k_2}$$

$= E_{k_1}\delta_{k_1k_2}$ **with HFB reference state**

$$+ \frac{1}{2!}\sum_{k_1k_2}\left\{\Omega^{20}_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + \Omega^{02}_{k_1k_2}\beta_{k_2}\beta_{k_1}\right\}$$ $= 0$

Residual interaction

$$+ \frac{1}{(2!)^2}\sum_{k_1k_2k_3k_4} \Omega^{22}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta_{k_4}\beta_{k_3}$$

$$+ \frac{1}{3!}\sum_{k_1k_2k_3k_4}\left\{\Omega^{31}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta_{k_4} + \Omega^{13}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta_{k_4}\beta_{k_3}\beta_{k_2}\right\}$$

$$+ \frac{1}{4!}\sum_{k_1k_2k_3k_4}\left\{\Omega^{40}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4} + \Omega^{04}_{k_1k_2k_3k_4}\beta_{k_4}\beta_{k_3}\beta_{k_2}\beta_{k_1}\right\}$$

$$+ \Omega^{[6]}$$

Each $\Omega^{ij}_{k_1\ldots k_i k_{i+1}\ldots k_{i+j}}$ **is**

***fully anti-symmetric**

***expressed in terms of** $\{t_{pq},\ \bar{v}_{pqrs},\ \bar{w}_{pqrstu}\}$ $\{U_{pk},\ V_{pk}\}$

NO2B approximation

Very good in closed shell (1% error)

[S. Binder *et al.*, PRC87 (2013) 021303]

Bogoliubov CC equations

Schrödinger equation

$$\Omega|\Psi\rangle = \Omega_0|\Psi\rangle$$

xe^{-T}

$$\bar{\Omega}|\Phi\rangle = \Omega_0|\Phi\rangle$$

$$(\Omega e^{\mathcal{T}})_c|\Phi\rangle = \Omega_0|\Phi\rangle$$

Size extensive

Non-hermitian similarity-transformed grand potential

$$\bar{\Omega} \equiv e^{-\mathcal{T}}\,\Omega\, e^{\mathcal{T}}$$

Baker-Campbell-Hausdorff + Wick theorem

$$\bar{\Omega} = \sum_{n=0}^{4} (\Omega \mathcal{T}^n)_c$$

Expansion naturally terminates

Energy equation

$$\langle\Phi|(\Omega e^{\mathcal{T}})_c|\Phi\rangle = \Omega_0$$

+ equation to constrain λ / $\dfrac{\langle\Psi|A|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \mathrm{A}$

Amplitude equation to find $\mathcal{T}_n$

$$\langle\Phi^{\alpha\beta\dots}|(\Omega e^{\mathcal{T}})_c|\Phi\rangle_C = 0$$

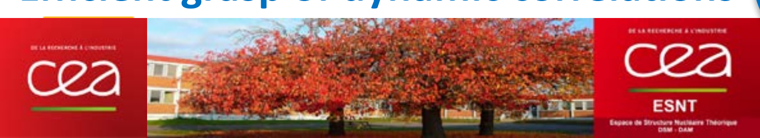
Truncate $\mathcal{T}$ beyond a certain $\mathcal{T}_n$
Retaining $\mathcal{T}_1$ and $\mathcal{T}_2$ defines BCCSD
Infinite-order method
Efficient grasp of dynamic correlations

BCC with Singles and Doubles

$$\Omega_0 = \langle\Phi|\Omega(1+\mathcal{T}_1+\mathcal{T}_2+\tfrac{1}{2}\mathcal{T}_1^2)|\Phi\rangle_C$$

$$0 = \langle\Phi^{\alpha\beta}|\Omega(1+\mathcal{T}_1+\tfrac{1}{2}\mathcal{T}_1^2+\tfrac{1}{3!}\mathcal{T}_1^3+\mathcal{T}_2+\mathcal{T}_1\mathcal{T}_2)|\Phi\rangle_C$$

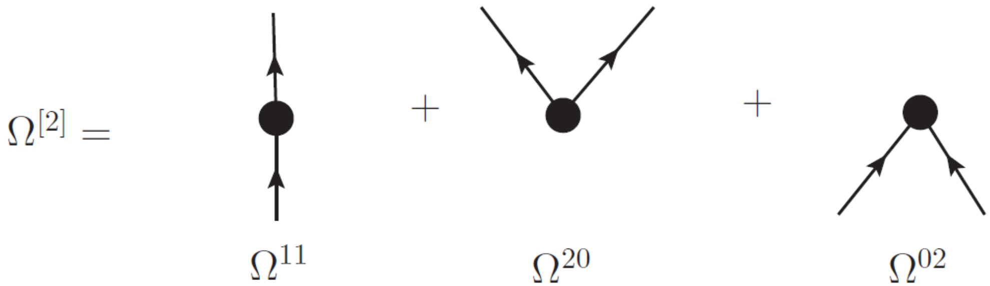
$$0 = \langle\Phi^{\alpha\beta\gamma\delta}|\Omega(1+\mathcal{T}_1+\mathcal{T}_2+\tfrac{1}{2}\mathcal{T}_1^2+\tfrac{1}{2}\mathcal{T}_2^2 +\mathcal{T}_1\mathcal{T}_2+\tfrac{1}{3!}\mathcal{T}_1^3+\tfrac{1}{4!}\mathcal{T}_1^4+\tfrac{1}{2}\mathcal{T}_1^2\mathcal{T}_2)|\Phi\rangle_C$$

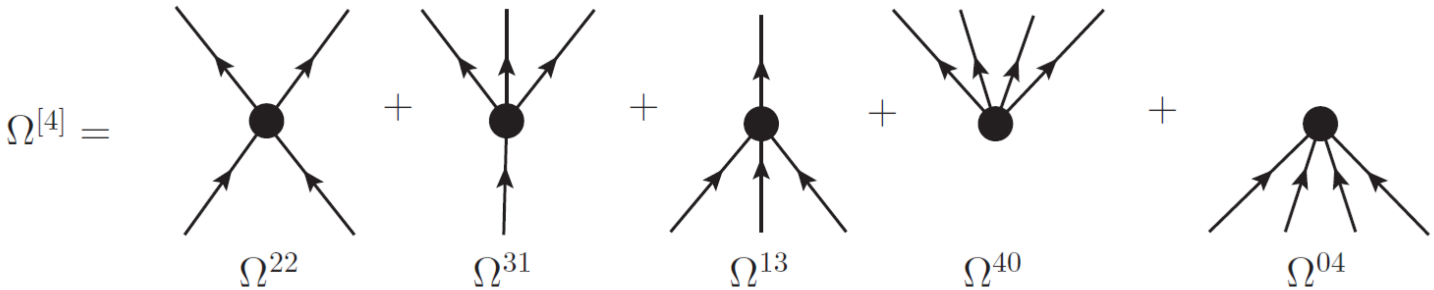


Incorporates standard single-reference CC as a particular case

Diagrammatic and BCCSD equations (1)

Grand potential at normal-ordered two-body level





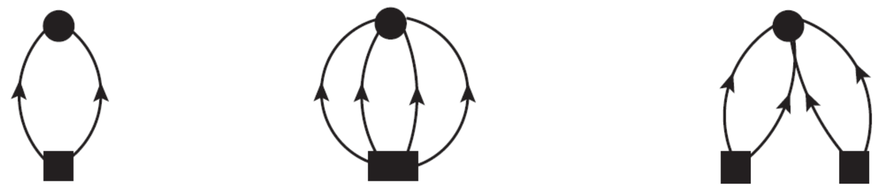
Cluster amplitudes at BCCSD level

- Generate all distinct connected diagrams
- Label external lines according to bra
- Sum over all internal lines
- Associate matrix elements to each vertex
  - $(n!)^{-1}$ factor for n equivalent internal lines
  - $(k!)^{-1}$ factor for k equivalent cluster vertices
  - $(-1)^n$ factor for n crossing lines
- Add permutation for inequivalent external lines

Diagrammatic and BCCSD equations (2)

Energy equation

$$\Omega_0 \quad = \quad \langle \Phi | \Omega (\mathcal{T}_1 + \mathcal{T}_2 + \tfrac{1}{2}\mathcal{T}_1^2) | \Phi \rangle_C$$



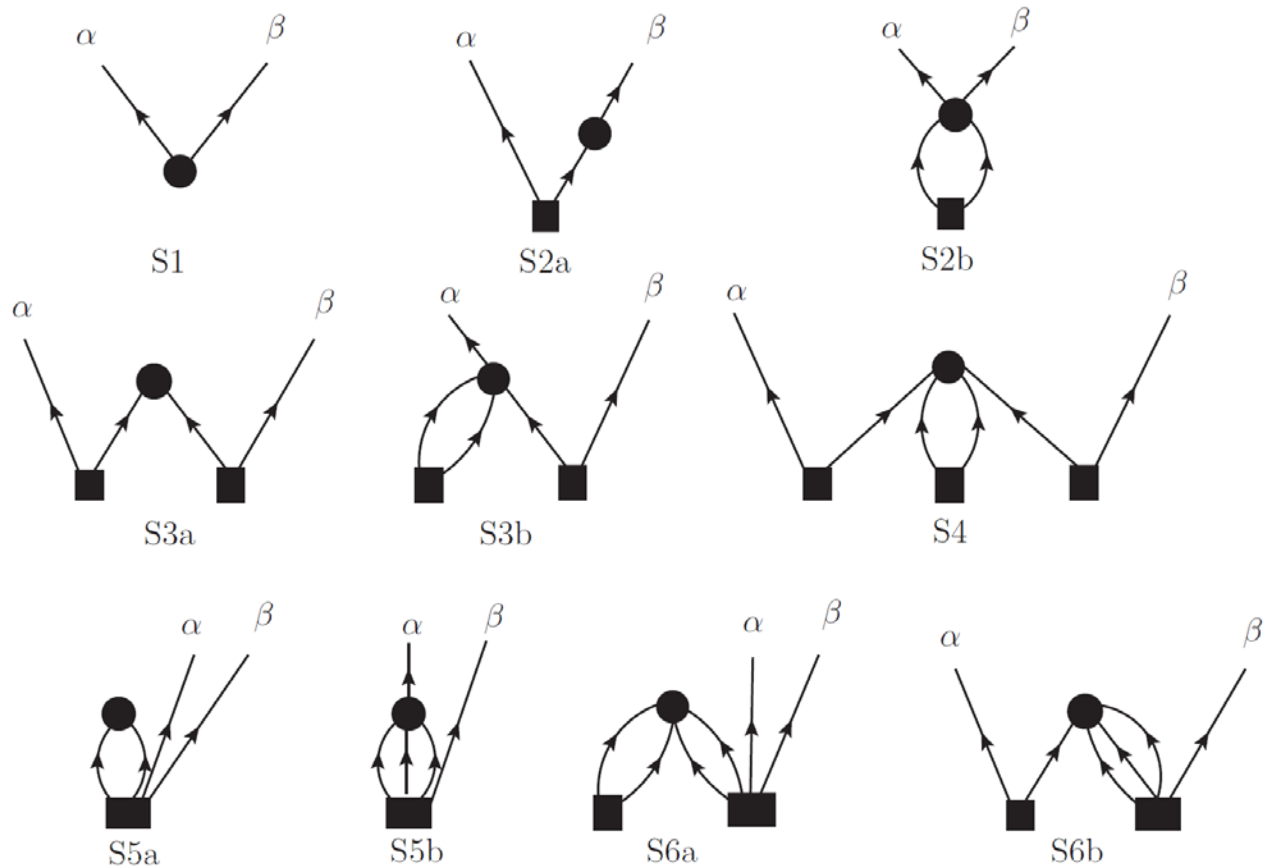
Single amplitude equation

No distinction between particles and holes

Fewer diagrams than in CCSD

Similar for double amplitude equation

Can be extended to
(1) residual 3NF $\Omega^{[6]}$
(2) triples $\mathcal{T}_3$



$$0 \quad = \quad \langle \Phi^{\alpha\beta} | \Omega (1 + \mathcal{T}_1 + \tfrac{1}{2}\mathcal{T}_1^2 + \tfrac{1}{3!}\mathcal{T}_1^3 + \mathcal{T}_2 + \mathcal{T}_1\mathcal{T}_2) | \Phi \rangle_C$$

Part II.a.

Pairing Hamiltonian from BCCD

[T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, T. Duguet, PRC89, 054305 (2014)]

Set up

Attractive pairing grand potential

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

Pair operators

$$N_p = a_{p\uparrow}^\dagger a_{p\uparrow} + a_{p\downarrow}^\dagger a_{p\downarrow}$$
$$P_p^\dagger = a_{p\uparrow}^\dagger a_{p\downarrow}^\dagger$$

SU(2) algebra

$$[P_p, P_q^\dagger] = +\delta_{pq}(1 - N_p)$$
$$[N_p, P_q] = -2\,\delta_{pq} P_p$$
$$[N_p, P_q^\dagger] = +2\,\delta_{pq} P_p^\dagger$$

Doubly-degenerate picket fence model $\epsilon_p = p\,\Delta\epsilon$

Model for, e.g., deformed nuclei

Exact ground-state energy

- **Diagonalization within seniority-0 subspace**

  [A. Volya, B.A. Brown, W. Zelevinsky, PLB509, 37 (2001)]

- **Richardson solution**

  [R.W. Richardson, PL3, 277 (1963), PR141 (1966)]

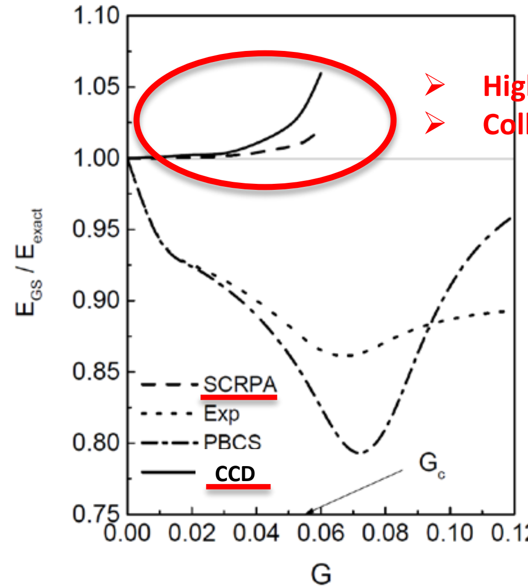
*Cheaper than full diagonalization (√)
*Still scales exponentially
->Limited to ~40 levels at half filling

Look for highly accurate many-body methods that

- scale polynomial with system size
- can be applied to more realistic Hamiltonians

Typical approximate methods

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



[J. Dukelsky *et al.*, NPA714, 63 (2003)]

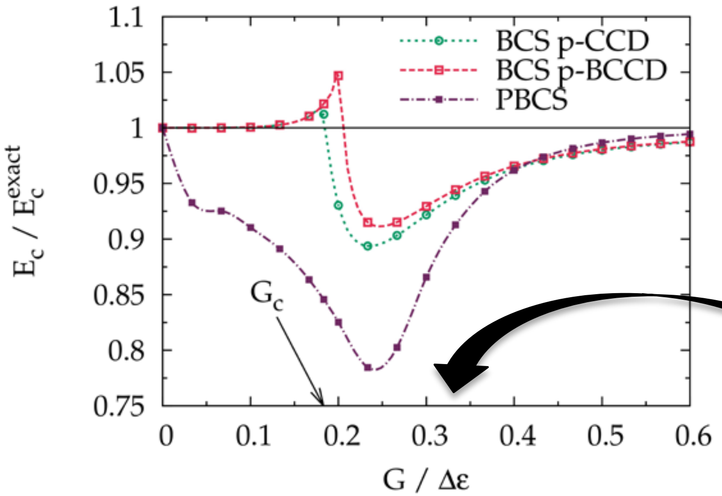
- High accuracy in normal phase
- Collapse near superfluid transition

What about BCCD?

*100 levels
*Half filling
*Δε = 300keV
*$G_c/\Delta\epsilon$ =0.18

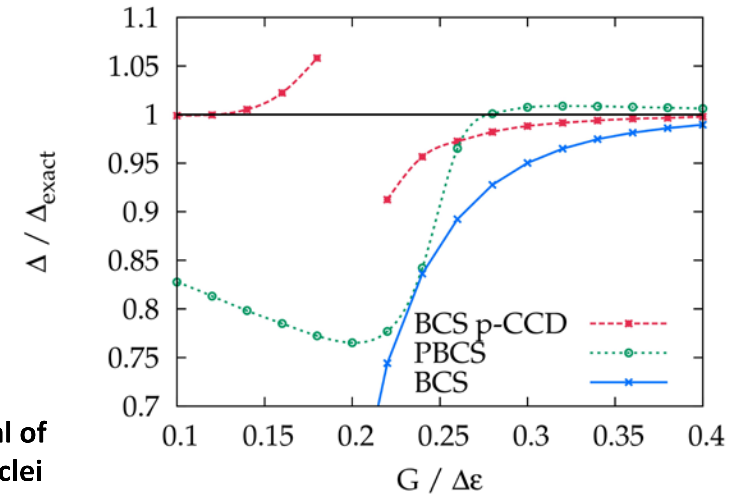
Results for 100 levels at half filling

Correlation energy



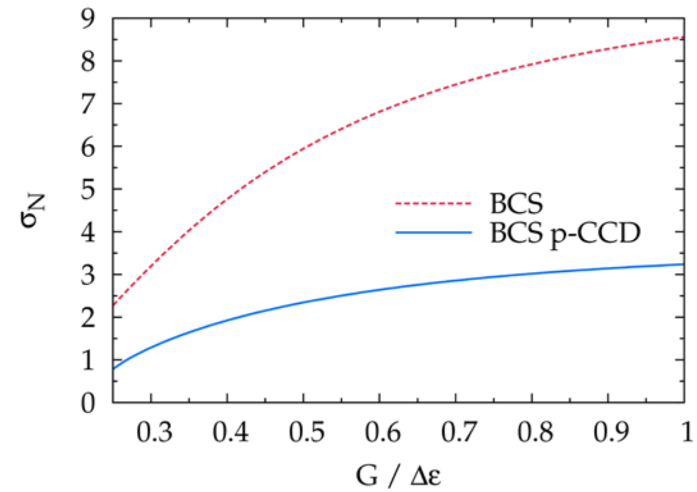
Regime typical of rare-earth nuclei

Pairing "gap"



$$\Delta_c = G \sum_p \left[\langle\Psi|P_p^\dagger P_p|\Psi\rangle - \frac{1}{4}\langle\Psi|N_p|\Psi\rangle^2 \right]$$

Variance in A



- High accuracy in normal & superfluid phases
- Superior to PBCS in regime of interest
- Superiority improves with system size
- Doubles reduce symmetry breaking vs BCS
- Conclusions valid away from half filling
- Symmetry restoration crucial near closed shell

[*PNR Bogoliubov CC theory*, T. Duguet, in preparation (2014)]

Triples correction will further improve

Phase transition wrongly of first order
Second-order character recovered from singles

Test calculations of semi-magic N/Z=8 nuclei

Set up

- NNLO$_{opt}$ 2NF (Λ = 500 MeV/c)
  [A. Ekstrom *et al.*, PRL110, 192502 (2013)]
- No 3NF yet
- HO basis
  - N_{max} = 6
  - hw = 26 and 50,53,55,58 MeV
- m-scheme code

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, in preparation (2014)]

Ground-state binding energy

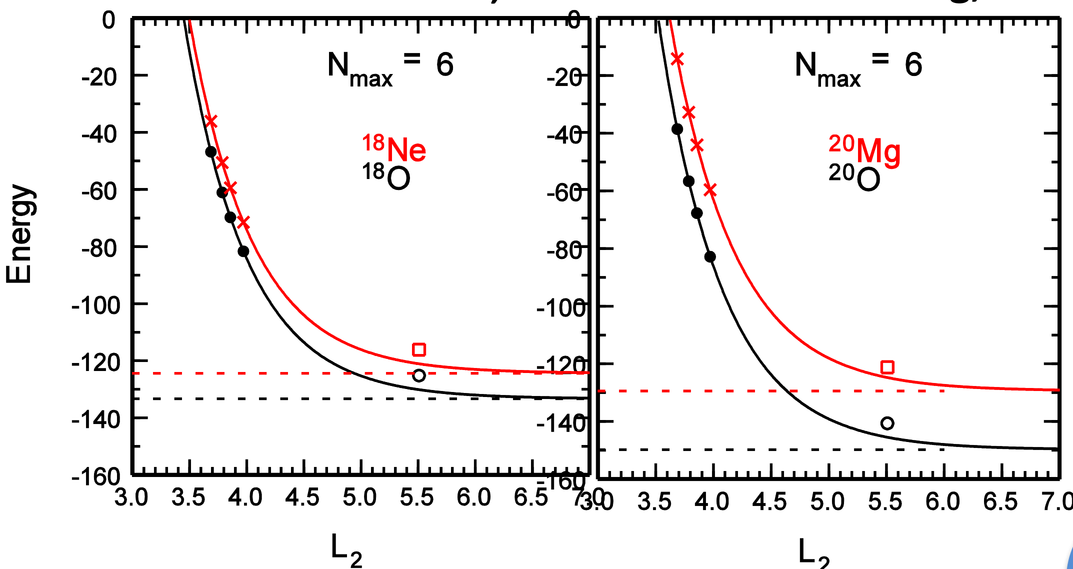
Preliminary

Accessible via 2PA-EOM-CCSD
[G. Jansen *et al.*, PRC83 (2011) 054306]
3p-1h on top of ^{16}O

Only accessible via BCCSD
(can do any number of valence nucleons)

BCCSD = CCSD to the ev level in doubly closed-shell 16O

+ 2 nucleons = ^{18}Ne, ^{18}O **+ 4 nucleons = ^{20}Mg, ^{20}O**



Nucleus	$E_{\min}$	$E^{CCSD}_{N_{\max}=6}$	E_∞	$E^{CCSD}_{N_{\max}=12}$
^{16}O	-119.211	-119.211	-124.905	-123.453
^{18}O	-125.2	-126.476	-133.284	-132.990
^{20}O	-140.672	n/a	-149.788	n/a
^{18}Ne	-116.141	-117.927	-124.351	-124.850
^{20}Mg	-121.186	n/a	-129.410	n/a

Infrared extrapolation from hw=50,53,55,58MeV
[R. Furnstahl *et al.*, (2014) arXiv:1408.0252]

$$E(L) = E_\infty + A_\infty e^{-2k_\infty L}$$

where

$$b = \sqrt{\hbar/(M\omega)}$$

$$L = \sqrt{2(N + 3/2 + 2)}b$$

Extends SR-CC to genuinely open-shells!
- Scales as $(n_h+n_p)^6$

~1.5 MeV > 2PA-EOM-CCSD in $^{18}0$ and ^{18}Mg
- Critical to restore A near closed shell

Storage of $\mathcal{T}_2$ in m scheme beyond N_{max} = 8?
- More involved distribution of $\mathcal{T}_2$
- Use SVD

[T. Kinoshita *et al.*, JCP 119 (2003) 7756]
- Code in J-coupled scheme

Conclusions and perspectives

Conclusions

- Development of Bogoliubov CC theory for genuinely open-shell nuclei
- Parallel effort to Gorkov-SCGF and MR-IMSRG
- m-scheme implementation at the singles and doubles level
  - *First proof-of-principle results*
  - *Allows for the treatment of doubly-open-shell systems*
  - *Currently limited to N_{max} = 8 due to storage scheme*

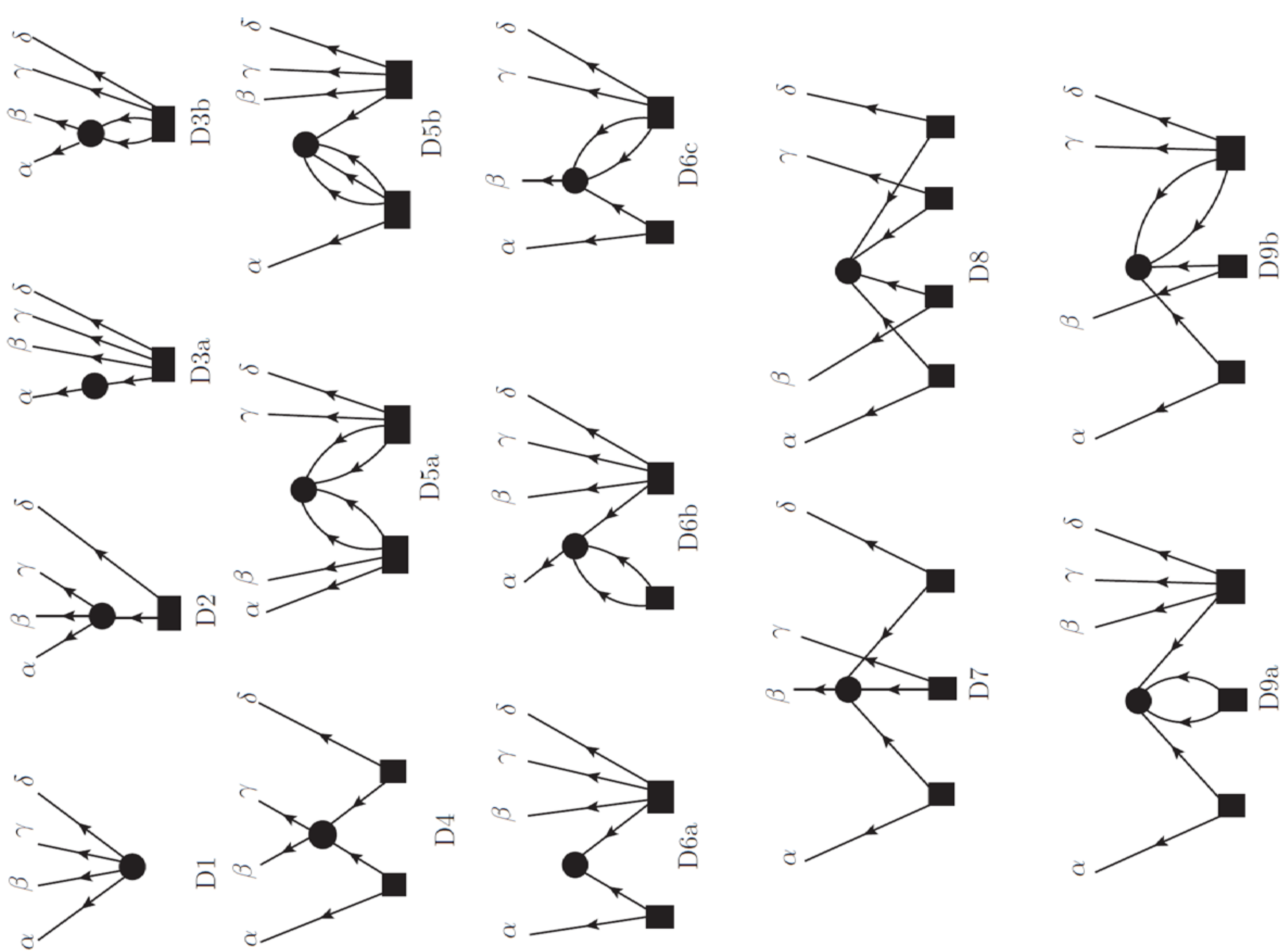
Future

- Develop option(s) to go to larger bases
- Implementation of 3NF at normal-ordered two-body level
- Extend to Equation-Of-Motion Bogoliubov CC theory
- Wealth of potential applications
  - *Problems of experimental interest*
  - *Cross-benchmarking with Gorkov-SCGF and MR-IMSRG*
- Symmetry-restored Bogoliubov CC theory and applications

Complementary slides

Diagrammatic and BCCSD equations (3)

Double amplitude equation



$$
\begin{aligned}
0 &= \langle \Phi^{\alpha\beta\gamma\delta} | \Omega (1 + \mathcal{T}_1 + \mathcal{T}_2 + \tfrac{1}{2}\mathcal{T}_1^2 + \tfrac{1}{2}\mathcal{T}_2^2 \\
&\quad + \mathcal{T}_1\mathcal{T}_2 + \tfrac{1}{3!}\mathcal{T}_1^3 + \tfrac{1}{4!}\mathcal{T}_1^4 + \tfrac{1}{2}\mathcal{T}_1^2\mathcal{T}_2) | \Phi \rangle_C
\end{aligned}
$$