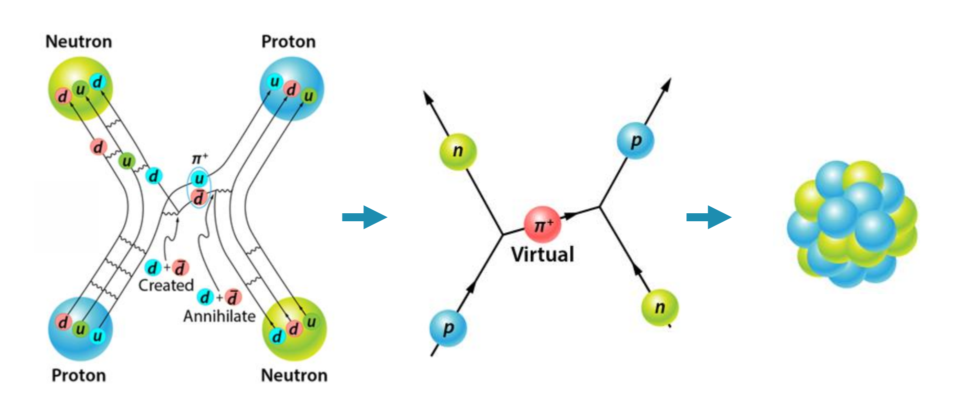
Bogoliubov Coupled Cluster theory for open-shell nuclei



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GDR NBODY

11/01/2022

Outline

- “Ab initio” many-body approach to nuclear systems
- Open-shell frontier
- Bogoliubov coupled cluster (BCC) theory
- Scalability
- Results
- Outlook

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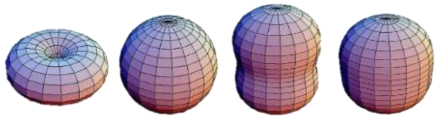
Huge diversity of nuclear phenomena

The atomic nucleus is a strongly correlated self-bound many-body quantum system and therefore intrinsically complex

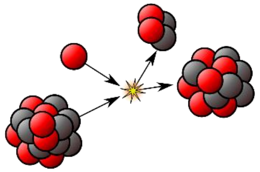
Ground-state properties:

Mass, binding energy, shape, moments, …



Nuclear reaction:

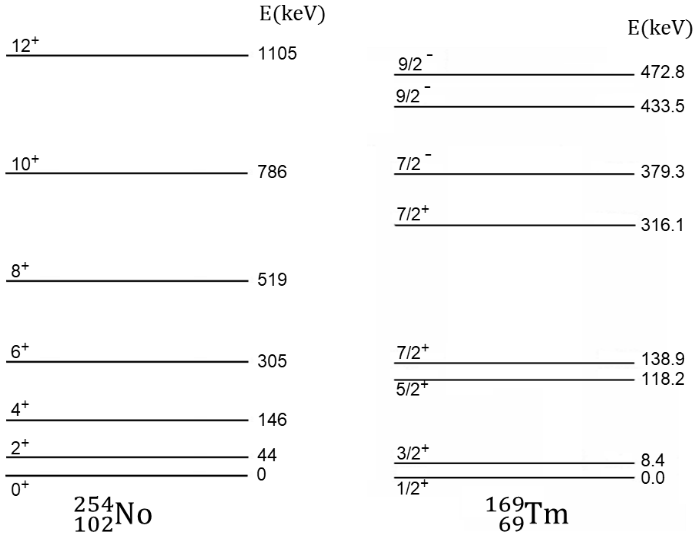
Fusion, knockout, transfer, …



Spectroscopy:

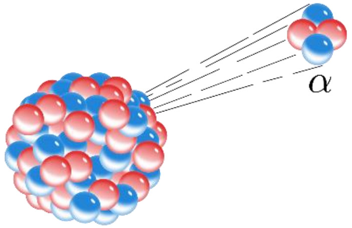
rotational & vibrational bands

Single-particle dominated excitations



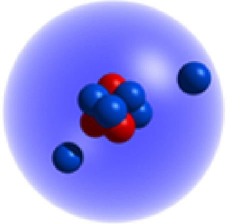
Radioactive decay:

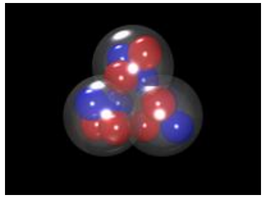
α, $\beta^{+/-}$, p, fission, …



Exotic structures:

Halo, clusters, …





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Huge diversity of nuclear phenomena

Many Models

- Examples
  - Liquid drop model
  - Rotational & vibrational models
  - Shell model
  - Nilsson model
  - …
- Short comings
  - Not straightforwardly improvable
  - No clear path to connect them

→

Effective Theories

- Resolves these short comings
  - Systematically improvable
  - Connections (reduction) possible

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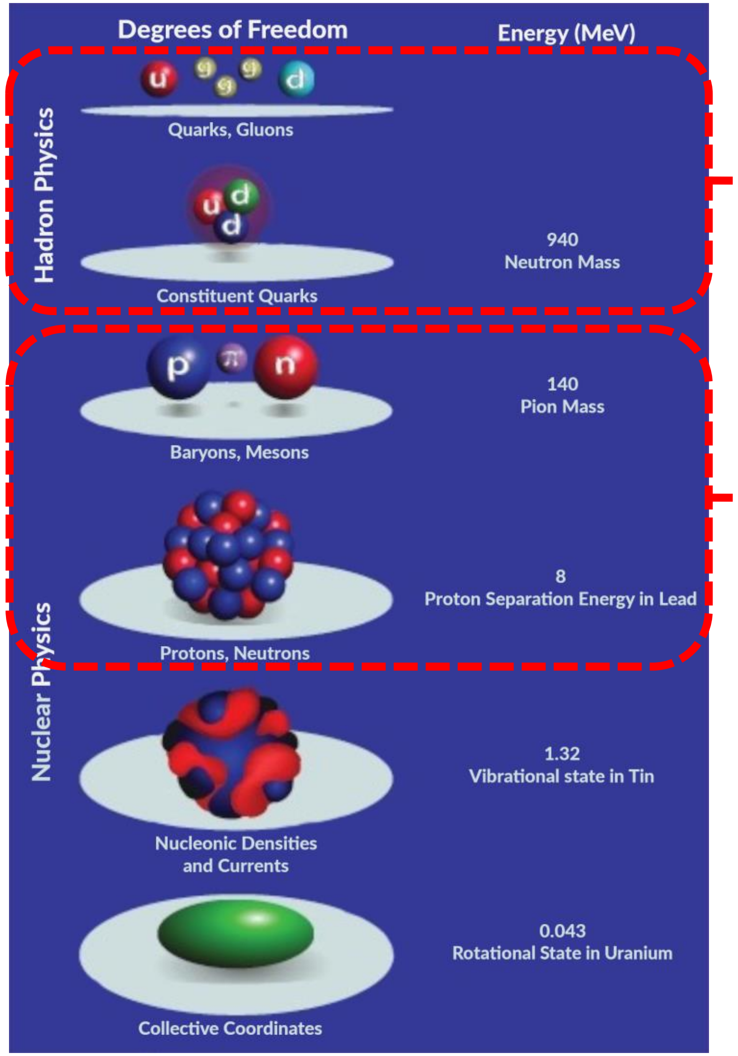
Effective field theory

Emergence of phenomena from effective description

More elementary description, reductionism



QCD

Chiral effective field theory (χ-EFT)

protons & neutrons as d.o.f.

Effective field theory (EFT)

1) Identifying appropriate degrees of freedom (d.o.f.)
2) ALL interactions complying with symmetries of underlying theory
3) Ordered in expansion governing hierarchy (power counting)
4) Fix low energy constants (LEC) from data (or underlying theory)

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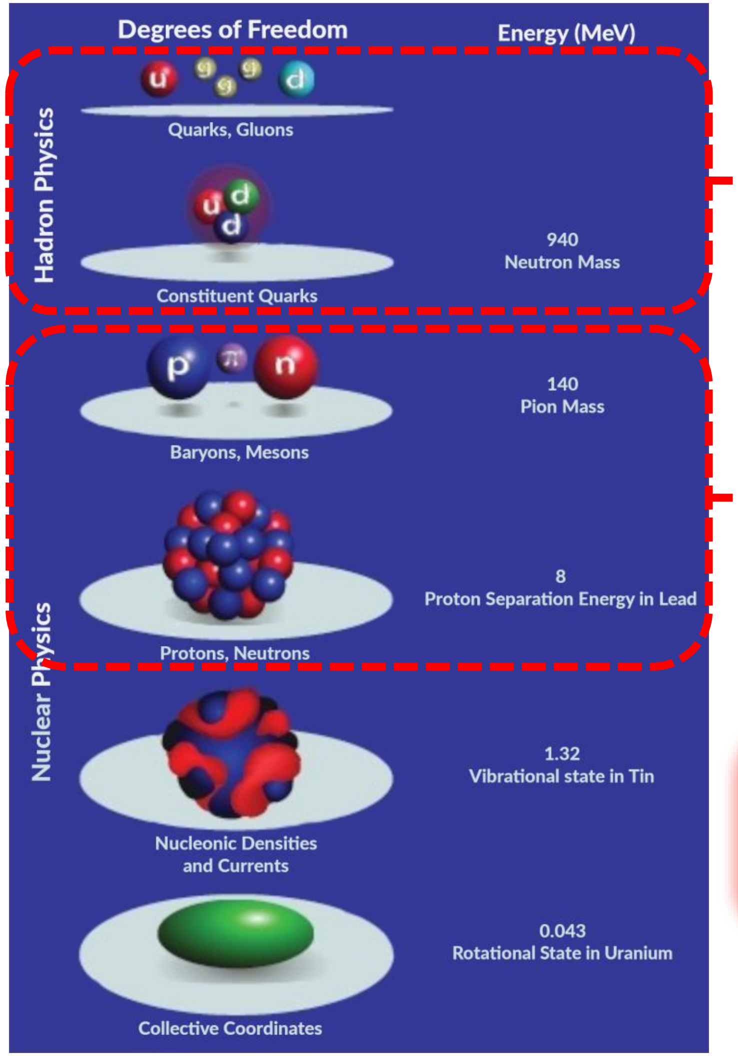
Effective field theory

Emergence of phenomena from effective description

More elementary description, reductionism



QCD

Chiral effective field theory (χ-EFT)

protons & neutrons as d.o.f.

***"Ab initio"* approach:**
Application of χ-EFT to describe the nucleus

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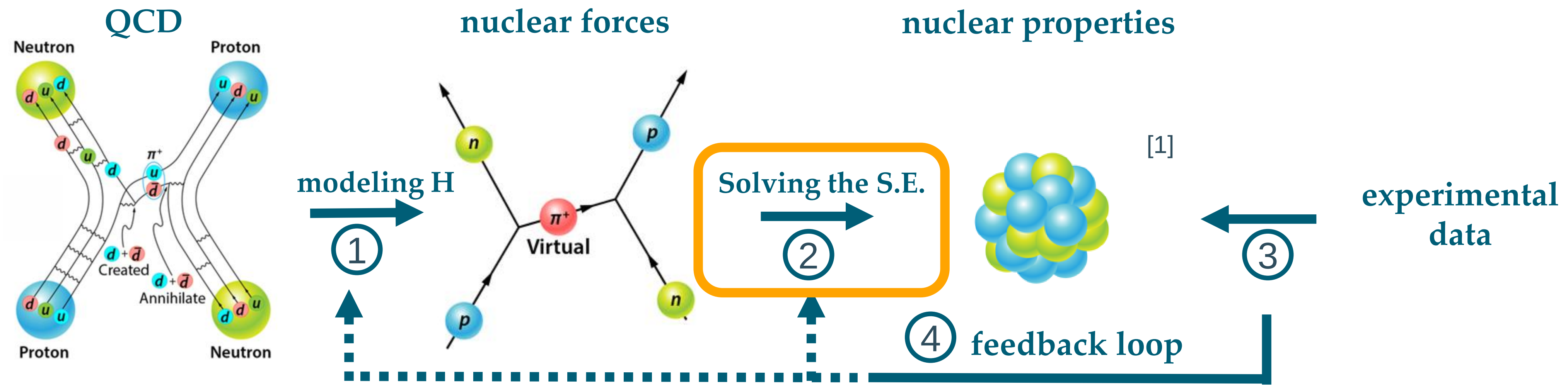
"*Ab initio*" approach to nuclear structure

Assumptions

- Structure-less protons and neutrons as d.o.f.
  - All nucleons active (no inert core)
- Only elementary interactions between them
  - Sound connection to QCD
  - All possible interactions allowed by symmetry
  - Up to A-body forces (in principle)

Ab initio **("from scratch") scheme =**
solve A-body Schrödinger equation (S.E.)

$$\hat{H}|\Psi_n^A\rangle = E_n^A|\Psi_n^A\rangle$$



[1]: APS/Alan Stonebraker

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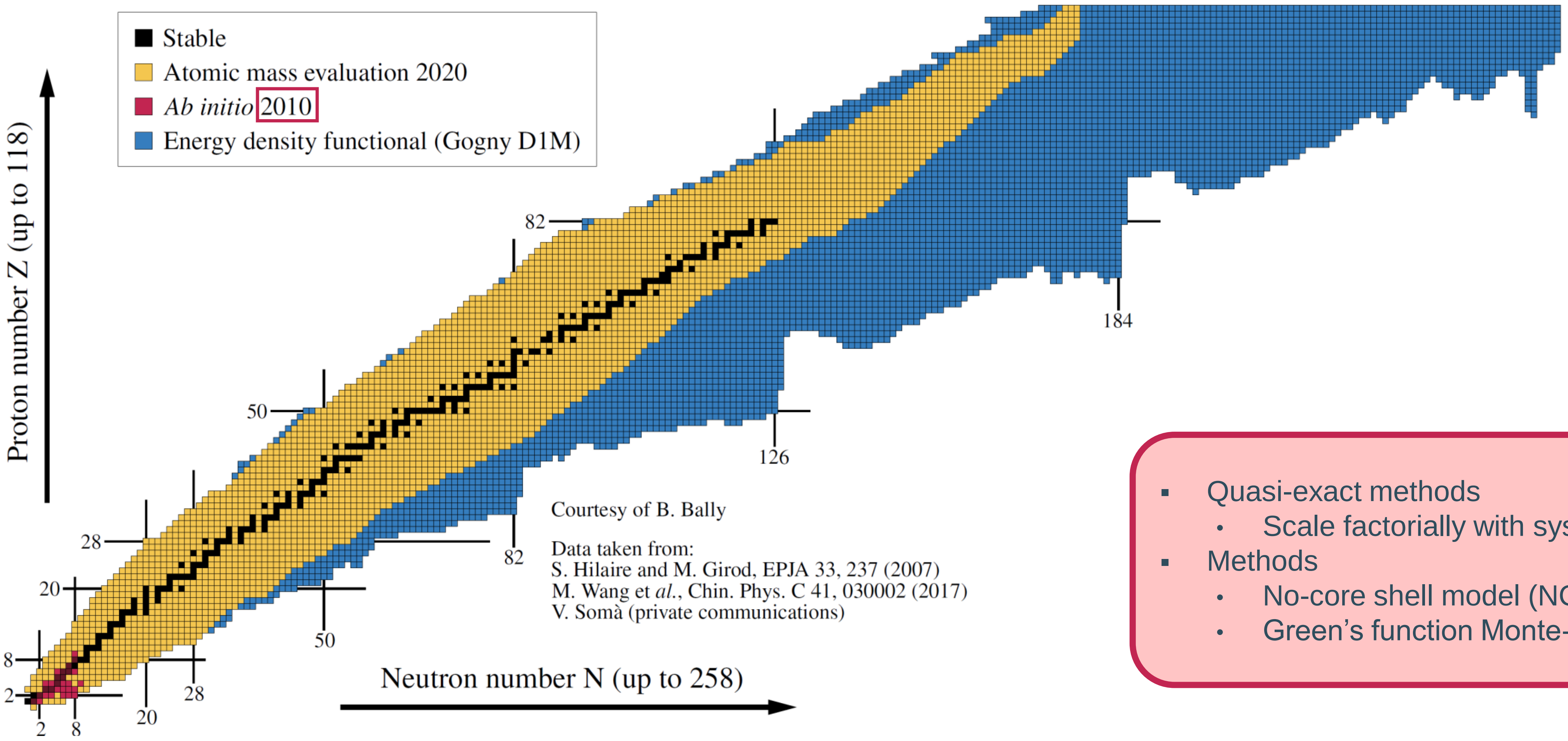
② Solving the Schrödinger equation



- Quasi-exact methods
  - Scale factorially with system size
- Methods
  - No-core shell model (NCSM)
  - Green's function Monte-Carlo (GFMC)

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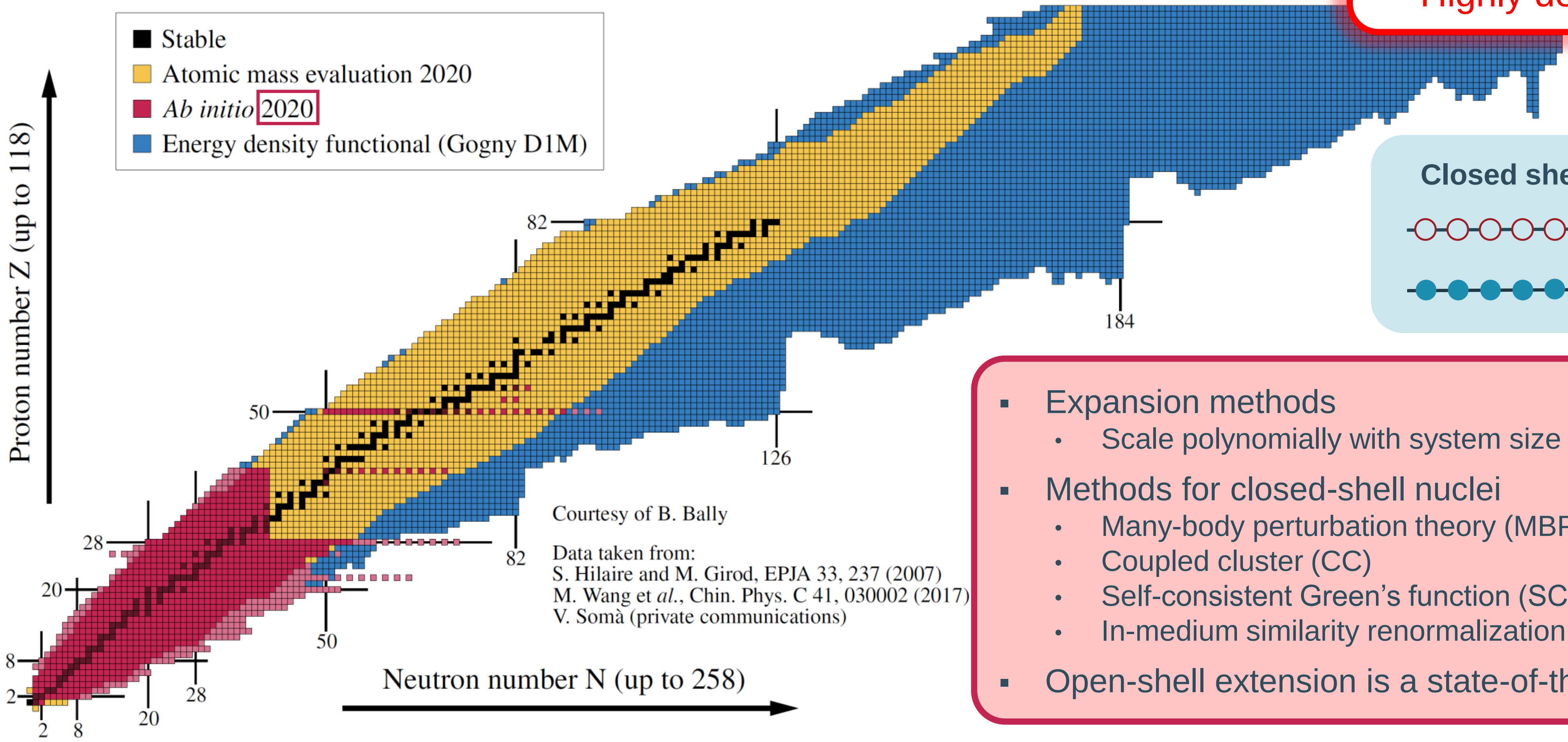
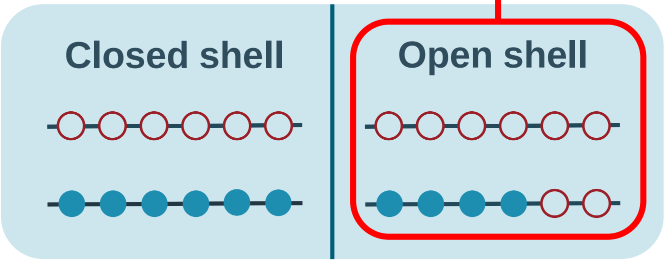
② Solving the Schrödinger equation



Vast majority
- Two types of fermions
- Highly degenerate shells



- Expansion methods
  - Scale polynomially with system size
- Methods for closed-shell nuclei
  - Many-body perturbation theory (MBPT)
  - Coupled cluster (CC)
  - Self-consistent Green's function (SCGF)
  - In-medium similarity renormalization group (IMSRG)
- Open-shell extension is a state-of-the-art challenge

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Open-shell systems

Expansion method: $\hat{H} = \hat{H}_0 + \hat{H}_1 \longrightarrow \begin{cases} \hat{H}_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle \\ |\Psi_n^A\rangle = \hat{\mathcal{W}}|\Phi_n\rangle \end{cases}$

Beyond mean field ($\hat{H}_1$)

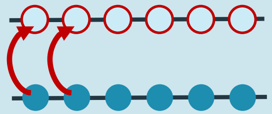
Mean field method ($\hat{H}_0$):
Hartree-Fock-Bogoliubov (HFB)

GS: $|\Phi\rangle$

Symmetry conserving

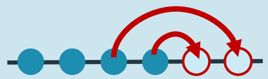
$$[\hat{H}_0, \hat{A}] = 0$$
$$[\hat{H}_1, \hat{A}] = 0$$

closed shell



non-degenerate
good starting point

open shell



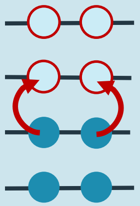
degenerate
IR divergence

Bogoliubov transformation

Symmetry breaking

$$[\hat{H}_0, \hat{A}] \neq 0$$
$$[\hat{H}_1, \hat{A}] \neq 0$$

open → closed shell



non-degenerate
good starting point
pairing incorporated

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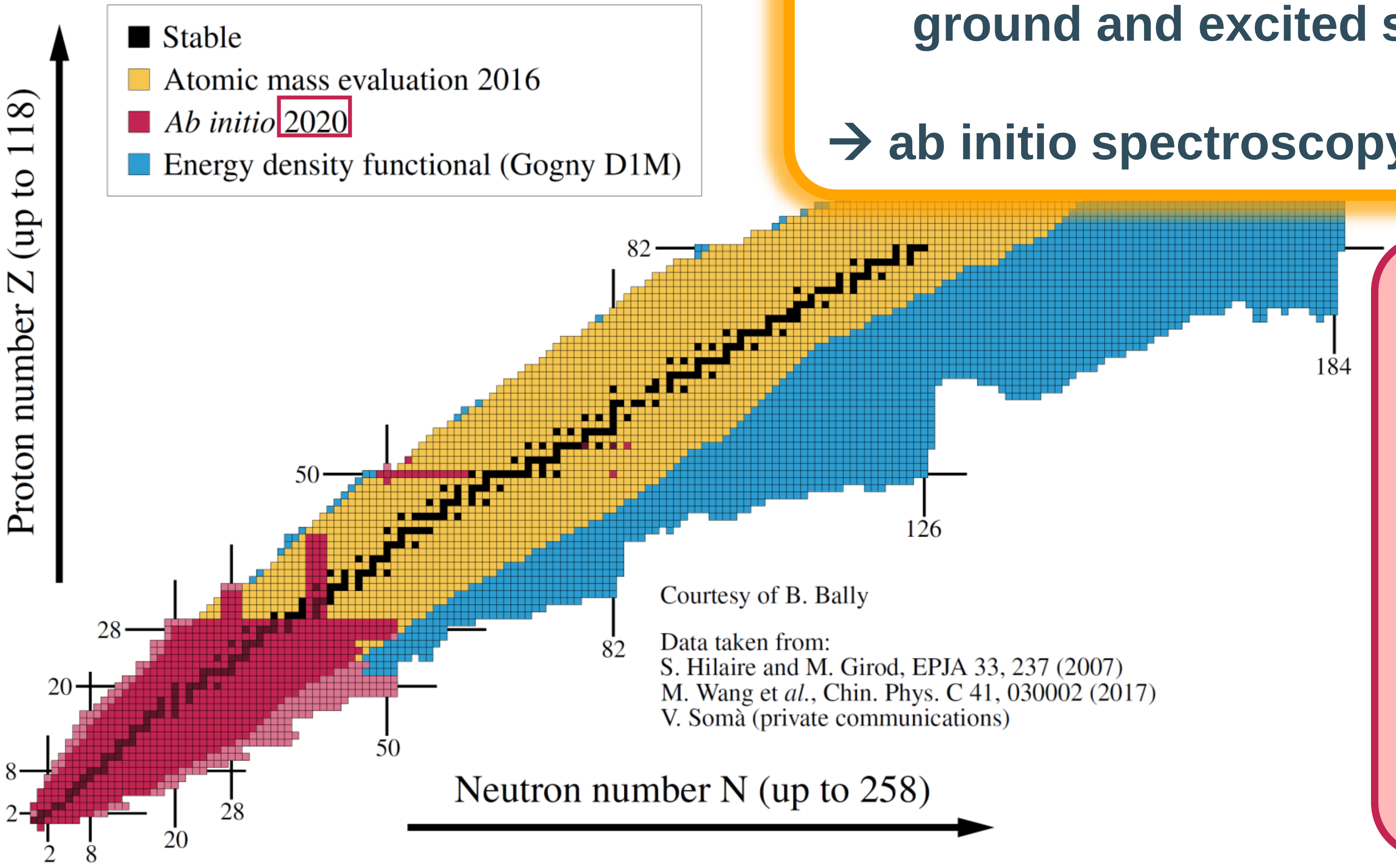
② Solving the Schrödinger equation

High-precision non-perturbative many-body method for ground and excited states of singly open-shell nuclei

→ ab initio spectroscopy along complete semi-magic chains



Expansion methods for open-shell nuclei

Single-reference method			
	Formalized	Implemented	
BMBPT	✓	✓	[2]
GSCGF	✓	✓	[3]
(EOM-)BCC	(✗) ✓	(✗) ✗	[4]
Multi-reference method			
PGCM-PT	✓	✓	[5]

[2] A.Tichai, P.Arthuis, T. Duguet et al. *Phys. Lett.* **B 786** 195 (2018)
[3] V. Somà, T. Duguet, C. Barbieri, *Phys. Rev. C* **84** 064317 (2011)
[4] A.Signoracci, T. Duguet et al. *Phys. Rev. C* **91** 064320 (2015)
[5] M. Frosini, T. Duguet, J.-P. Ebran, V. Somà, arXiv:2110.15737 (2021)

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Bogoliubov Coupled Cluster

Beyond mean field ← $\hat{H}_1$

Expansion method: $\hat{H} = \hat{H}_0 + \hat{H}_1$ → $\begin{cases} \hat{H}_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle \\ |\Psi_n^A\rangle = \hat{\mathcal{W}}|\Phi_n\rangle \end{cases}$

GS: $|\Phi\rangle$

$\hat{H}_0$ → Mean field method: Hartree-Fock-Bogoliubov (HFB)

BCC → $|\Psi_0^A\rangle = e^{\hat{\mathcal{T}}}|\Phi\rangle$

EOM-BCC → $|\Psi_n^A\rangle = \hat{\mathcal{R}}_n|\Psi_0^A\rangle$, $|\Psi_n^{A\pm1}\rangle = \hat{\mathcal{R}}_n^{\pm1}|\Psi_0^A\rangle$

Quasi-particle cluster operator

$$\hat{\mathcal{T}} \equiv \hat{\mathcal{T}}_1 + \hat{\mathcal{T}}_2 + \hat{\mathcal{T}}_3 + \cdots$$

BCCSD: Singles, Doubles

Singles → $\hat{\mathcal{T}}_1 \equiv \frac{1}{2!}\sum_{k_1k_2} t_{k_1k_2}\beta_{k_1}^\dagger\beta_{k_2}^\dagger$

Doubles → $\hat{\mathcal{T}}_2 \equiv \frac{1}{4!}\sum_{k_1k_2k_3k_4} t_{k_1k_2k_3k_4}\beta_{k_1}^\dagger\beta_{k_2}^\dagger\beta_{k_3}^\dagger\beta_{k_4}^\dagger$

Triples → $\hat{\mathcal{T}}_3 \equiv \frac{1}{6!}\sum_{k_1k_2k_3k_4k_5k_6} t_{k_1k_2k_3k_4k_5k_6}\beta_{k_1}^\dagger\beta_{k_2}^\dagger\beta_{k_3}^\dagger\beta_{k_4}^\dagger\beta_{k_5}^\dagger\beta_{k_6}^\dagger$

excitation amplitudes → Solutions of a set of non-linear algebraic equations which can be solved iteratively

Quasi-particle creation operators

unitary mix of ordinary particle creation and annihilation operators $\{c_p^\dagger, c_p\}$

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

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

⚠ $\hat{A}|\Psi_0\rangle \equiv \hat{A}\left(e^{\hat{\mathcal{T}}_1+\hat{\mathcal{T}}_2}|\Phi\rangle\right) \neq A|\Psi_0\rangle$ → monitor $\langle A\rangle$

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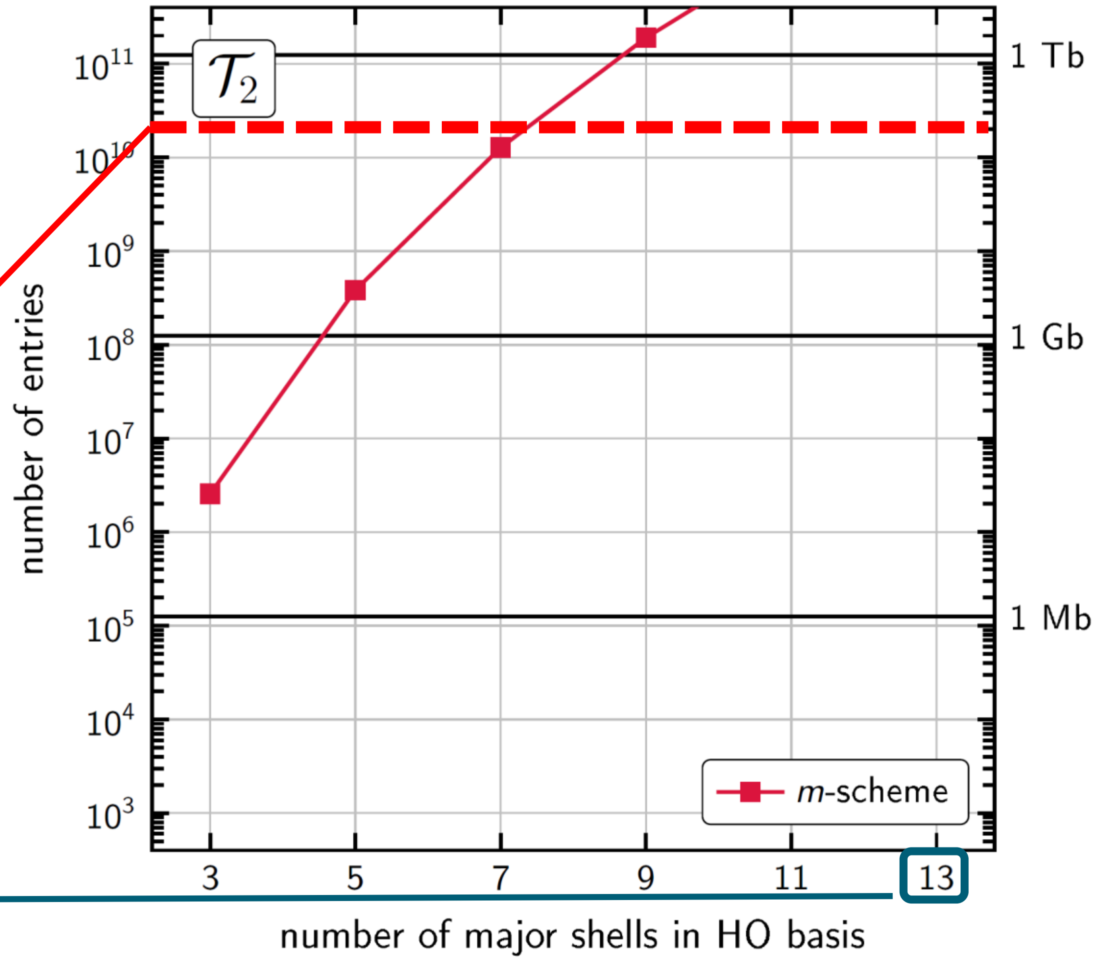
Scalability

m-scheme BCC

- Direct implementation of the BCC equations

✕ not scalable to large model spaces

Computational wall: ≈ 200Gb of RAM



Model space size required for precision calculations

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Scalability

m-scheme BCC

- Direct implementation of the BCC equations

✗ not scalable to large model spaces

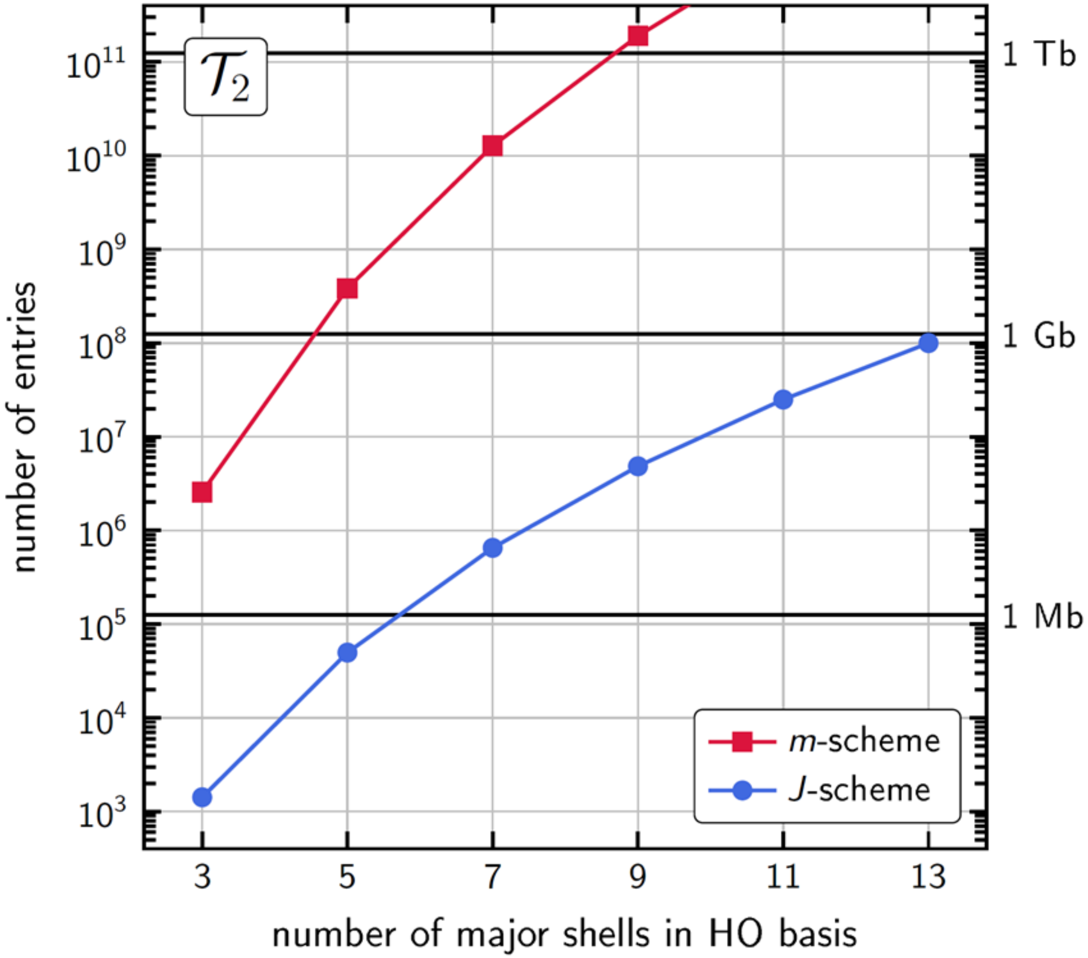
Angular momentum coupling (AMC)

J-scheme BCC

- Exploit shared rotational symmetry of $\hat{H}$ and computational basis
  - **m-degeneracy much larger than in QC → larger gain**

✓ Resolves scalability problem

- Spherical BCC equations much more involved
  - **Assisted with automated AMC tools [6]**
- Benchmarked w.r.t. m-scheme code (small model spaces)



[6] A. Tichai et al., *Eur. Phys. J. A* **56** 10 272 (2020)

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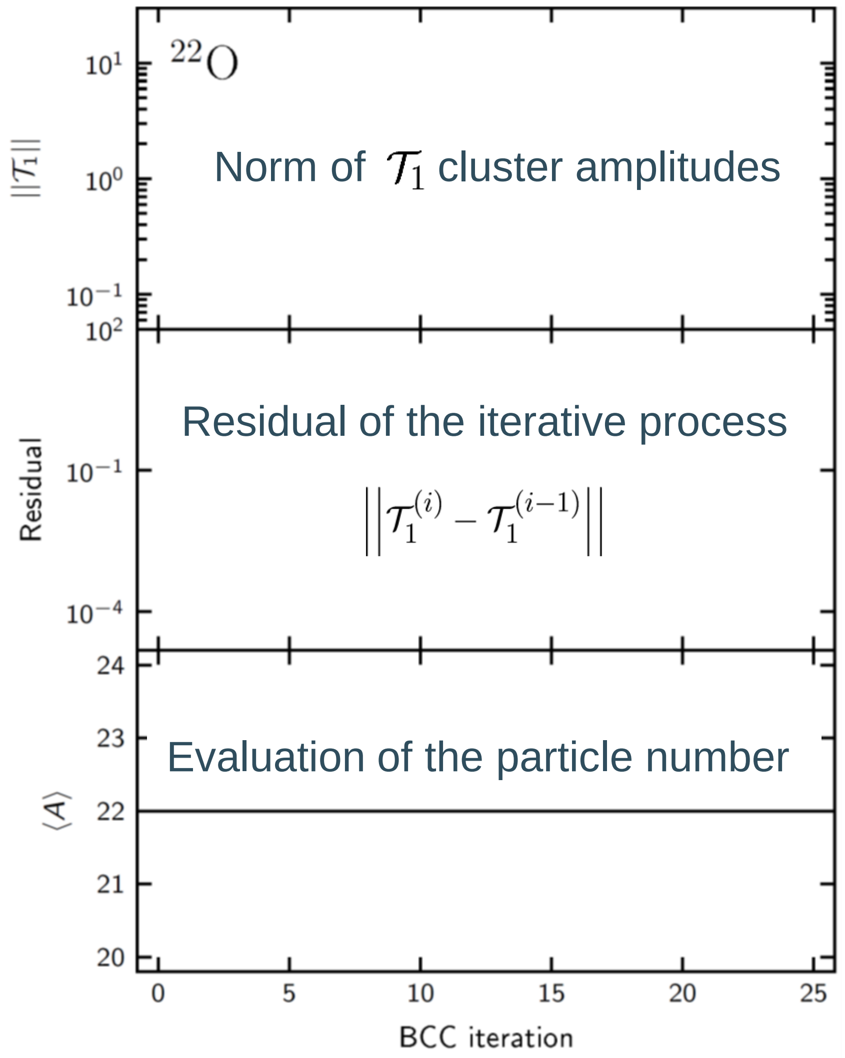
Results

- m-scheme BCCSD
- Ground-state ^{22}O
- 5 major shells in computational basis



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m-scheme BCCSD ^{22}O

Initial results

- ✗ Iterative process diverges

⇩ Enforce convergence with mixing techniques ⇩

Simple mixing

- ✓ Resolves divergence
- ✓ In agreement with results in *Signorracci et al.* [4]
- ✗ Convergence is very slow

⇩ Convergence acceleration method ⇩

Direct Inversion of the Iterative Subspace (DIIS)

- ✓ Much faster convergence
- ✗ Average particle number has shifted

⇩ particle number adjustment proposed in [4] ⇩

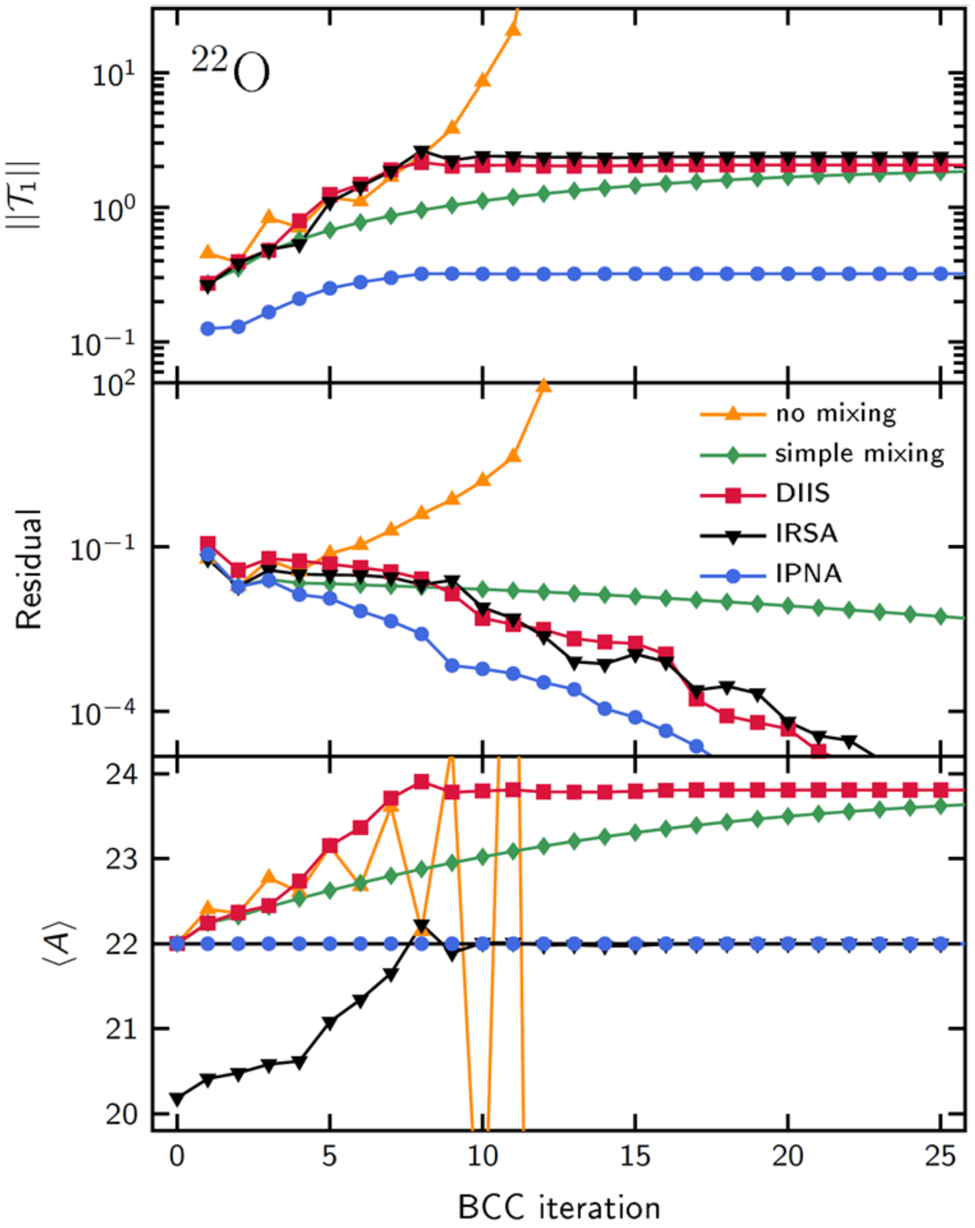
Iterative reference state adjustment (IRSA)

- ✓ BCC solution correct particle number on average
- ✗ Computationally very intensive
- ✗ Suitable reference state does not always exist

⇩ Novel particle number adjustment ⇩

Internal particle number adjustment (IPNA)

- ✓ particle number constrained in each BCC iteration
- ✓ BCC converges even faster
- ✓ Cluster amplitudes are reduced



[4] A.Signoracci, T. Duguet et al. *Phys. Rev. C* **91** 064320 (2015)

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Outlook

My PhD project . . .

Restoring particle number

Ab initio spectroscopy

Spectroscopic observables

Formulate and implement EOM-BCC

First full-fledged BCCSD application
→ NN + 3N forces, large model space, particle-number adjusted

Implement and benchmark J-scheme BCCSD
→ **extend automated angular momentum coupling tools**

Developed novel particle-number-adjustment scheme
→ Universal, accelerated convergence further and reduced cluster amplitudes

Accelerated convergence with DIIS

Implemented m-scheme BCCSD

Collaborators

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