Role of pairing in semi-magic nuclear ground states based on Bogoliubov coupled-cluster calculations

Pepijn Demol

ESNT "Where has the nuclear pairing gone?"- CEA Saclay
20 May 2025

Content

1. Correlation expansion methods and symmetry breaking
2. Bogoliubov many-body perturbation theory
3. Recent results from Bogoliubov coupled-cluster (BCC) theory
4. Pairing properties studied at HFB and BCC level

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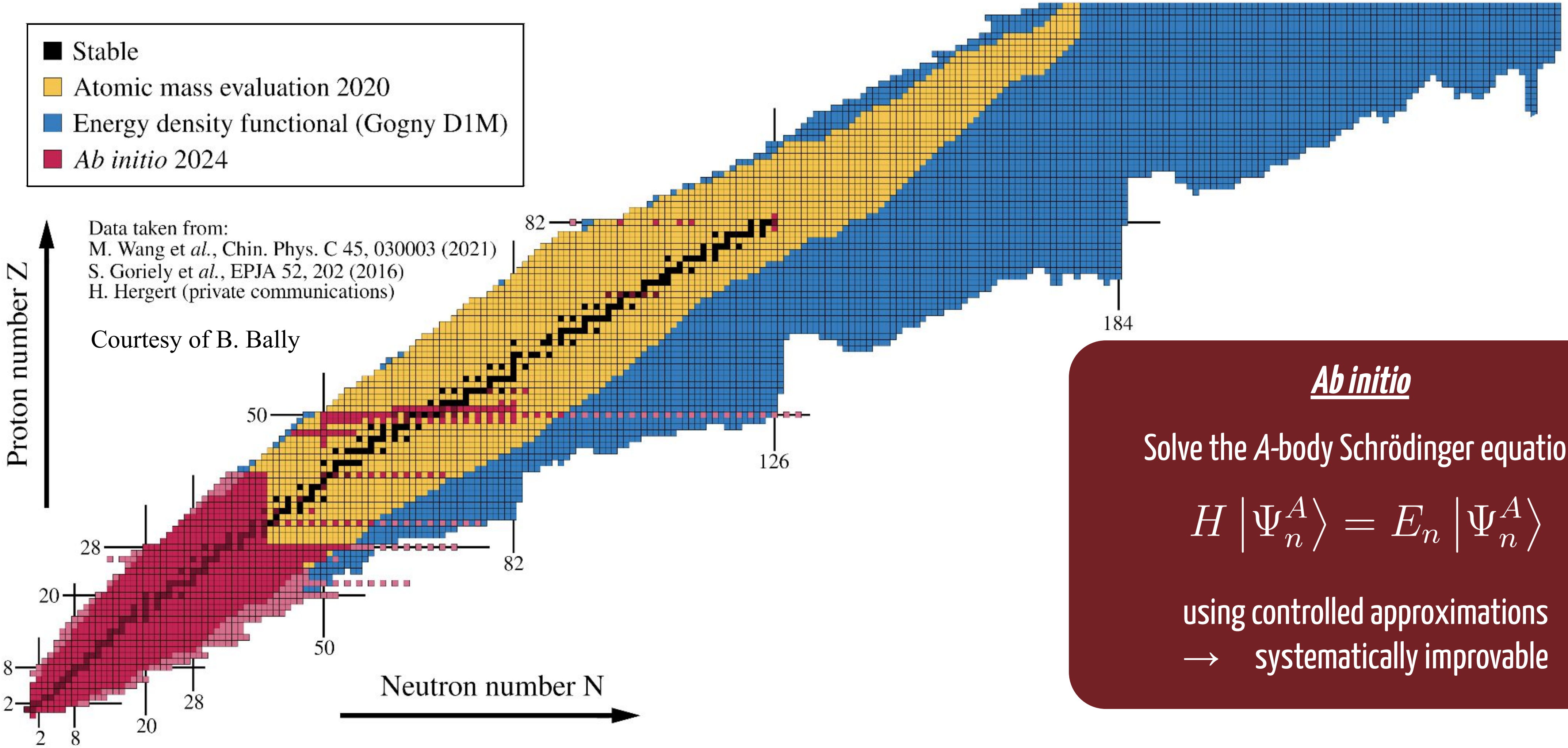
Ab initio approach to nuclear structure



Ab initio

Solve the *A*-body Schrödinger equation:

$$H \left|\Psi_n^A\right\rangle = E_n \left|\Psi_n^A\right\rangle$$

using controlled approximations

$\longrightarrow$ systematically improvable

$\longrightarrow$ **Pushing *ab initio* requires computationally affordable (polynomial) many-body methods**

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Correlation expansion methods

$$H\left|\Psi_n^A\right\rangle = E_n\left|\Psi_n^A\right\rangle$$

Mean-field-like $H_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle$

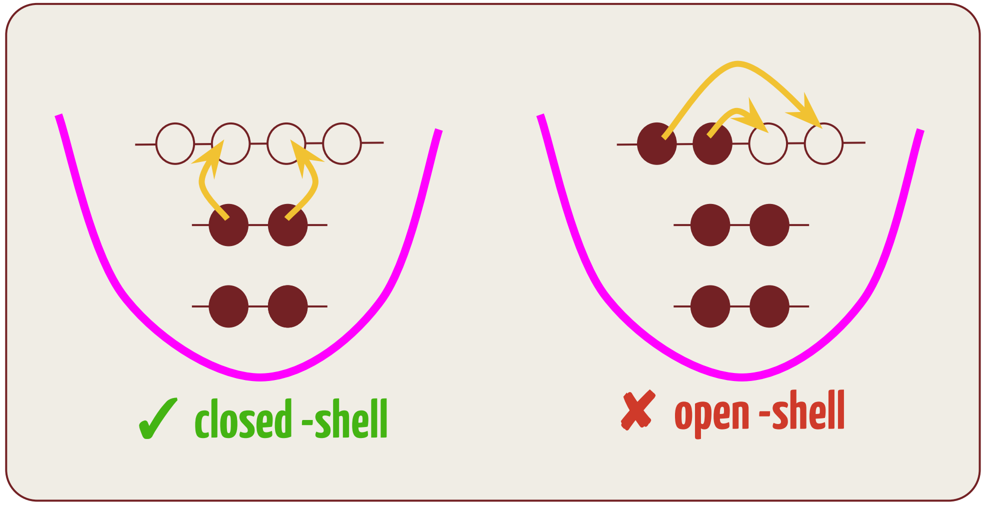
Partitioning: $H = H_0 + H_1$ → Correlation expansion $|\Psi_n^A\rangle = \mathcal{W}_n|\Phi_n\rangle$

Many-body perturbation theory (MBPT)

$\mathcal{W}$: Taylor expansion in powers of H_1

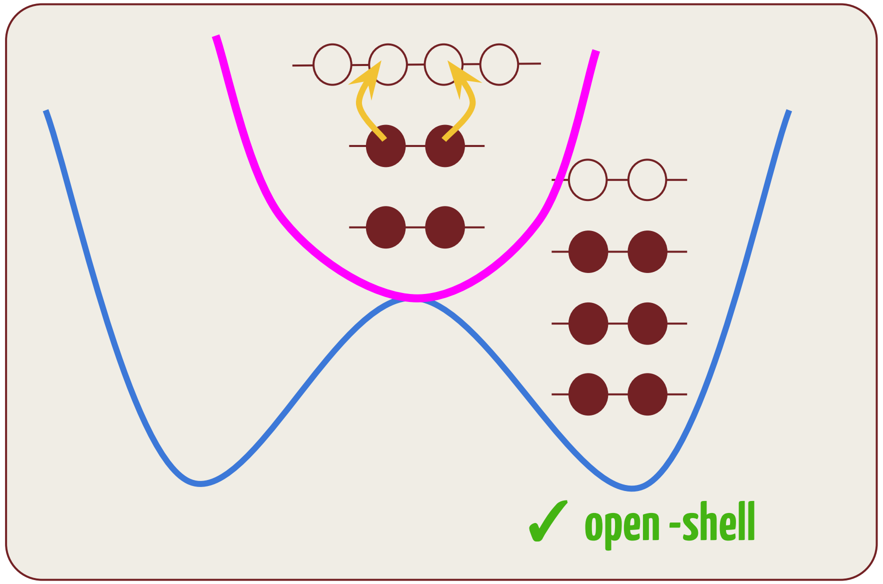
Coupled-cluster theory (CC)

$\mathcal{W} = e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T}(H_1)$

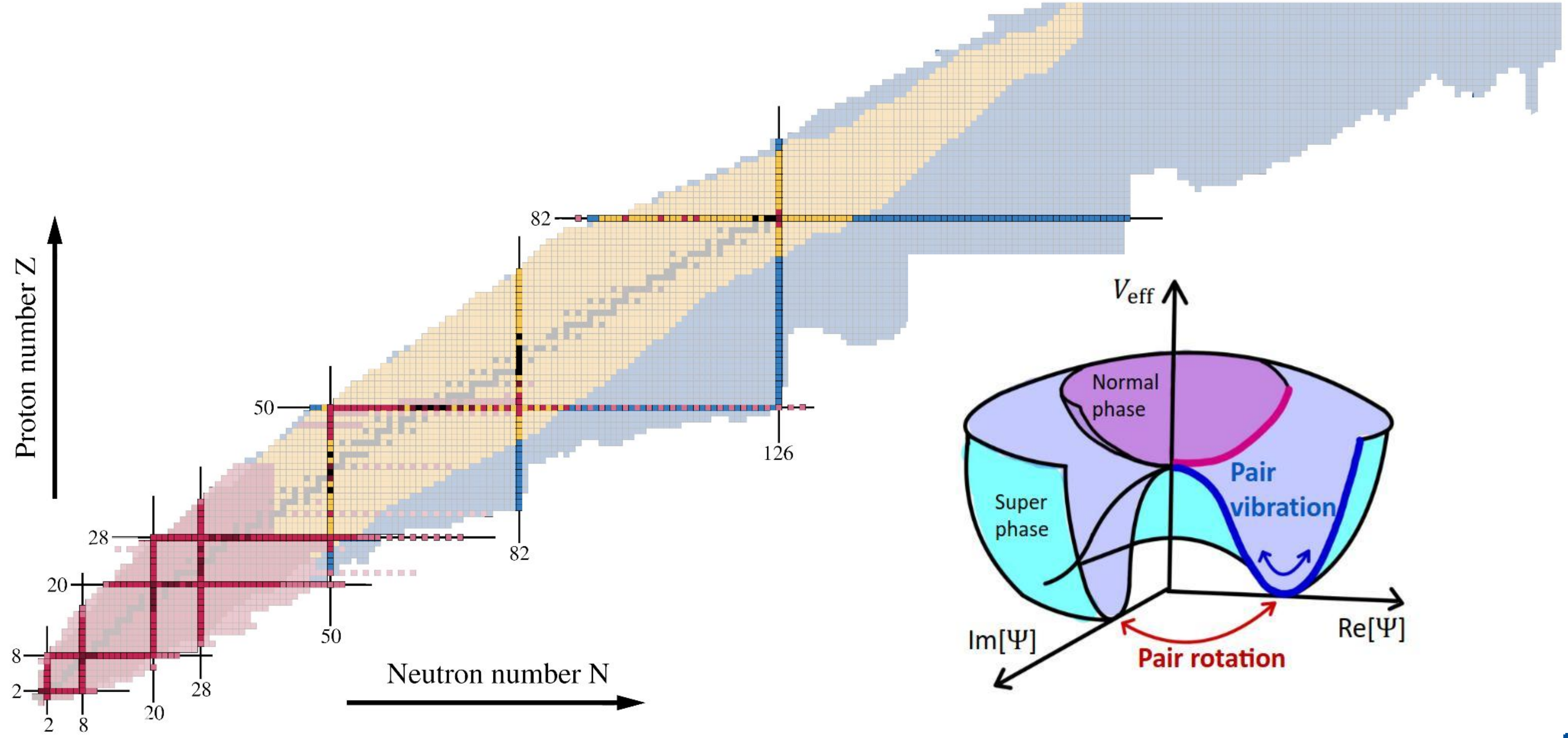


Symmetry breaking of H_0 & H_1

Lifts degeneracy



Semi-magic nuclei spontaneously break U(1) symmetry associated with pairing correlations



U(1) broken correlation expansion methods

Hartree-Fock-Bogoliubov (HFB) $\Omega_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle \longrightarrow A|\Phi_n\rangle \neq \mathrm{A}|\Phi_n\rangle$

<u>Partitioning:</u> $\cancel{H = H_0 + H_1}$

Correlation expansion $|\Psi_n^A\rangle = \mathcal{W}_n|\Phi_n\rangle$

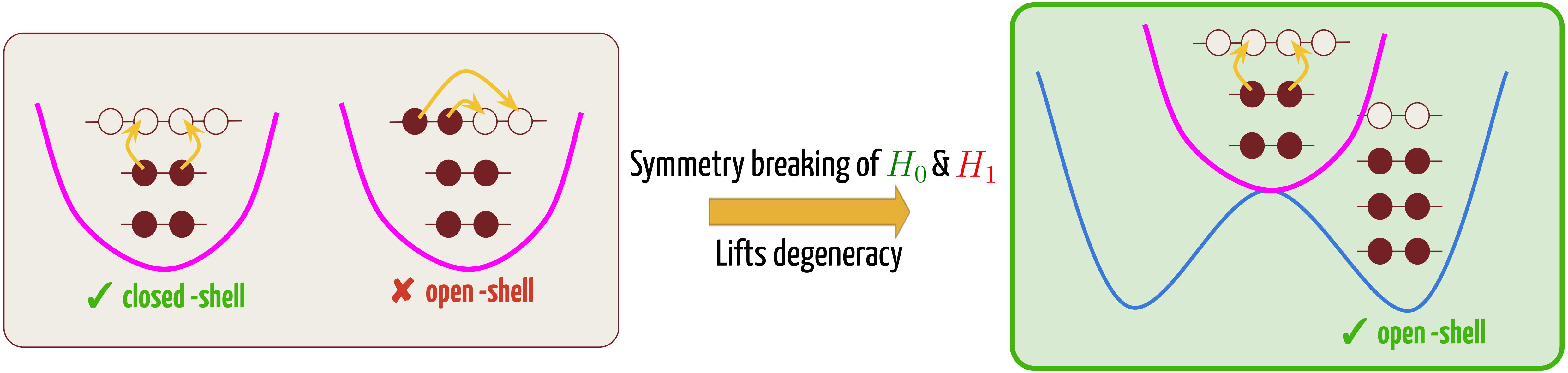
Grand potential: $\Omega = H - \lambda A = \Omega_0 + \Omega_1$

Bogoliubov many-body perturbation theory (BMBPT)

$\mathcal{W}$: Taylor expansion in powers of Ω_1

Bogoliubov coupled-cluster theory (BCC)

$\mathcal{W} = e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T}(\Omega_1)$



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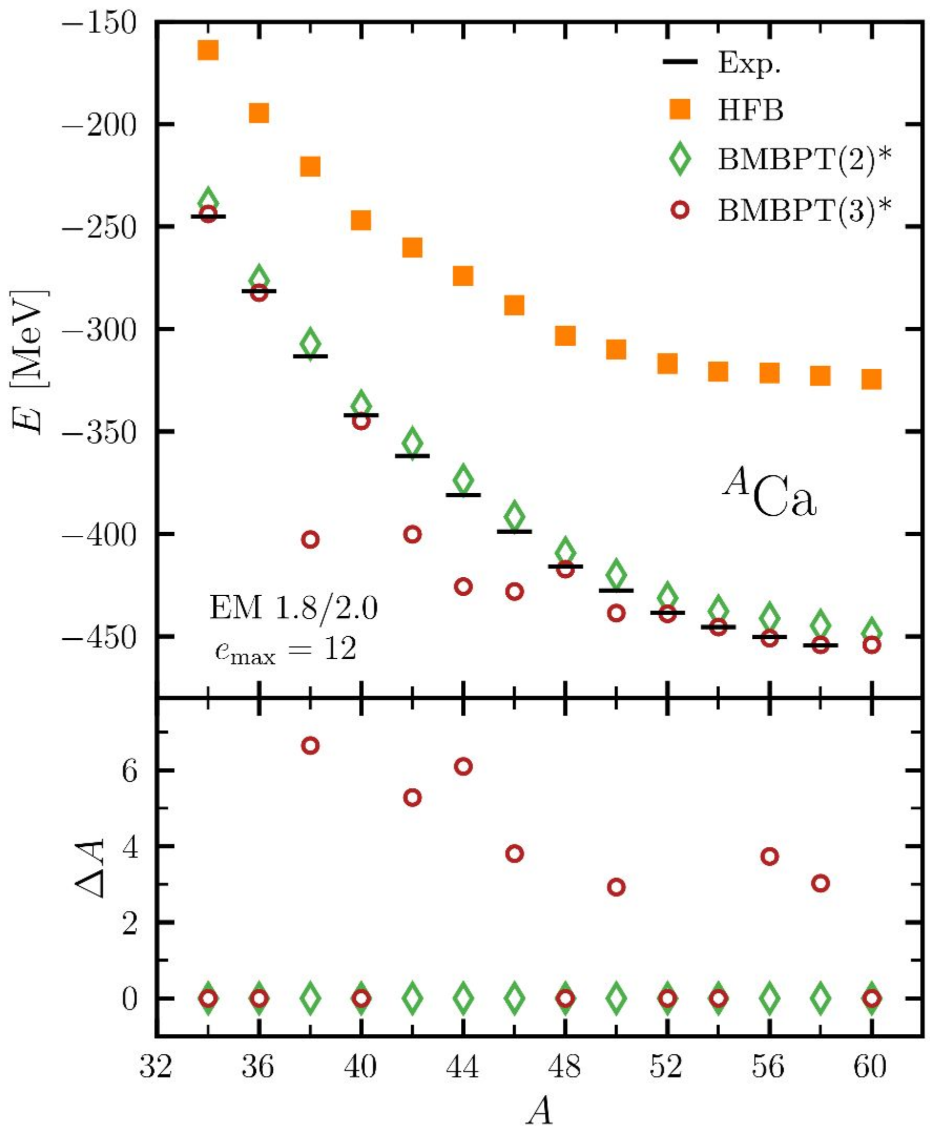
Bogoliubov many-body perturbation theory



- BMBPT(2 & 3) binding energy with EM(1.8/2.0) chiral EFT interaction
- BMBPT(2) gives satisfactory description
- BMBPT(3) flawed by large shift of average particle number

$\rightarrow$ U(1) breaking expansions require constraint on $\langle A \rangle$

BMBPT - particle number constraint

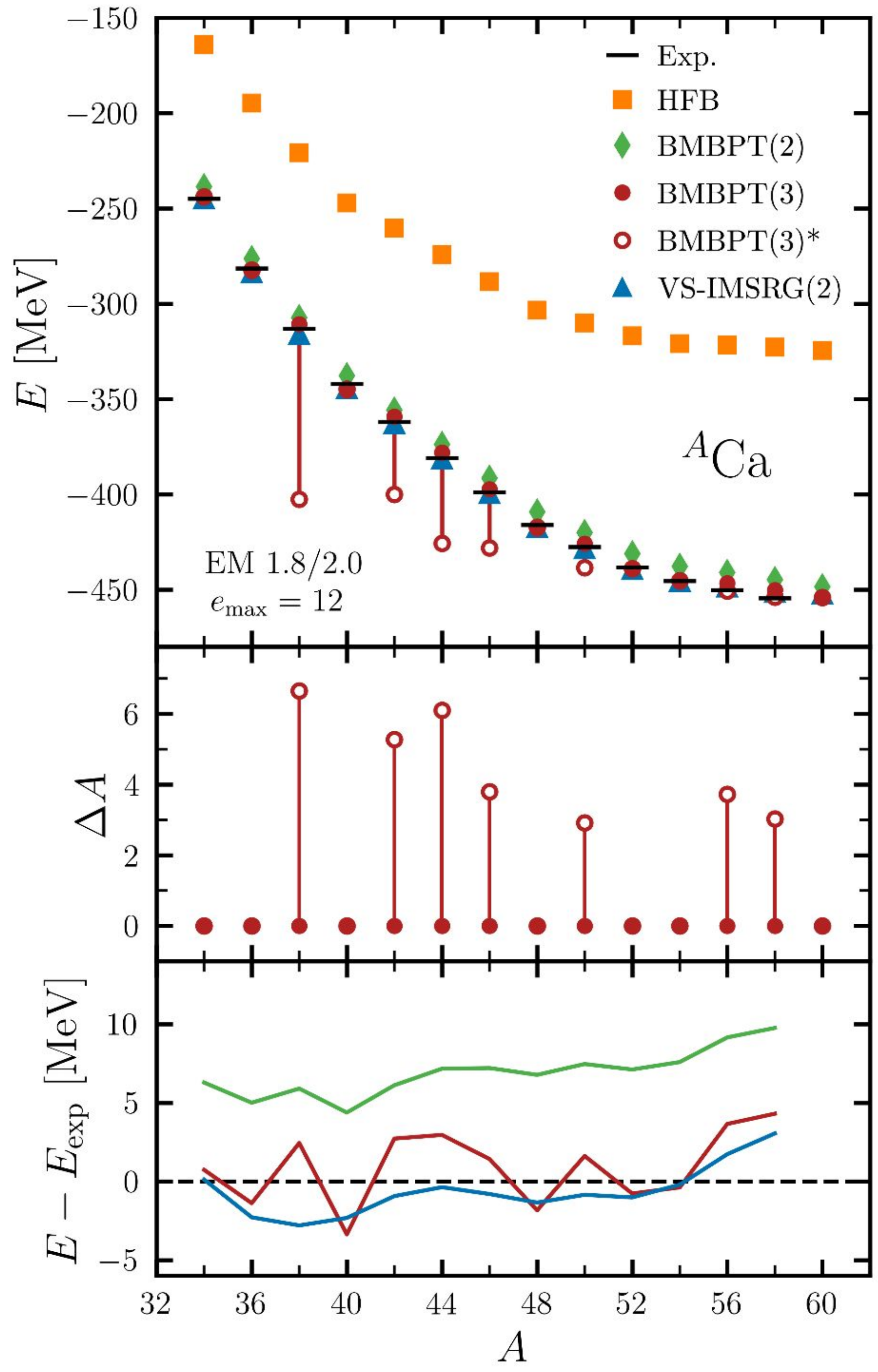
- Order-by-order particle number constraint
- Order-dependent chemical potential

$$\Omega^{(P)} = H - \lambda^{(P)} A \qquad \text{[@ BMBPT(P)]}$$

- $\lambda^{(P)}$ obtained as a root of an order P–1 polynomial equation

PD. T. Duguet, A. Tichai, EPJA **61** (2025).

- Constrained BMBPT(3) in good agreement with VS-IMSRG(2) & exp.



ULB

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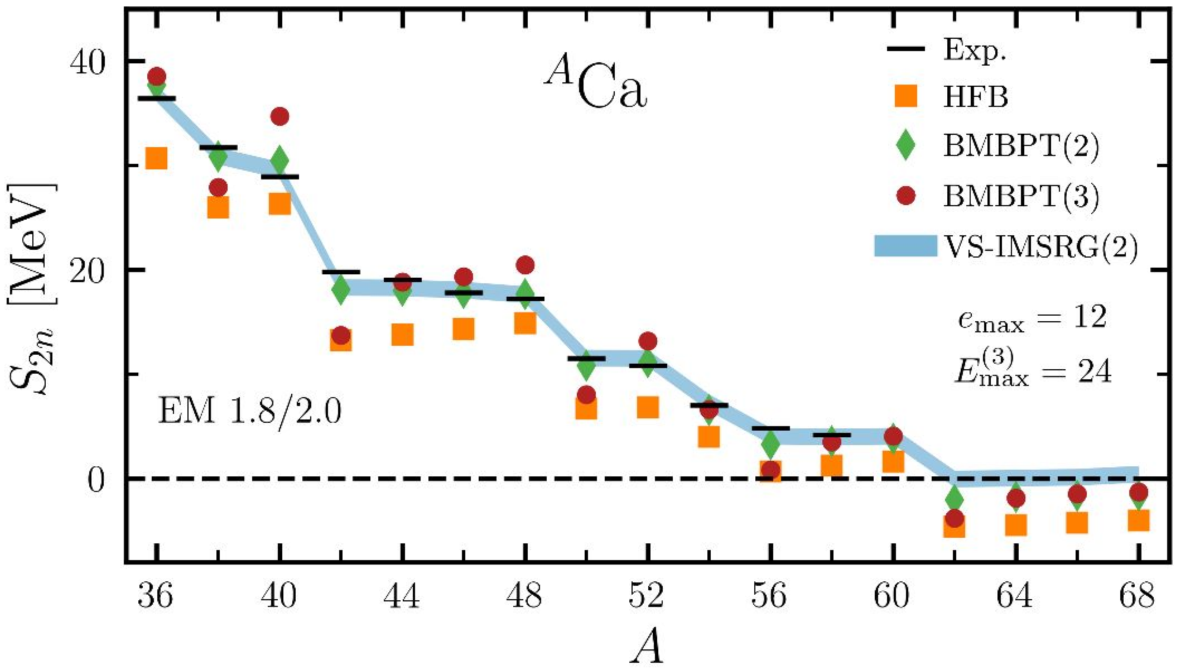

- Constrained BMBPT(3) in good agreement with VS-IMSRG(2) & exp.
- S_{2n} affected by strong sensitivity to isotope-dependent particle-number constraint

$\longrightarrow$ Non-perturbative expansion: Bogoliubov coupled-cluster theory

Content

Bogoliubov coupled-cluster (BCC) theory

Bogoliubov coupled-cluster theory (BCC)
$\mathcal{W} = e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T}(\Omega_1)$

A. Signoracci, et al. PRC **91** (2015).

Exponential ansatz: $|\Psi_0^A\rangle = e^{\mathcal{T}}|\Phi\rangle$

Quasi-particle cluster operator: $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \cdots$

BCCSD

$$\mathcal{T}_1 \equiv \frac{1}{2!}\sum_{k_1 k_2} t_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2}$$ [singles]

$$\mathcal{T}_2 \equiv \frac{1}{4!}\sum_{k_1 k_2 k_3 k_4} t_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$ [doubles]

$$\mathcal{T}_3 \equiv \frac{1}{6!}\sum_{k_1 k_2 k_3 k_4 k_5 k_6} t_{k_1 k_2 k_3 k_4 k_5 k_6} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} \beta^\dagger_{k_5} \beta^\dagger_{k_6}$$ [triples]

Quasi-particle excitation operators : mix of ordinary single-particle creation and annihilation operators $\beta^\dagger_k = \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p$

Excitation amplitudes : solutions of set of non-linear algebraic equations which must be solved iteratively

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Applying BCCSD: energies

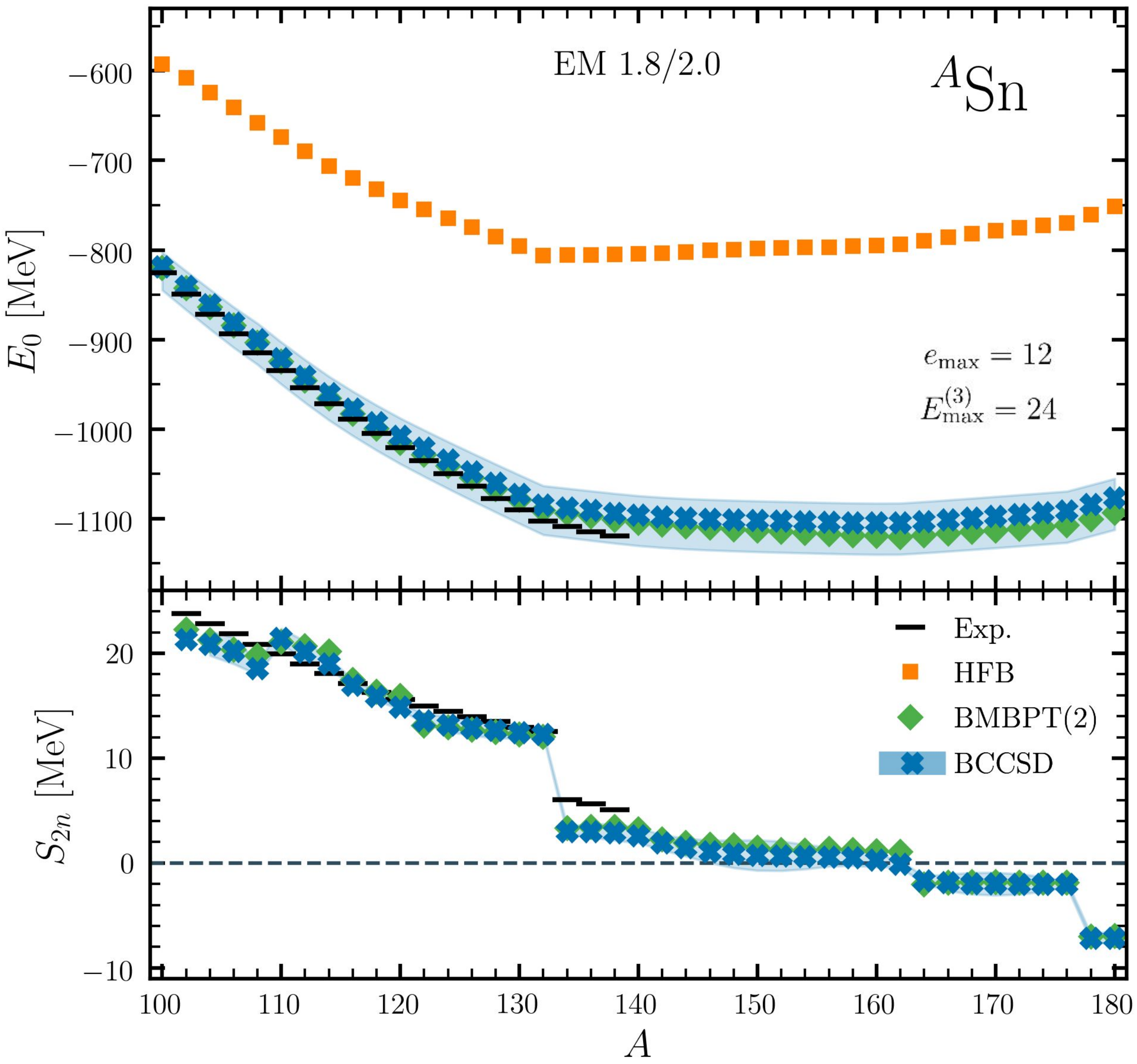
- Ground-state energy along Sn chain: ^{100}Sn – ^{180}Sn

  A. Tichai, PD, T. Duguet, PLB **851** (2024).

- BCCSD agrees with experiment within error band
  $\longrightarrow$ dominated by lacking triples excitations $\mathcal{T}_3$

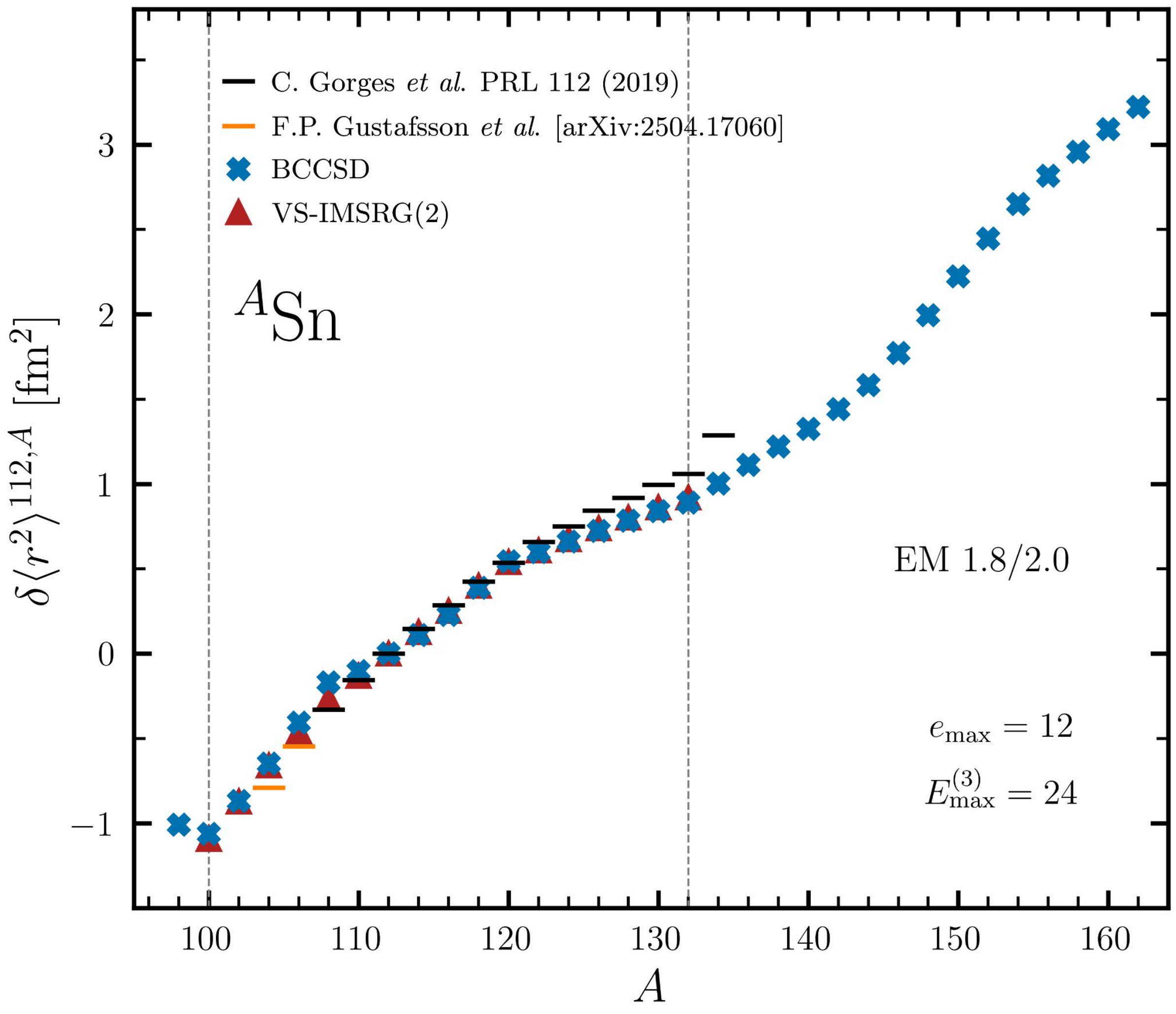
- BMBPT(2) performs well (soft interaction)

- Flat trend in S_{2n}
  $\longrightarrow$ drip line location is fine tuned



Applying BCCSD to tin: charge radii

- BCCSD radii in good agreement with VS-IMSRG(2)
  $\longrightarrow$ no core and scalable to large open shells

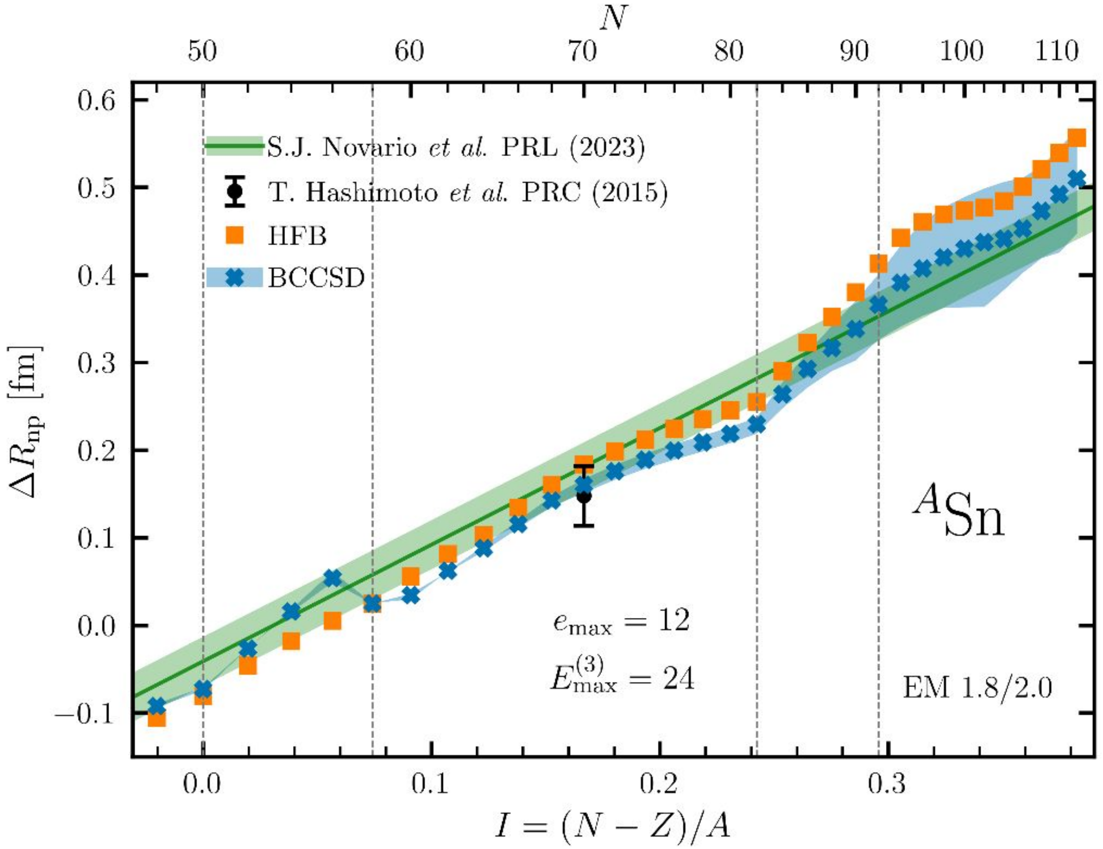


PD, T. Duguet, A. Tichai (unpublished)

Applying BCCSD to tin: neutron skin thickness

- BCCSD radii in good agreement with VS-IMSRG(2)
  ⟶ no core and scalable to large open shells

- Neutron skin thickness proportional to isospin asymmetry
  ⟶ studied for closed-shell nuclei using CC
  S.J. Novario et al., PRL **130** (2023)
  ⟶ confirmed in open-shell tin isotopes using BCC
  PD, PhD thesis (2024)



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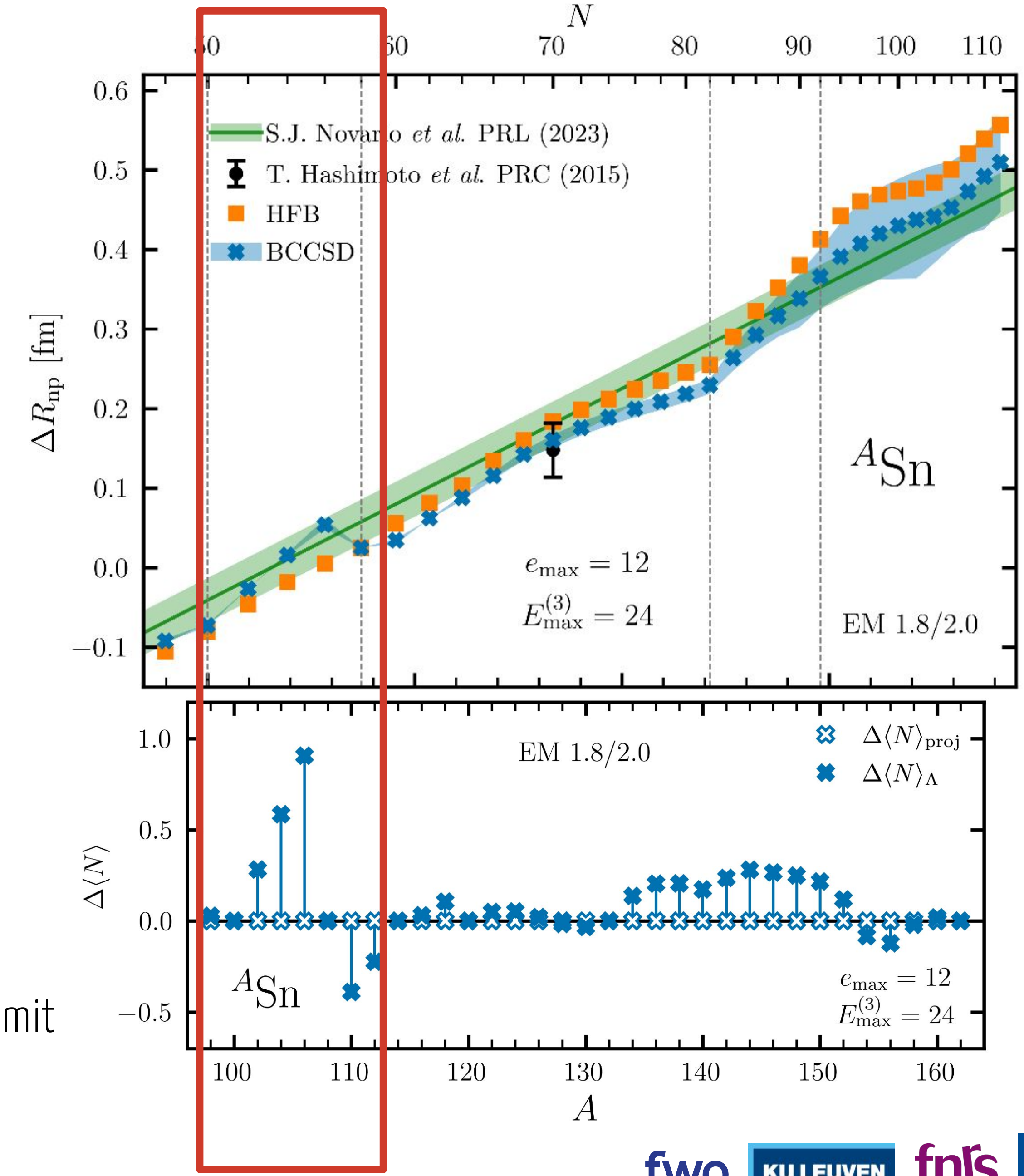
- Bump at N=56 due to residual neutron number shift ?

Now: 0= $\boxed{\Delta\langle N\rangle_{\text{proj}} \equiv \langle\Phi|N - \mathrm{N}_0|\Psi\rangle}$

$$\Delta\langle N\rangle_{\Lambda} \equiv \langle\Psi|N - \mathrm{N}_0|\Psi\rangle$$

Both yield 0 in the exact limit



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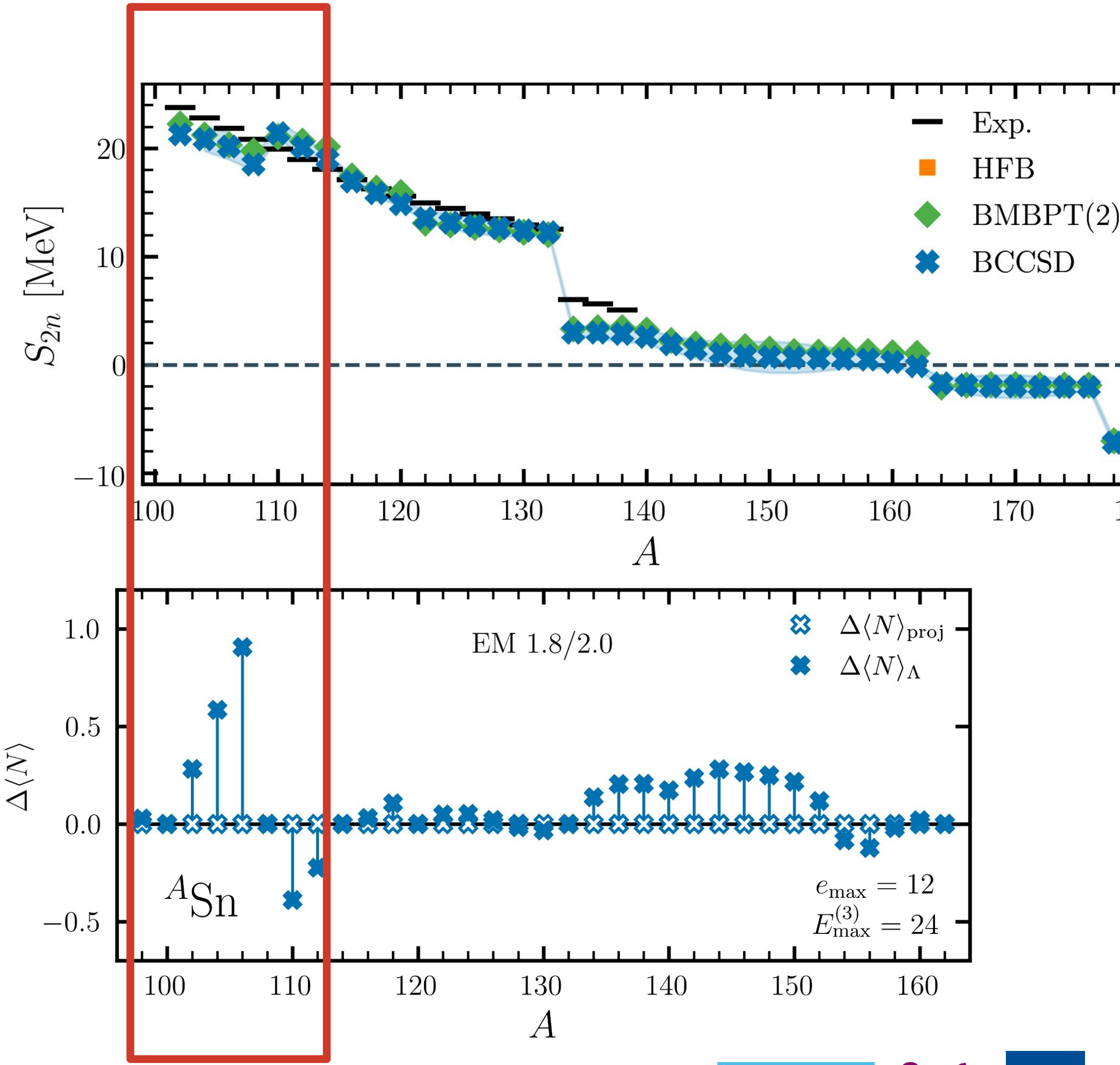
$$\left.\begin{aligned}\Delta\langle N\rangle_{\mathrm{proj}} &\equiv \langle\Phi|N - \mathrm{N}_0|\Psi\rangle \\ \text{Goal: } 0 = \boxed{\Delta\langle N\rangle_{\Lambda} \equiv \langle\Psi|N - \mathrm{N}_0|\Psi\rangle}\end{aligned}\right\}$$ Both yield 0 in the exact limit



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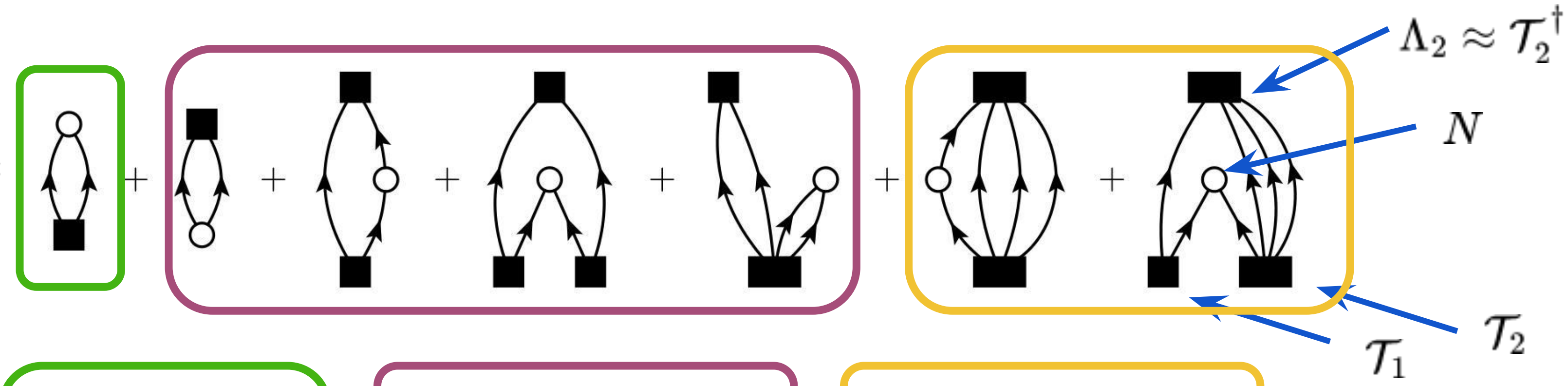
Particle-number constraint in BCCSD

$$\Delta\langle N\rangle_\Lambda \equiv \langle\Psi|N-\mathrm{N}_0|\Psi\rangle =$$



$$= \underbrace{\boxed{\langle\Phi|N-\mathrm{N}_0|\Psi\rangle}}_{\Delta\langle N\rangle_{\mathrm{proj}}} + \boxed{\langle\Phi|\Lambda_1(N-\mathrm{N}_0)|\Psi\rangle} + \boxed{\langle\Phi|\Lambda_2(N-\mathrm{N}_0)|\Psi\rangle}$$

- Adjust the chemical potential at each iteration of the cluster amplitude equation: $\Omega^{(i)} = H - \lambda^{(i)} A$
- Update is <u>linear</u> in $\boldsymbol{\Omega}$: $\mathcal{T}^{(i+1)} = I(\mathcal{T}^{(i)}, \Omega^{(i)}) = I(\mathcal{T}^{(i)}, H) + \lambda^{(i)} f(\mathcal{T}^{(i)}, N)$

$\longrightarrow$ constraining $\Delta\langle N\rangle_{\mathrm{proj}}$ is *trivial* : <u>one</u> additional update of <u>singles</u> at each BCC iteration

$\longrightarrow$ constraining $\Delta\langle N\rangle_\Lambda$ is *slightly more involved* : <u>several</u> additional updates of <u>singles</u> at each BCC iteration

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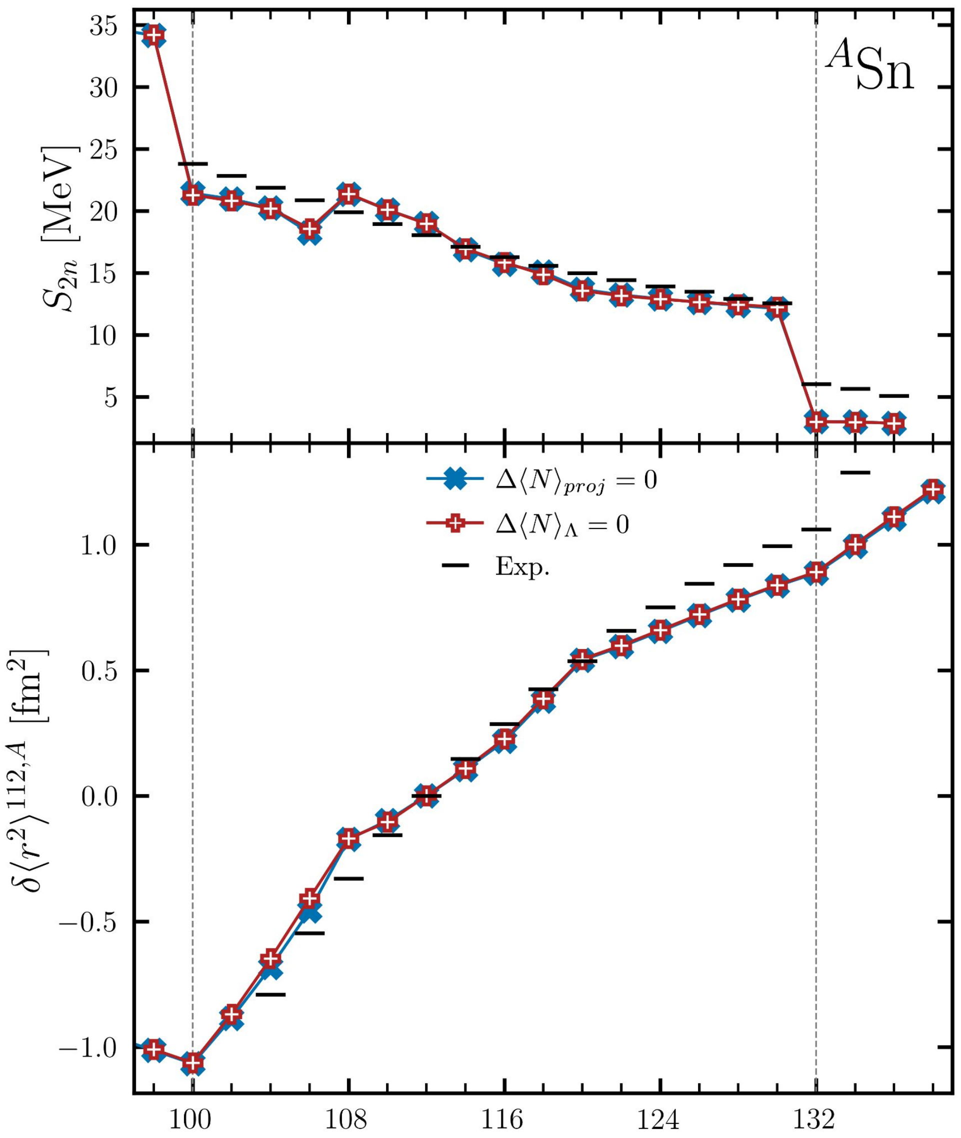
Particle-number constraint in BCCSD

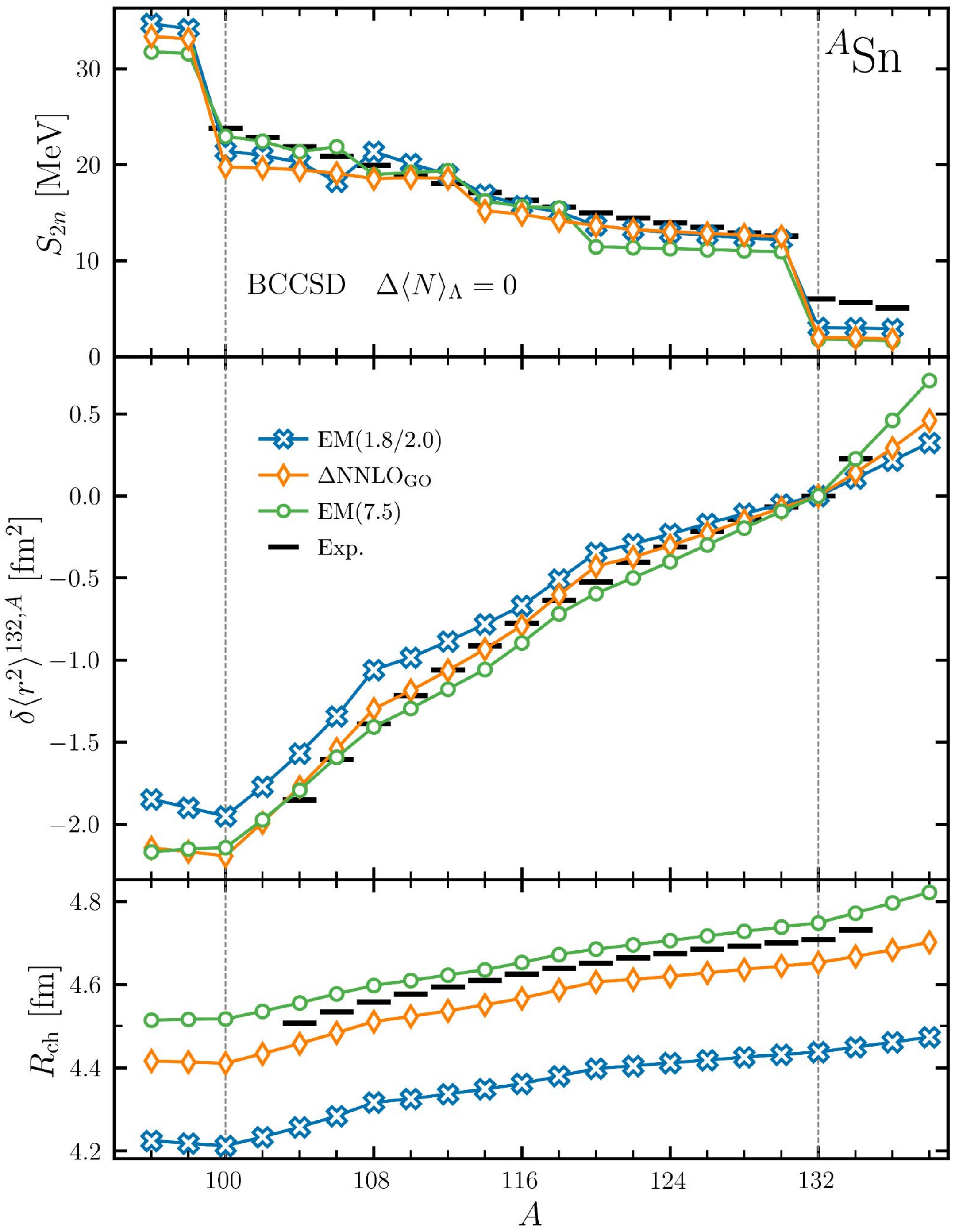
- Constraining $\Delta\langle N\rangle_\Lambda$ has <u>very little effect</u> on the energy and radius

  $\longrightarrow$ dependence on the interaction?

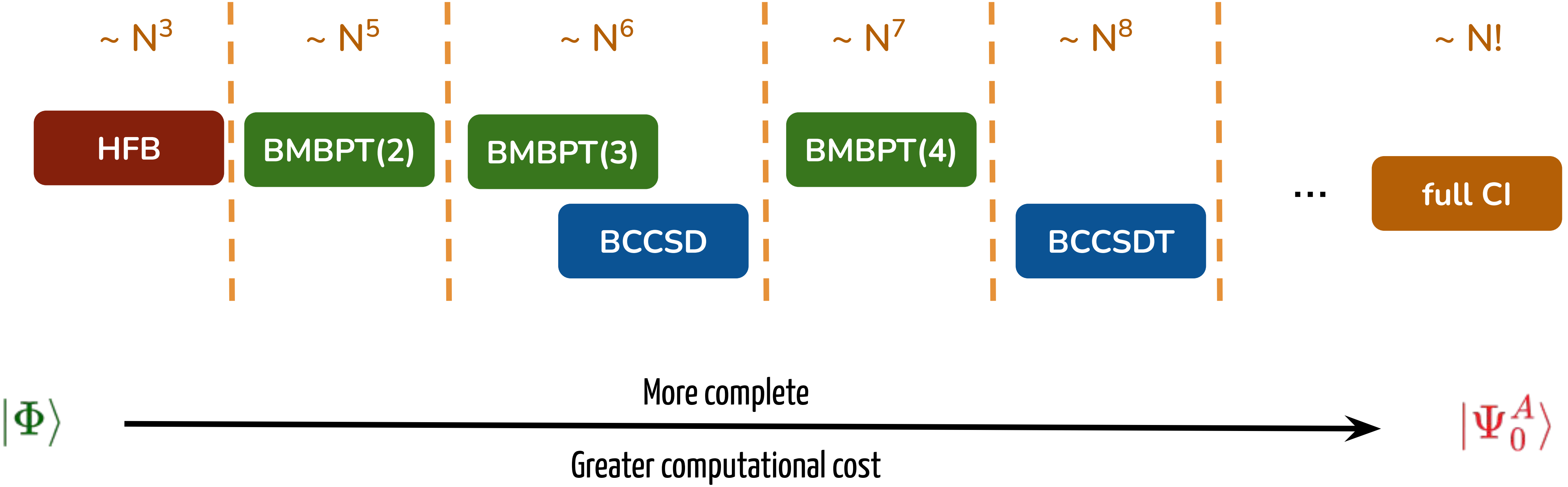


Particle-number constraint in BCCSD

- Constraining $\Delta\langle N\rangle_\Lambda$ has <u>very little effect</u> on the energy and radius
  $\longrightarrow$ dependence on the interaction?
- BCCSD results for EM(1.8/2.0), ΔNNLO$_{GO}$ and EM(7.5)
- Kink at N = 82 shell closure well reproduced by the EM(7.5) interaction



Towards a more complete account of correlations



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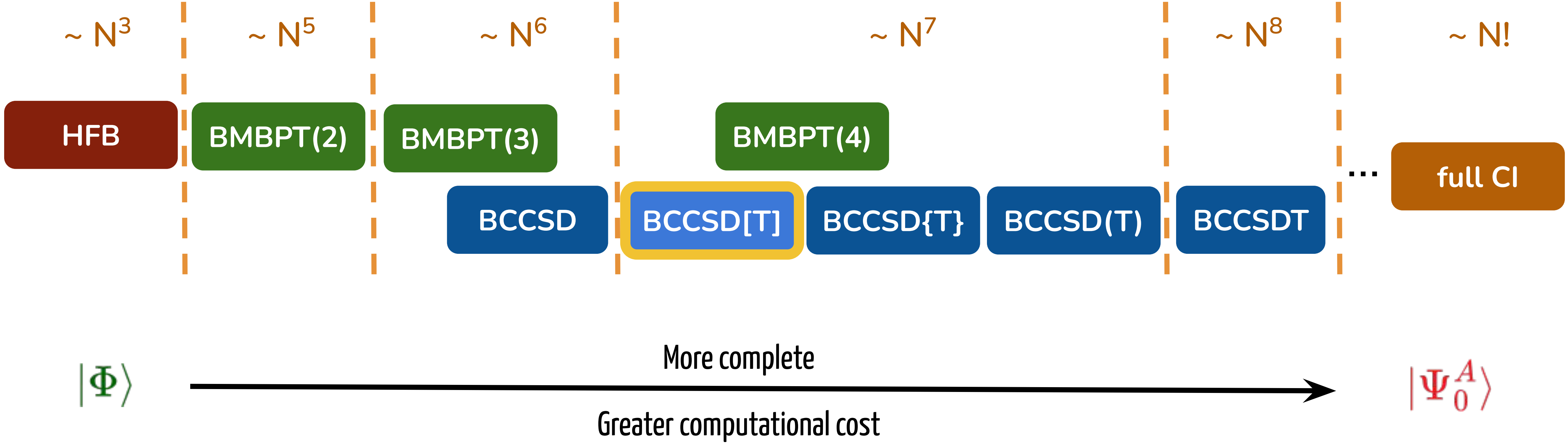
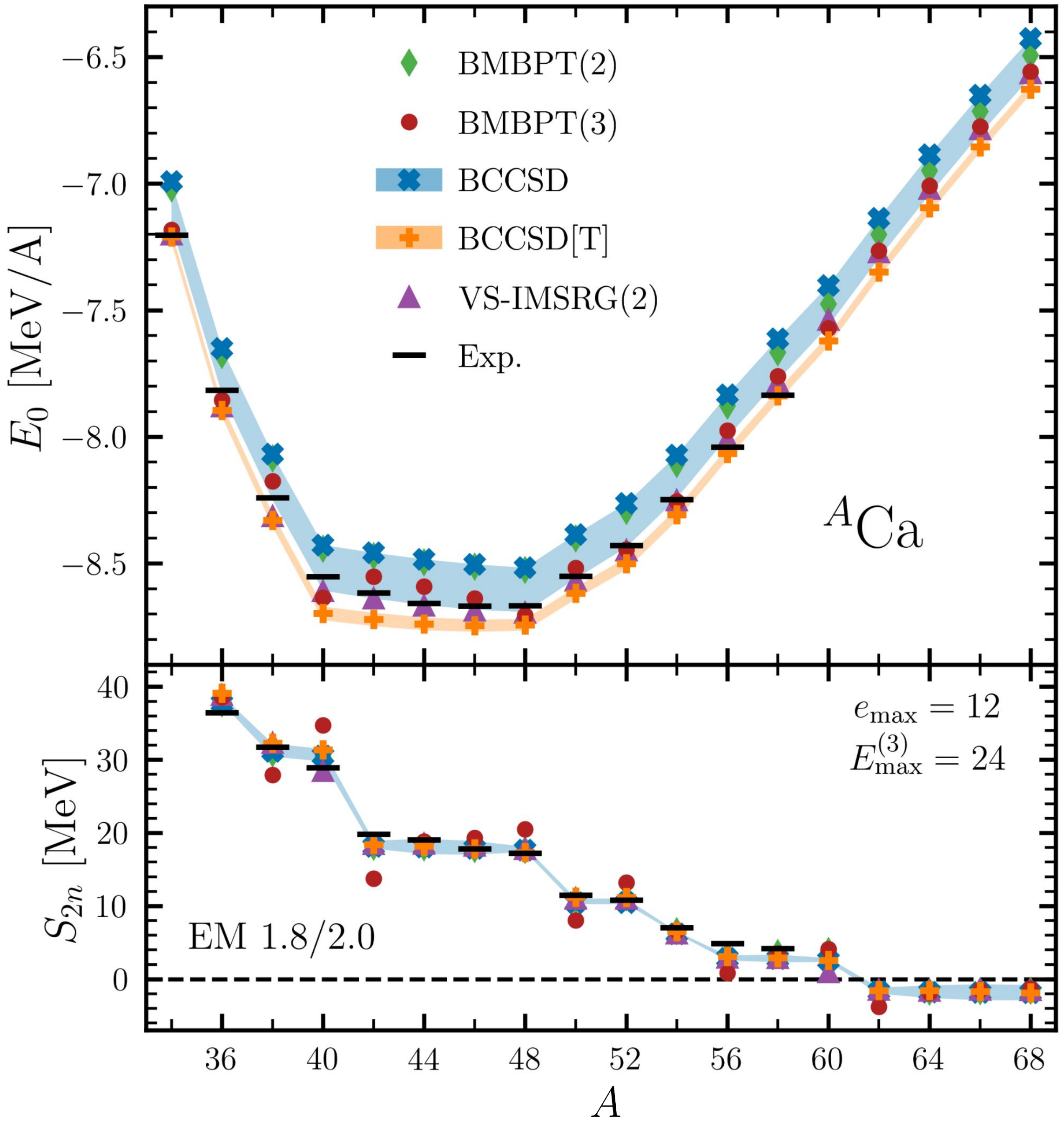


First application of BCCSD[T]: calcium energies

U. Vernik, PD, T. Duguet, A. Tichai (unpublished)

- BCCSD[T] prediction in good agreement with VS-IMSRG(2)
- Sub-percent accuracy on binding energies for Ca and Ni
- Further improvement expected from Λ-BCCSD(T)

⟶ Application of BCCSD[T] for Sn isotopes are underway



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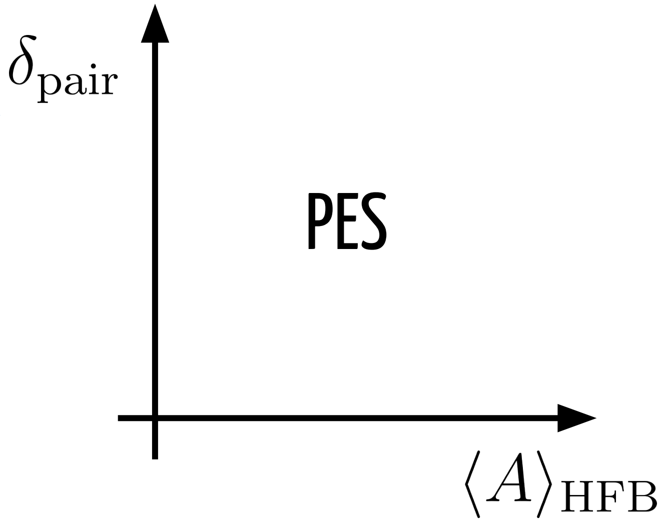
Pairing potential energy surface

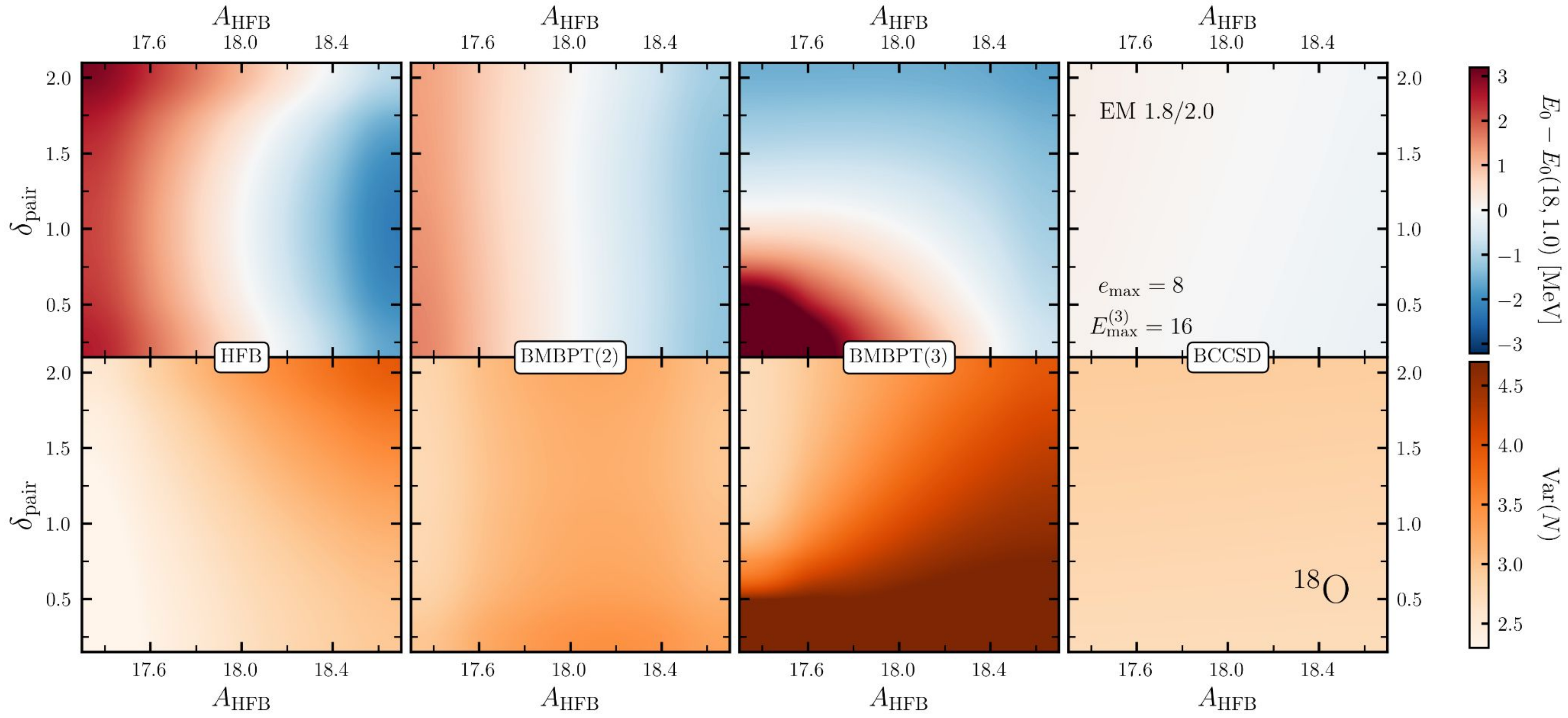


Scaling the HFB pairing field:

$$\begin{pmatrix} h - \lambda & \delta_{\text{pair}} \times \Delta \\ -\delta_{\text{pair}} \times \Delta^* & -(h-\lambda)^* \end{pmatrix}$$

$$\rightarrow \delta_{\text{pair}} \sim \text{Var}(A)_{\text{HFB}}$$

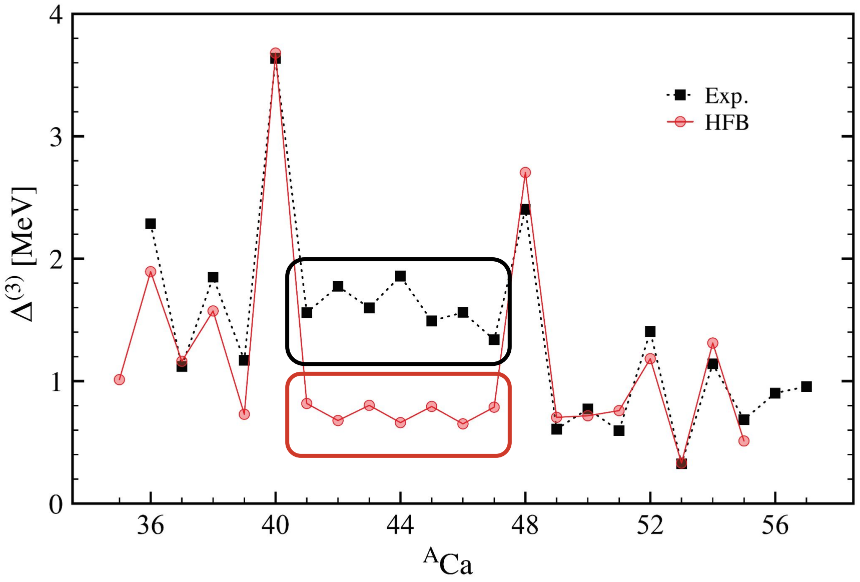
Pairing potential energy surface



→ In BCC: $e^{\mathcal{T}_1}$ acts as Thouless transformation absorbing the reference state dependence

T. Duguet, introductory lecture, last week

Ab initio sHFB calculations in Ca isotopes



Only 45% of experimental $\Delta^{(3)}$ in $f_{7/2}$ shell

→Consistent with semi empirical HFB with Skyrme mean-field…
…but even slightly lower (exponential sensitivity to "m*")

→Even smaller % in Sn isotopes **Talk by P. Demol**

Despite a^{1S0}=-18.5 fm and large BCS gap in INM

→Too low density of states from the ab initio HF field?

→ Anti-pairing from spin-orbit in finite nuclei Bertsch, Baroni, PRC (2009)

Similar results for other χ-EFT (based) interactions

→See **Talk by A. Ekström** for proper sensitivity analysis

Oscillation inverted… wrong curvature of the energy!

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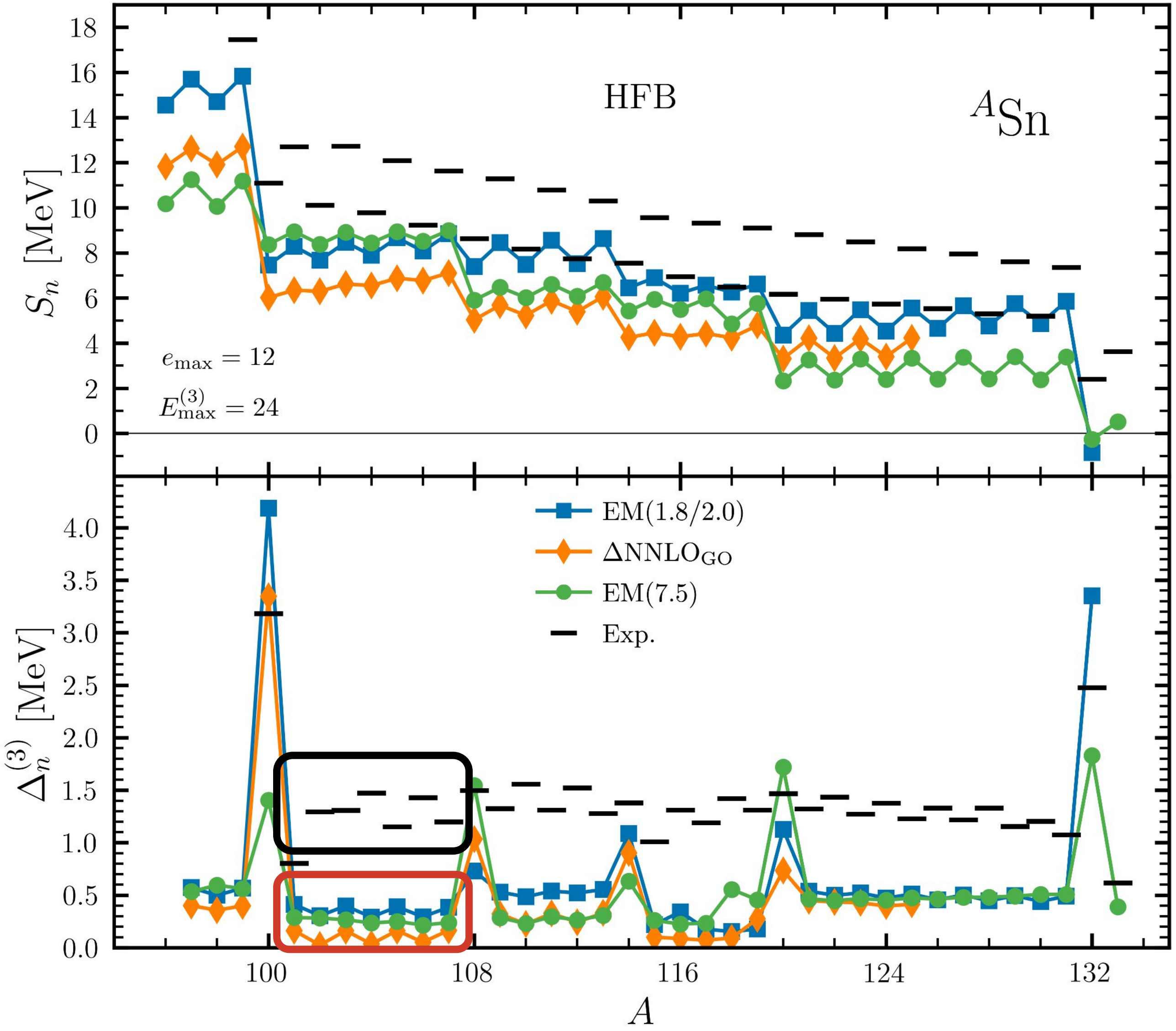
Static pairing: odd-even scattering at mean-field level in Sn isotopes



EM(1.8/2.0) : ~ 27 %

ΔNNLO$_{GO}$: ~ 8 %

EM(7.5) : ~ 19 %

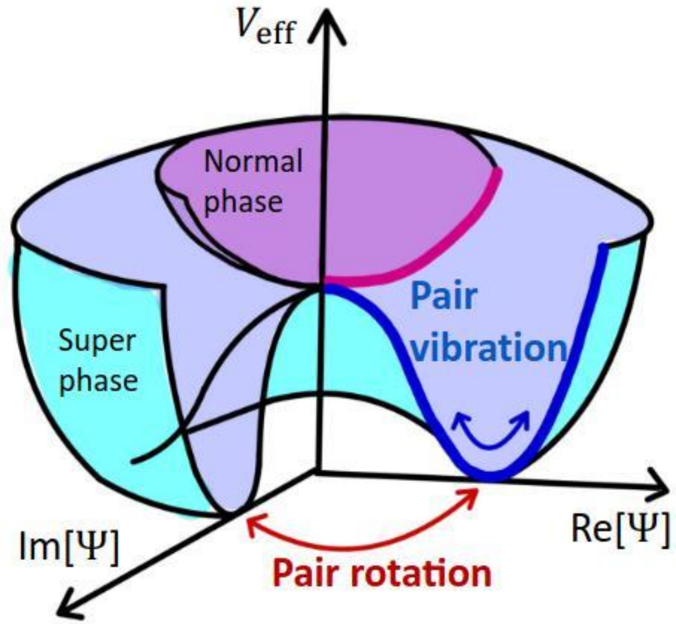
- Motivates the extension BCC to odd isotopes

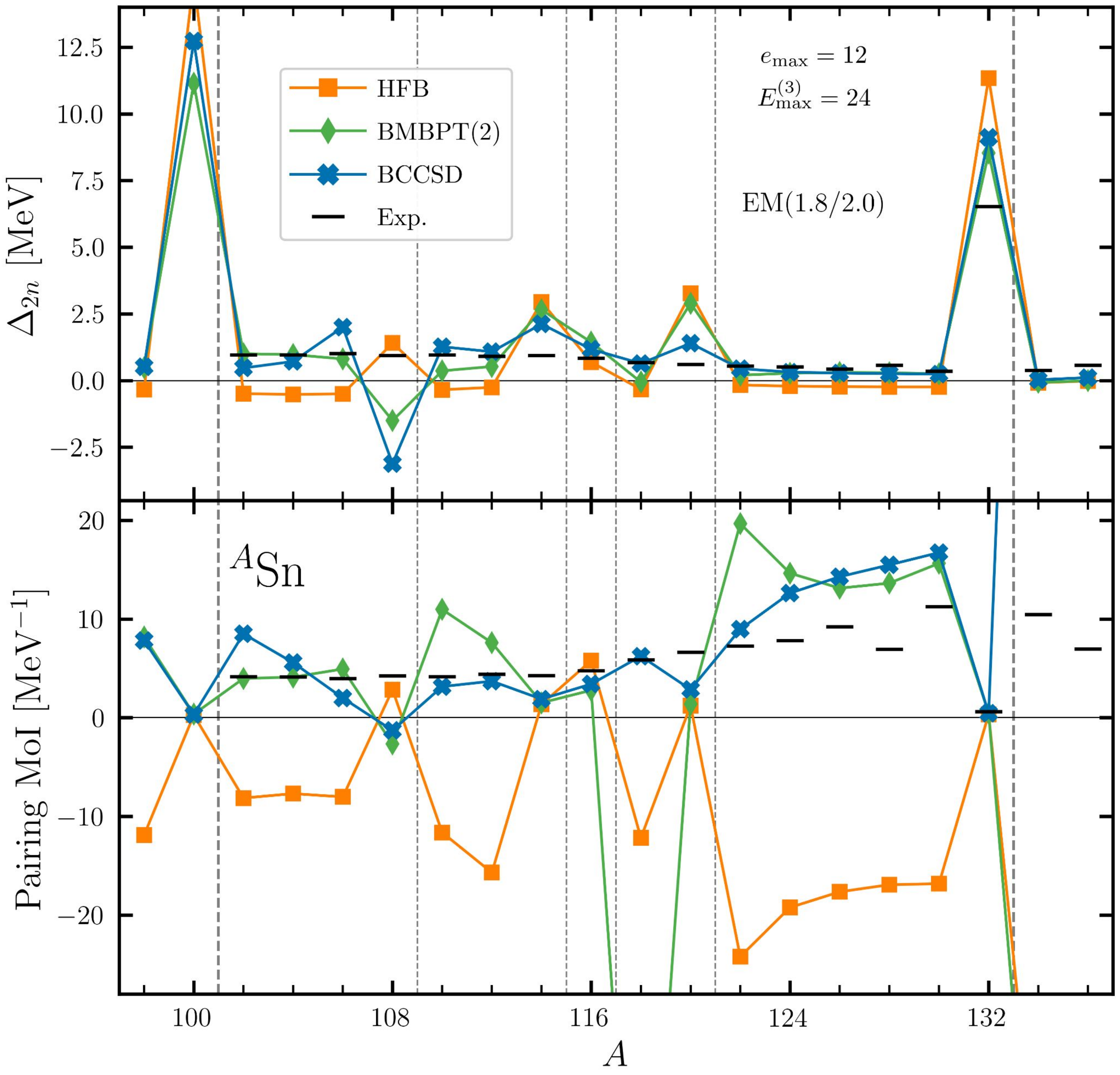
  ⟶ requires equation-of-motion (EOM) techniques

Dynamic pairing in Sn isotopes

Pairing moment of inertia (MoI):

$$\mathcal{I}(N) = \frac{4}{E(N-2) - 2E(N) + E(N+2)}$$





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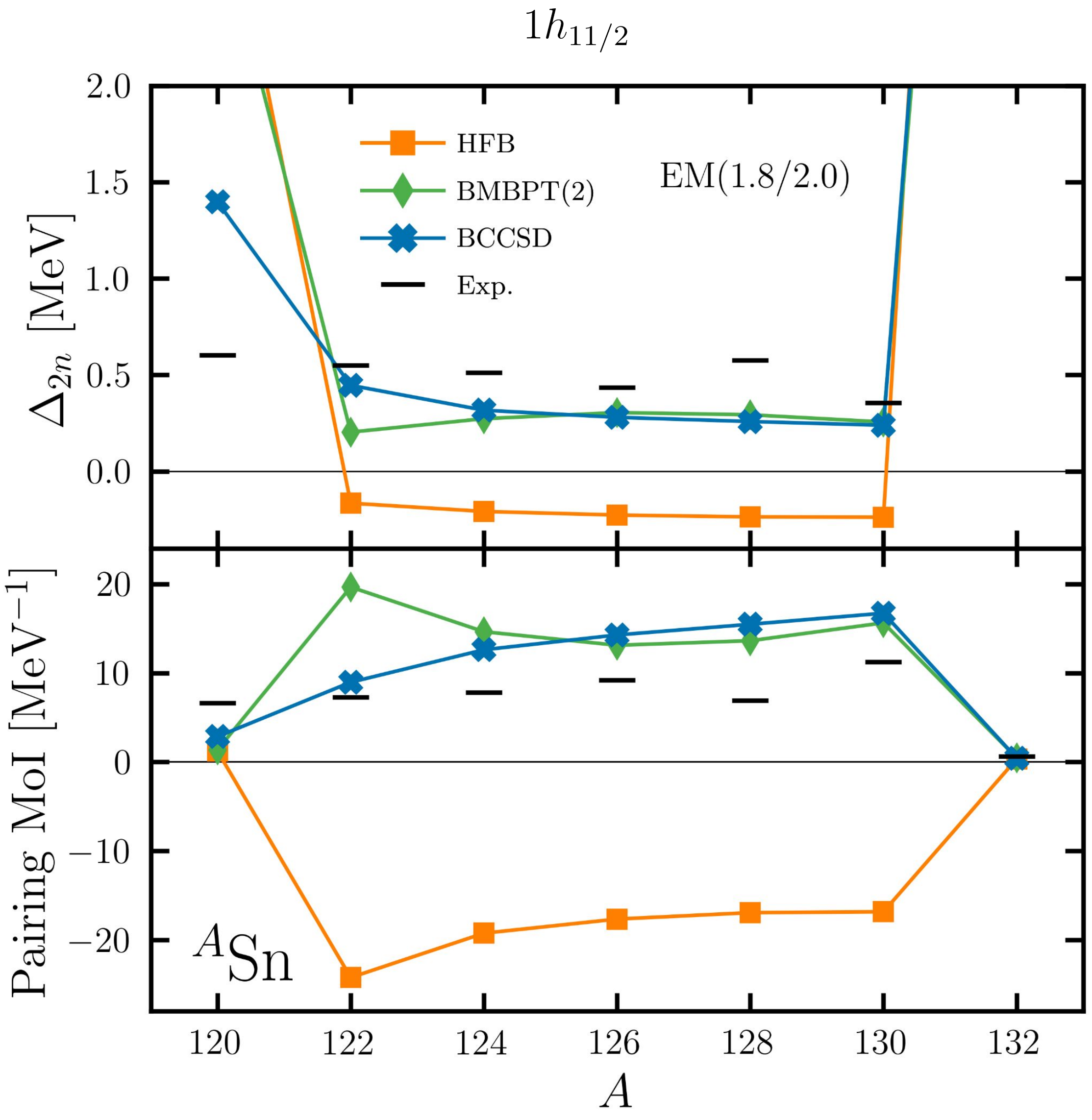
- HFB predicts <u>negative</u> Δ_{2n} and pairing MoI
  $\longrightarrow$ E is concave rather than convex

- Correlations captured by BCCSD turn Δ_{2n} <u>positive</u>

A. Scalesi et al. EPJA **60** (2024)



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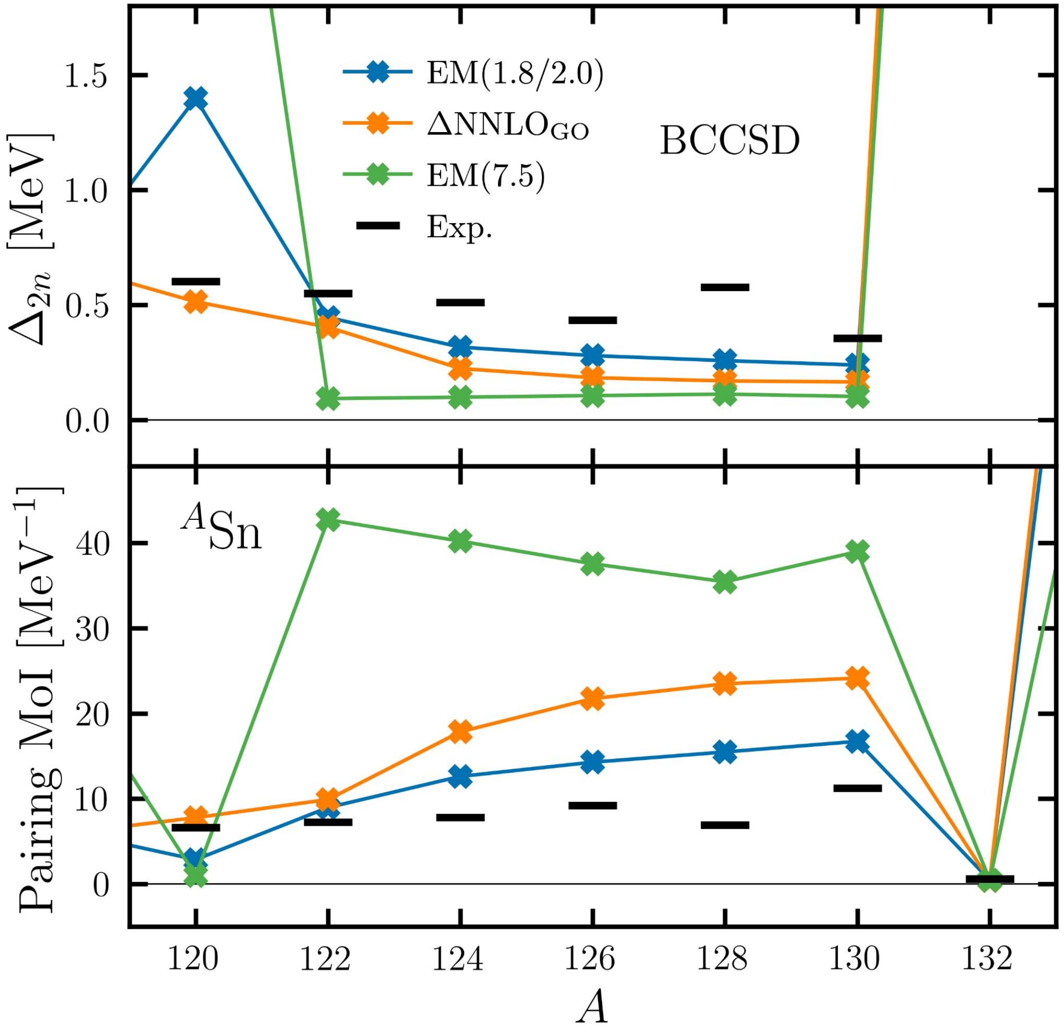
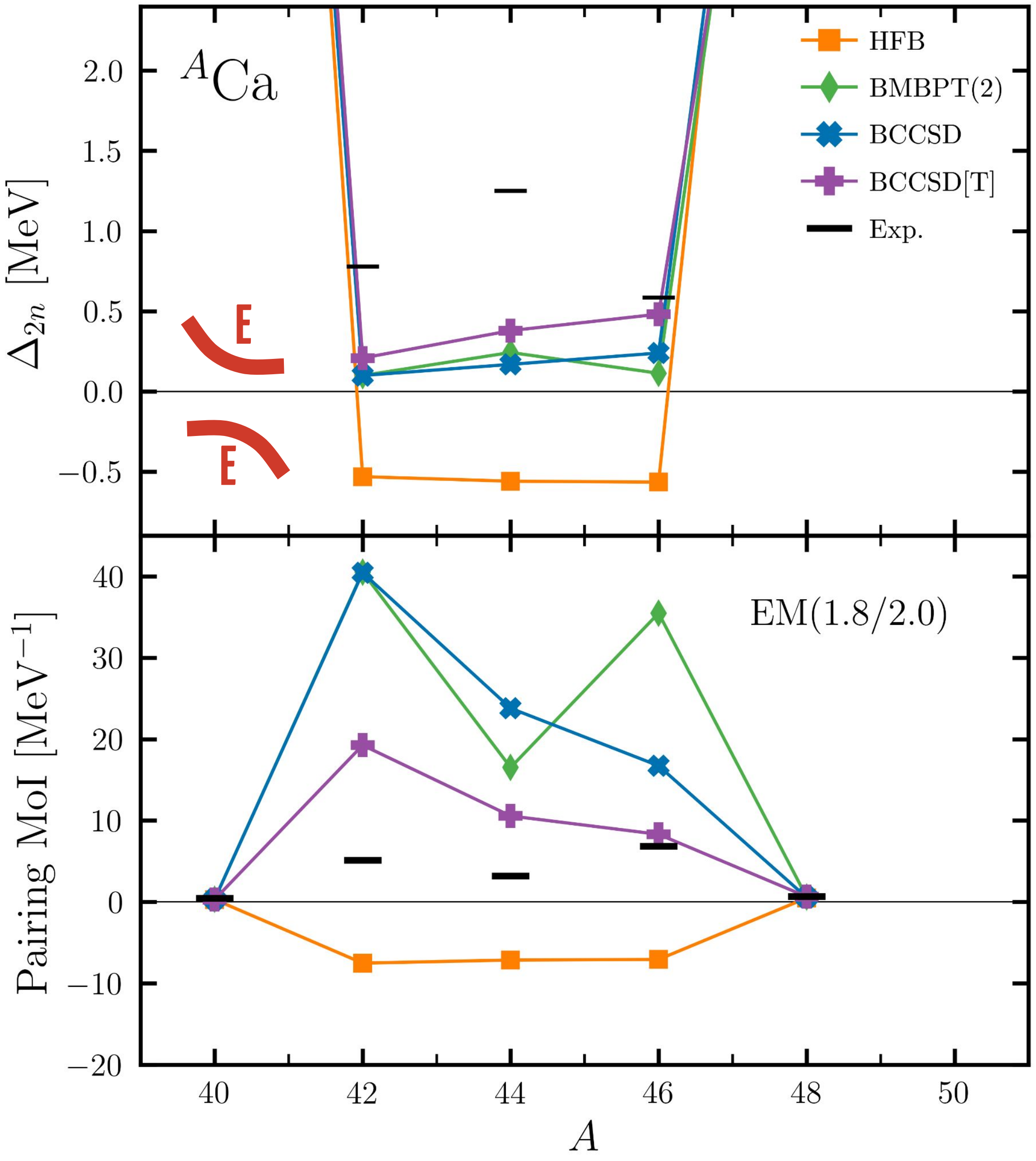
$\longrightarrow$ True for several interactions: EM(1.8/2.0), ΔNNLO$_{GO}$, EM(7.5)



Dynamic pairing in Ca isotopes

- BCCSD[T]: inclusion of triples further improve Δ_{2n} and pairing MoI

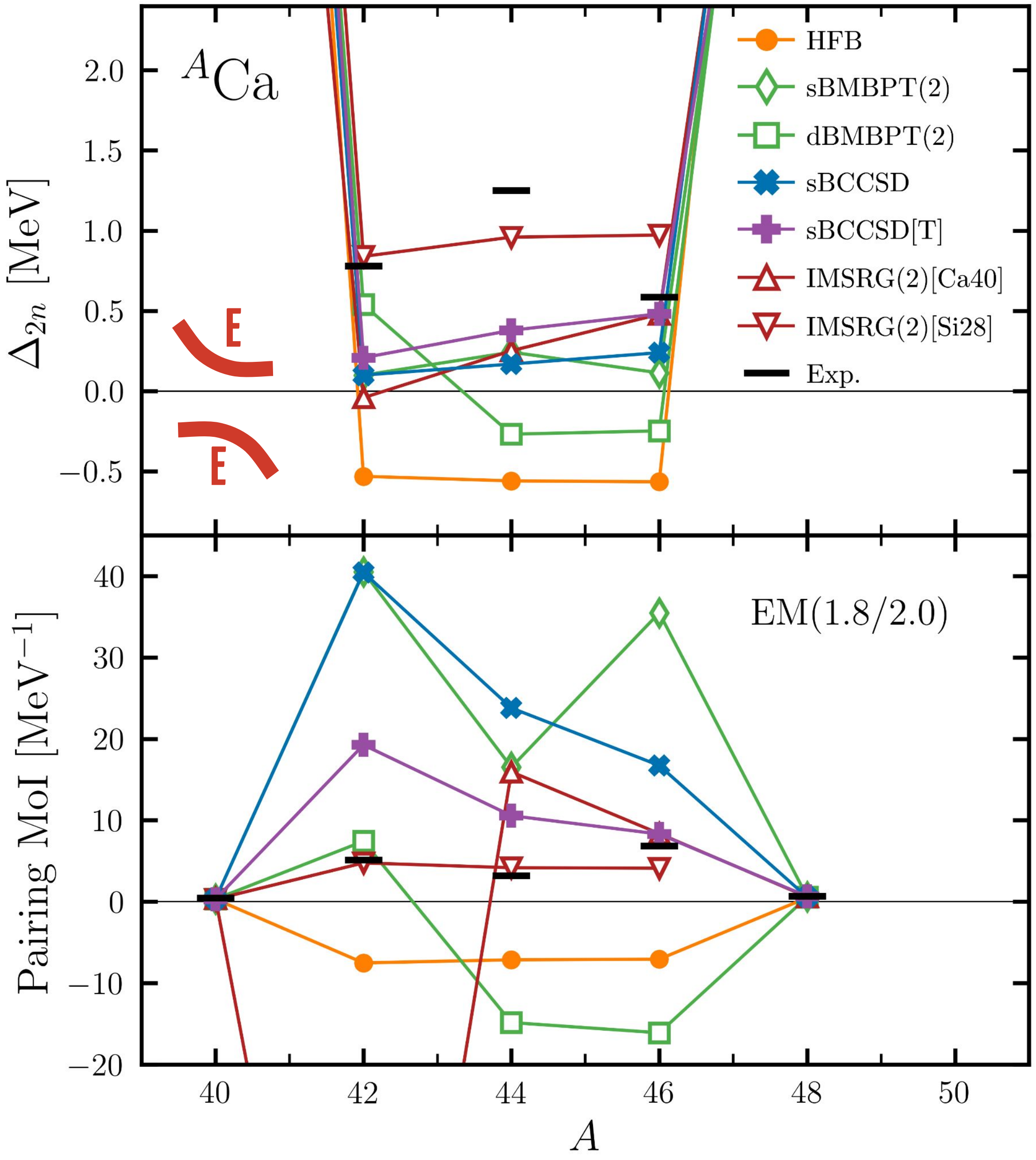


A. Scalesi et al. EPJA **60** (2024)

Dynamic pairing in Ca isotopes

- BCCSD[T]: inclusion of triples further improve Δ_{2n} and pairing MoI
- Comparing several complementary many-body methods
  - VS-IMSRG(2) with Si28 core reproduces Δ_{2n} the best

    ... but VS-IMSRG(3) worsens description again ...



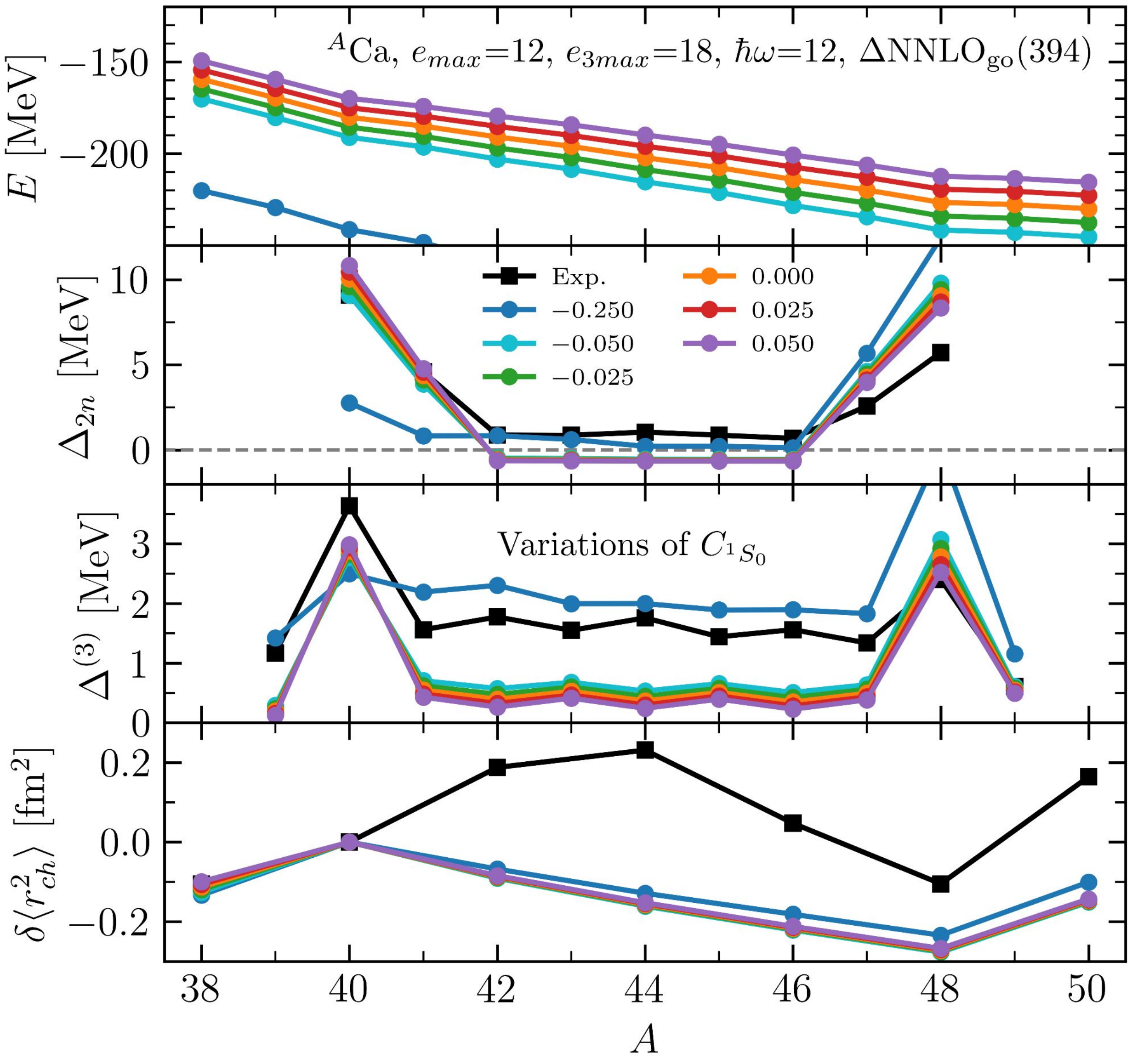
More things to learn: boosting the pairing

- Inspired by Andreas Ekström's presentation last week

  $\longrightarrow$ repeat by simple δ_{pair} scaling of HFB pairing field

$$\begin{pmatrix} h-\lambda & \delta_{\mathrm{pair}}\times\Delta \\ -\delta_{\mathrm{pair}}\times\Delta^* & -(h-\lambda)^* \end{pmatrix}$$

Courtesy of: A. Scalesi, A. Ekström



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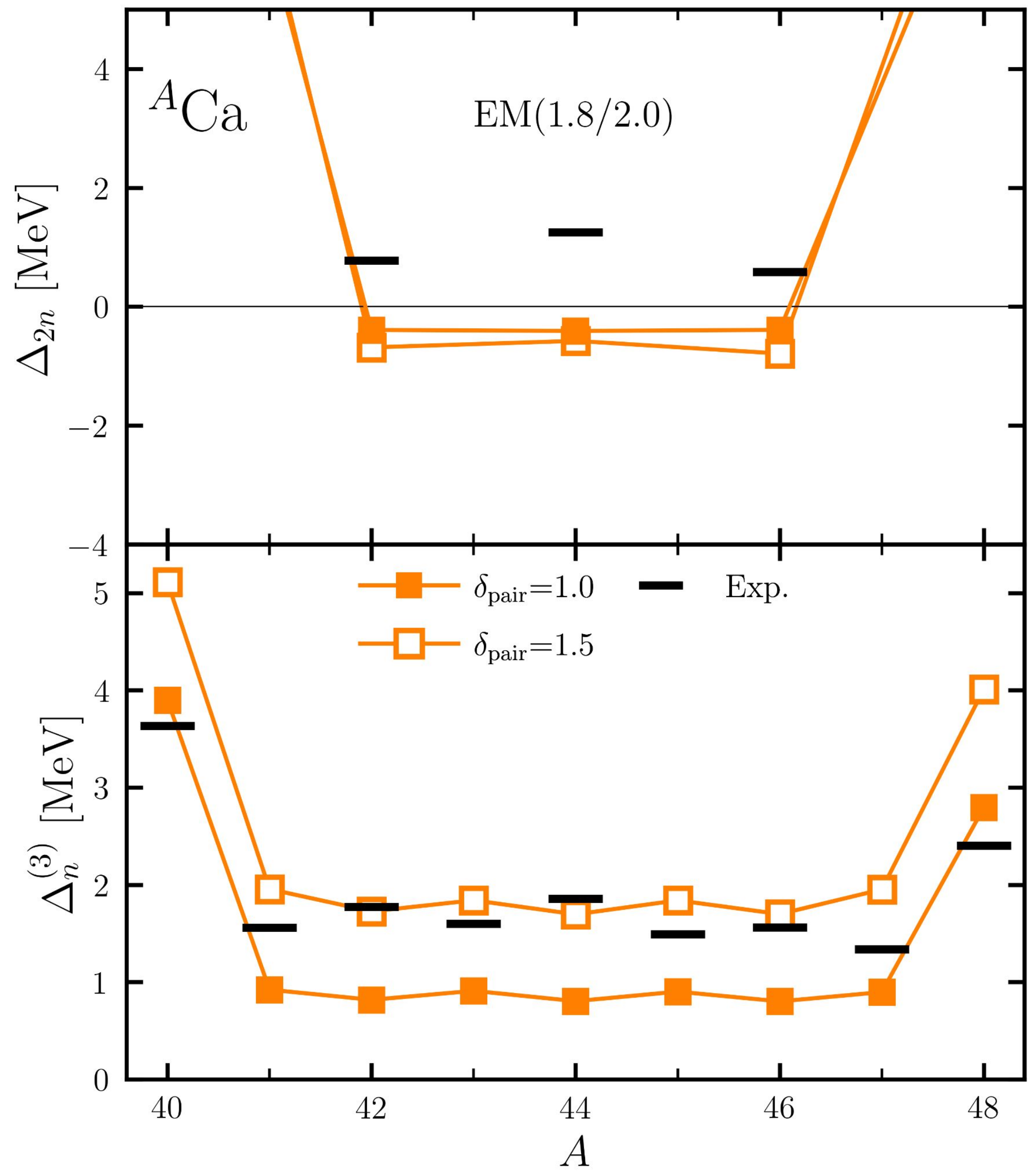
- Boosting HFB pairing field by 50% brings $\Delta_n^{(3)}$ to exp: ~2 MeV
  … BUT Δ_{2n} barely affected, even slight negative shift (!)



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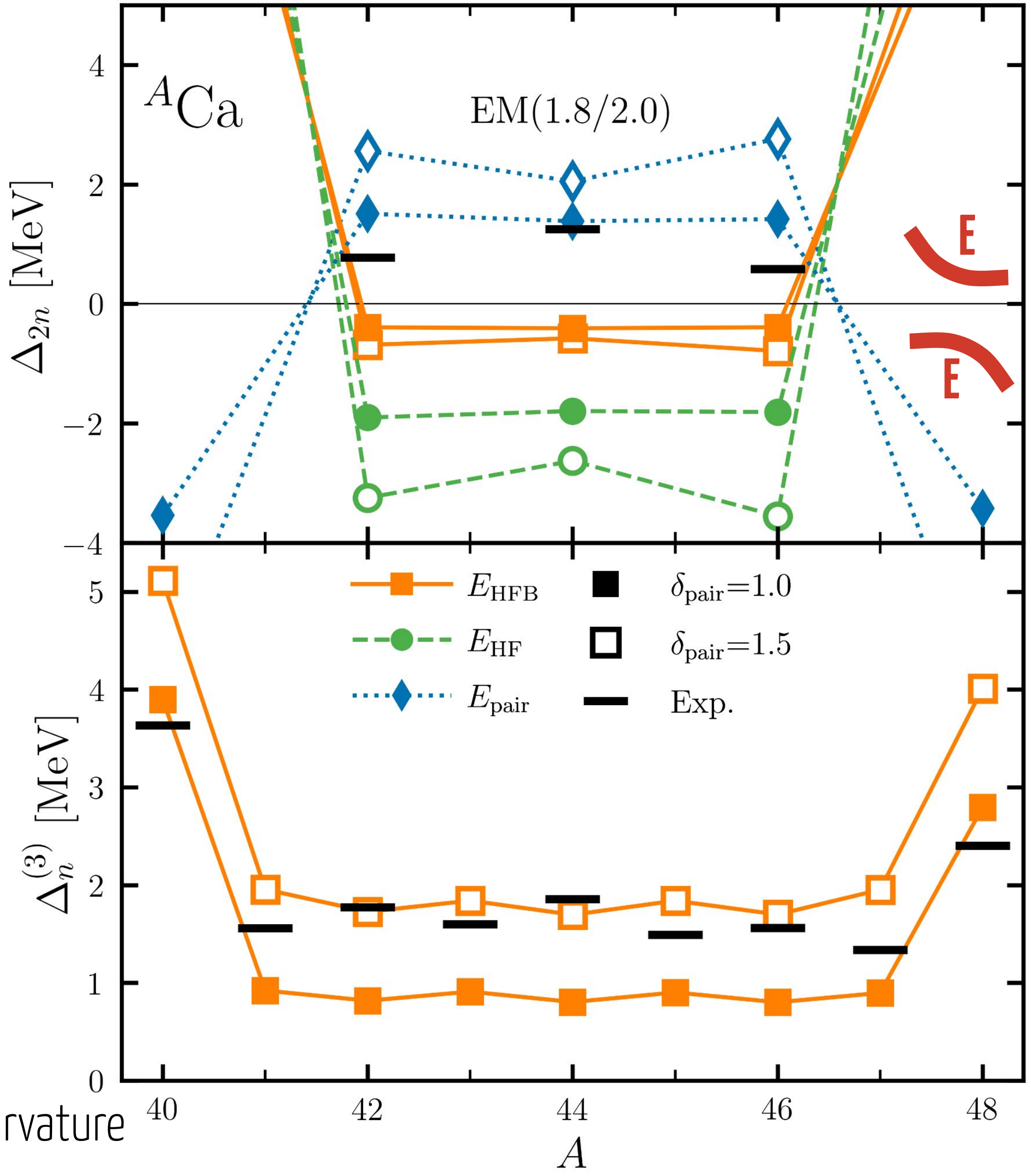
- Breaking down the HFB energy into HF and pairing energies

$$E_{\text{HFB}} = E_{\text{HF}} + E_{\text{pair}}$$

  $\longrightarrow$ compensation of normal and anomalous contribution to the curvature



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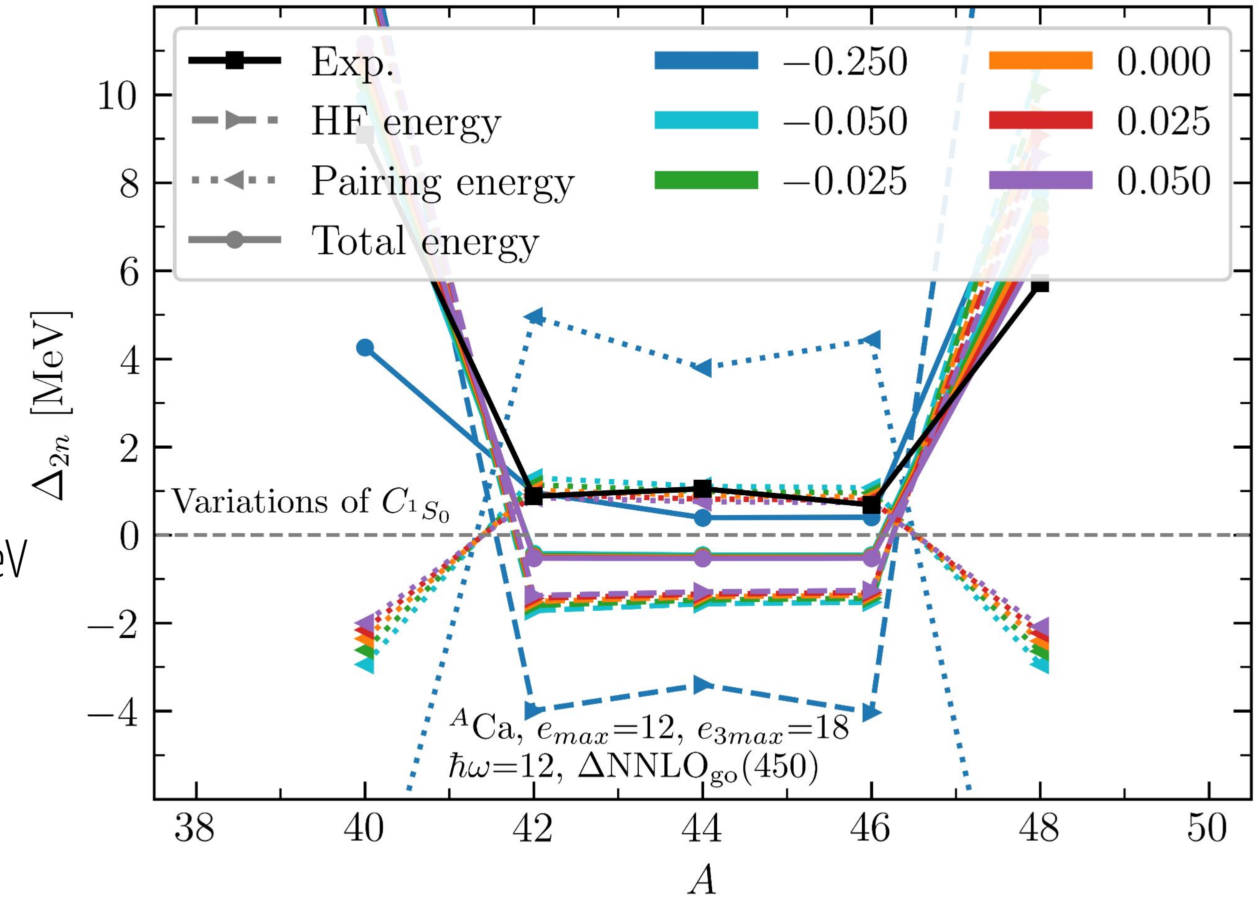
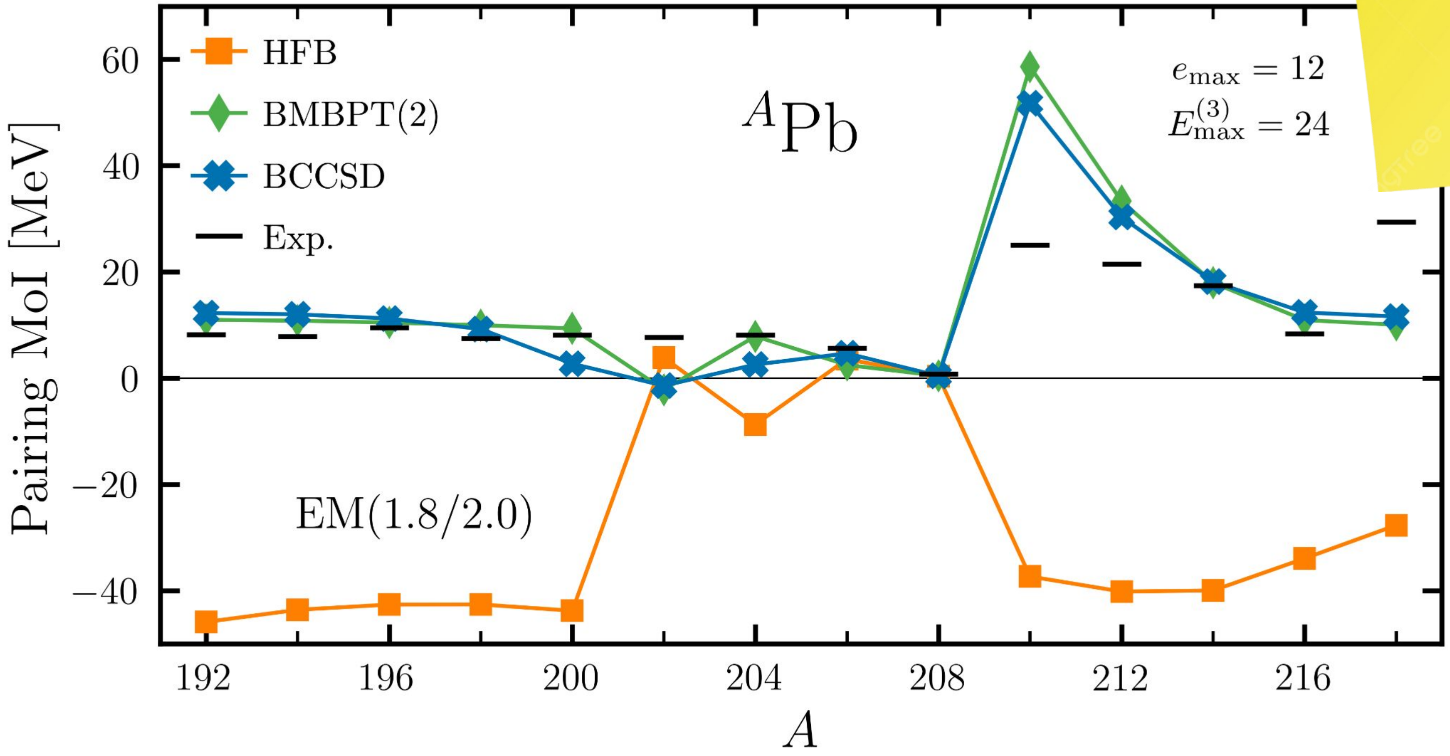
  $\longrightarrow$ compensation of normal and anomalous contribution to the curvature

- <u>Very new results from A. Scalesi</u>: similar observation with $C_{^1S_0}$ scaling
  $\longrightarrow$ at extreme scaling (blue), positive pairing curvature dominates negative HF curvature

<u>Courtesy of: A. Scalesi, A. Ekström</u>



Teaser for upcoming BCC applications



Side note

- "Only" eMax 12

TODO: error analysis

Conclusion

Bogoliubov coupled-cluster theory pushes *ab initio* frontiers to

- heavy nuclei thanks to its polynomial scaling
- open-shell systems via the breaking of U(1) symmetry
- high precision by incorporating (leading-order) triples excitations

$\longrightarrow$ Ideal many-body method to investigate pairing properties along semi-magic chains

"Where has the pairing gone?" $\longrightarrow$ Obscured by realistic mean-field ($\neq$ EDF), dynamical correlation are vital in *ab initio*

Next steps

Further developments of BCC foreseen

- odd isotopes & excited states via its equation of motion extension
- projection on particle number

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