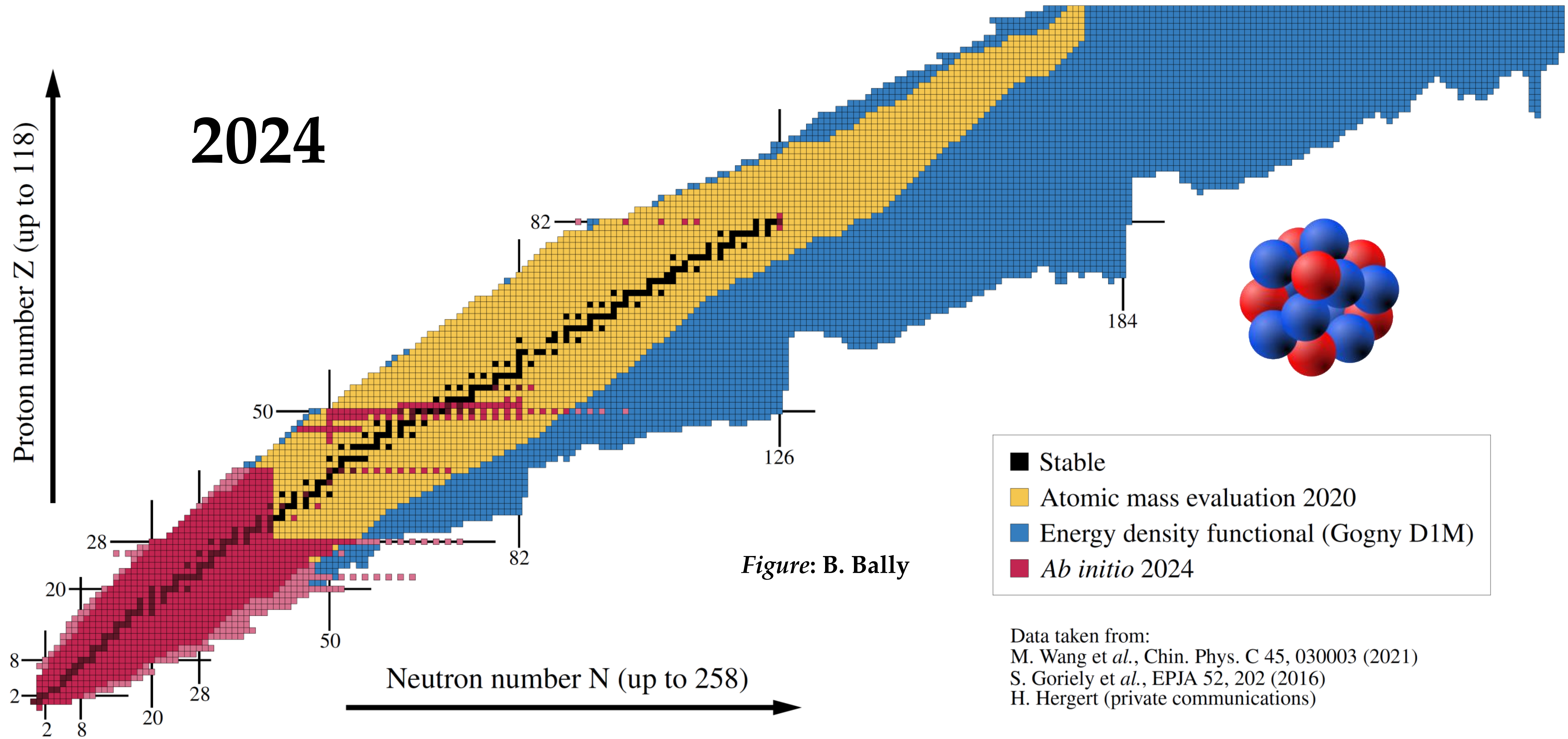
Ab initio description of singly and doubly open-shell nuclei at polynomial cost

Pairing and deformation versus dynamical correlations + going heavier and more neutron rich



HaloWeek'24 - Nuclei at and beyond the driplines
9–14 juin 2024 Chalmers University of Technology

Thomas DUGUET
DPhN, CEA-Saclay, France
IKS, KU Leuven, Belgium

Collaborators on ab initio many-body methods/calculations

CEA

B. Bally
J.-P. Ebran
M. Frosini
A. Porro
A. Roux
A. Scalesi
V. Somà
G. Stellin
L. Zurek

KU LEUVEN

P. Demol
U. Vernik

University of Surrey

C. Barbieri

The University of Tennessee / Oak Ridge National Laboratory

G. Hagen
T. Papenbrock

NSCL

H. Hergert

TRIUMF

P. Navratil

Technische Universität Darmstadt

A.Tichai
P. Arthuis
R. Roth

UAM Universidad Autónoma de Madrid

T. R. Rodriguez

Sun Yat-Sen University

J. M. Yao

Could have talked about halo…

I. Model-independent quantitative characterization method based on the matter density distribution

PHYSICAL REVIEW C **79**, 054308 (2009)

New analysis method of the halo phenomenon in finite many-fermion systems: First applications to medium-mass atomic nuclei

V. Rotival[1,2,*] and T. Duguet[2,3,4,†]

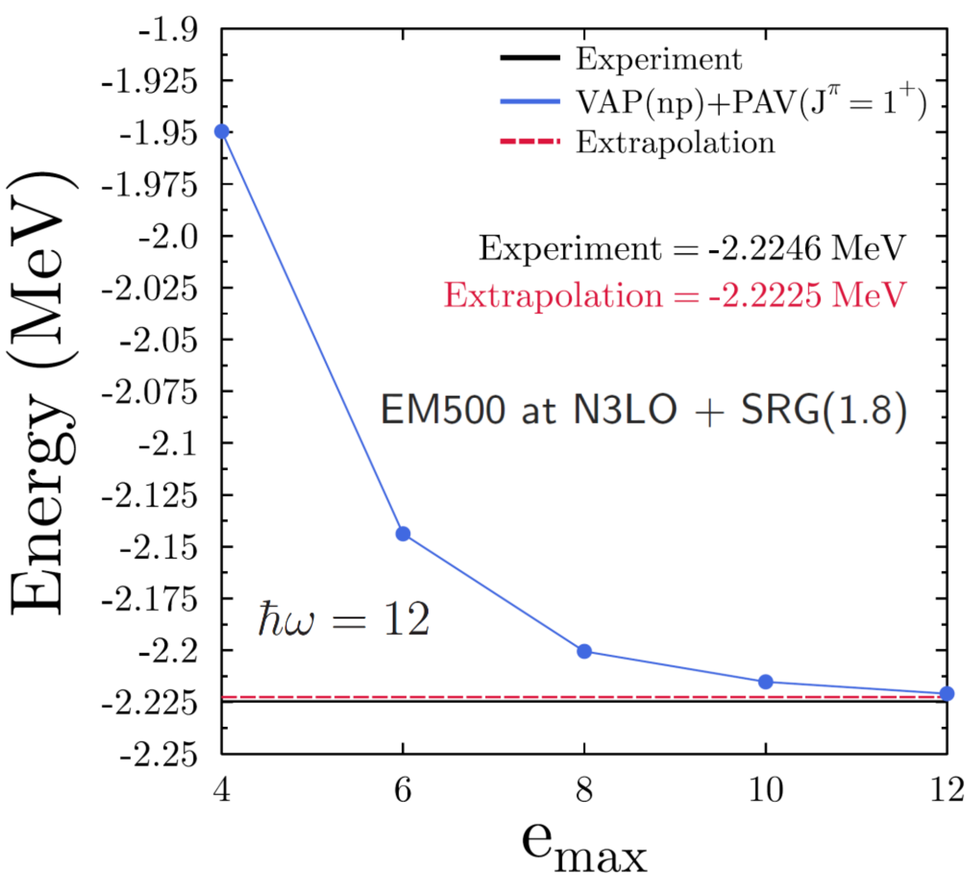
PHYSICAL REVIEW C **79**, 054309 (2009)

Halo phenomenon in finite many-fermion systems: Atom-positron complexes and large-scale study of atomic nuclei

V. Rotival,[1,2,*] K. Bennaceur,[3,4,†] and T. Duguet[2,4,5,‡]

II. Lightest halo (the deuteron…) can be described ab initio *exactly* at mean-field (« on steroid ») level

Bally *et al.*, unpublished



General Bogoliubov state
Breaking U(1)= np pairing
Breaking S(U2) = triax deformation
Breaking parity = Octupole
Break time reversal
+VAP on N=1 and Z=1
+PAV on N=1,Z=1,P=+,J=1

Quantity	Experiment	EM500	dVAP(pn)+PAV
J^π	1^+	1^+	1^+
E (MeV)	-2.2246	-2.2246	-2.222
Q_s (efm^2)	+0.286	+0.275*	[+0.25,+0.31]
μ (μ_N)	+0.857	?	[+0.860,+0.865]
a_2 (fm)	5.419(7)	5.417	5.49 (e_{max} = 10)
r_2 (fm)	1.753(8)	1.752	1.71 (e_{max} = 10)

M. Drissi, T. Duguet, V. Somà, EPJA (2020)

Implications about many-body approx. on π-less EFT renormalizability

Contents

- ◉ Ab initio expansion many-body methods for closed- and open-shell nuclei
- ◉ How many-body correlations come in at polynomial cost = pedagogical account
- ◉ Pushing to high accuracy and to heavier open-shell nuclei at polynomial cost

Contents

- Ab initio expansion many-body methods for closed- and open-shell nuclei
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Ab initio approach at polynomial cost

"Ab initio" theoretical scheme

1) From point-like nucleons = In medias res
2) Inter-nucleon interactions rooted into QCD = via effective field theory

Currently best realized by chiral effective field theory (χEFT) in A-body sector

$$H|\Psi_k^{\sigma}\rangle = E_k^{\tilde{\sigma}}|\Psi_k^{\sigma}\rangle \quad \textbf{with } \sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$$

Exponential → Polynomial cost

Systematic expansion of H

$$H = T + V_{\text{LO}} + V_{\text{NLO}} + V_{\text{N}^2\text{LO}} + \dots$$

Systematic expansion of | Ψ_k >

$$|\Psi_k^{\text{A}}\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \dots$$

Global philosophy

Approximate solution systematically improvable towards well-defined limit

\+

Uncertainties evaluation, quantify what is missing

Expansion many-body methods

$$H|\Psi_k^{\sigma}\rangle = E_k^{\tilde{\sigma}}|\Psi_k^{\sigma}\rangle \text{ with } \sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$$

$$[H, R(\theta)] = 0 \text{ with } G_H \equiv \{R(\theta), \theta \in \mathcal{D}_{G_H}\}$$

One-body Hilbert space

$$\mathcal{H}(1)$$

$$\dim \mathcal{H}(1) \equiv n_{\text{dim}}$$

A-body Hilbert space

$$\mathcal{H}_{\text{A}} = \mathcal{H}(1) \otimes \ldots \otimes \mathcal{H}(\text{A})$$

$$\dim \mathcal{H}(\text{A}) \equiv n_{\text{dim}}^{\text{A}}$$

« The curse of dimensionality »

Expansion many-body methods

Hamiltonian partitioning

$$H = H_0 + H_1$$

« Easy » to solve

Mean-field-like $= O(n_{\text{dim}}^4)$

Unperturbed state

$$H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$$

H_0 → **Symmetry?**

$|\Theta_k^{(0)}\rangle$ → **Nature of the state?**

Expansion many-body methods

$H|\Psi^{\sigma}_{k}\rangle = E^{\tilde{\sigma}}_{k}|\Psi^{\sigma}_{k}\rangle$ with $\sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$

$[H, R(\theta)] = 0$ with $G_H \equiv \{R(\theta), \theta \in \mathcal{D}_{G_H}\}$

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$\mathcal{H}_A = \mathcal{H}(1) \otimes \ldots \otimes \mathcal{H}(A)$

$\dim \mathcal{H}(A) \equiv n^{A}_{\text{dim}}$

Expansion many-body methods

Hamiltonian partitioning — **Unperturbed state**

$H = H_0 + H_1$ → « Easy » to solve → $H_0|\Theta^{(0)}_{k}\rangle = E^{(0)}_{k}|\Theta^{(0)}_{k}\rangle$

90% of the even-even nuclei

	Doubly closed shell	Singly open shell	Doubly open shell
H_0	$[H_0, R(\theta)] = 0$	$[H_0, e^{i\theta A}] \neq 0$	$[H_0, e^{i\vec{\theta}\cdot\vec{J}}] \neq 0$
$\|\Theta^{(0)}_{0}\rangle$	sHF	sHFB	dHF(B)
Static correlations	None	Superfluidity	Deformation (superfluidity)

► Empirically key

► Impossible to grasp otherwise at polynomial cost

Expansion many-body methods

$$H|\Psi_k^\sigma\rangle = E_k^{\tilde\sigma}|\Psi_k^\sigma\rangle \text{ with } \sigma \equiv JM\Pi NZ \equiv \tilde\sigma M$$

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Expansion many-body methods

Hamiltonian partitioning

$$H = H_0 + H_1$$

« Easy » to solve

Unperturbed state

$$H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$$

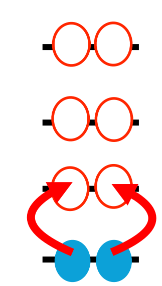
Expansion series

Fully correlated state

Wave operator

$$|\Psi_k^\sigma\rangle = \Omega_k|\Theta_k^{(0)}\rangle$$

Dynamical correlations due to H_1



Wave-operator expansion

Nature of the expansion?

Cost?

Expansion many-body methods

$H|\Psi_k^\sigma\rangle = E_k^{\tilde\sigma}|\Psi_k^\sigma\rangle$ with $\sigma \equiv JM\Pi NZ \equiv \tilde\sigma M$

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Expansion many-body methods

Hamiltonian partitioning | **Unperturbed state** | **Fully correlated state**

$H = H_0 + H_1$ → « Easy » to solve → $H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$ → Expansion series → $|\Psi_k^\sigma\rangle = \Omega_k|\Theta_k^{(0)}\rangle$

Wave operator (Ω_k)

Wave-operator expansion nature

$$\Omega_k \equiv \sum_{q=0}^{\infty \to q_{\text{max}}} c_q H_1^q \quad \textbf{Perturbative}$$

$$\Omega_k \equiv \sum_{q=0}^{\infty \to q_{\text{max}}} f_q(H_1) \quad \textbf{Non-perturbative}$$

→

$$|\Psi_k^\sigma\rangle = \sum_{q=0}^{\infty \to q_{\text{max}}} |\Theta_k^{(q)}\rangle$$

with

$$|\Theta_k^{(q)}\rangle = \sum_{\mu \neq k}^{\text{subset}(q)} C_{k\mu}^{(q)} |\Theta_\mu^{(0)}\rangle$$

- ▶ Tuncated expansion = n_{dim}^p cost
  → Systematically improvable
- ▶ Become quickly expansive as q ↗
  → **Typically $q_{\text{max}} \leq 3$**

Coefficients calculated at n_{dim}^p cost

Expansion many-body methods

$H|\Psi^{\sigma}_{k}\rangle = E^{\tilde{\sigma}}_{k}|\Psi^{\sigma}_{k}\rangle$ with $\sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$

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Expansion many-body methods

Hamiltonian partitioning — **Unperturbed state** — **Fully correlated state**

$H = H_0 + H_1$ → « Easy » to solve → $H_0|\Theta^{(0)}_{k}\rangle = E^{(0)}_{k}|\Theta^{(0)}_{k}\rangle$ → Expansion series → $|\Psi^{\sigma}_{k}\rangle = \Omega_k|\Theta^{(0)}_{k}\rangle$

Example: coupled cluster theories $\Omega_0 \equiv e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T} \equiv \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \ldots$

singles doubles triples

Closed-shell (unpaired) nuclei: standard CC

Hagen *et al.*, RPP (2014)

$|\Theta^{(0)}_{0}\rangle = \prod_{i=1}^{\text{A}} a^{\dagger}_{i}|0\rangle$ Slater determinant

np-nh excitations operator

$$\mathcal{T}_n \equiv \frac{1}{(n!)^2} \sum_{ab\ldots ij\ldots} \mathbf{t}^{ab\ldots}_{ij\ldots} a^{\dagger}_{a} a^{\dagger}_{b} \ldots a_j a_i$$

Unknowns found via coupled algebraic non-linear equations

→ Ex: CCSD = $A^2 n_{\text{dim}}^4$; CCSDT = $A^3 n_{\text{dim}}^5$

Open-shell (paired) nuclei: Bogoliubov CC extension

Signoracci *et al.*, PRC (2015)

$|\Theta^{(0)}_{0}\rangle = \prod \beta_k|0\rangle$ Bogoliubov vacuum

2n quasi-particle excitations operator

$$\mathcal{T}_n \equiv \frac{1}{(2n)!} \sum_{k_1 k_2 \ldots k_{2n}} \mathbf{t}^{2n0}_{k_1 k_2 \ldots k_{2n}} \beta^{\dagger}_{k_1} \beta^{\dagger}_{k_2} \ldots \beta^{\dagger}_{k_{2n}}$$

Unknowns found via coupled algebraic non-linear equations

→ Ex: BCCSD = n_{dim}^6 ; BCCSDT = n_{dim}^8

Expansion many-body methods

$H|\Psi_k^\sigma\rangle = E_k^{\tilde\sigma}|\Psi_k^\sigma\rangle$ **with** $\sigma \equiv JM\Pi NZ \equiv \tilde\sigma M$

$[H,R(\theta)] = 0$ **with** $G_H \equiv \{R(\theta), \theta \in \mathcal{D}_{G_H}\}$

One-body Hilbert space

$\mathcal{H}(1)$

$\dim \mathcal{H}(1) \equiv n_{\text{dim}}$

➡

A-body Hilbert space

$\mathcal{H}_A = \mathcal{H}(1) \otimes \ldots \otimes \mathcal{H}(A)$

$\dim \mathcal{H}(A) \equiv n_{\text{dim}}^A$

Expansion many-body methods

Hamiltonian partitioning — **Unperturbed state** — **Fully correlated state**

$H = H_0 + H_1$ → (**« Easy » to solve**) → $H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$ → (**Expansion series**) → $|\Psi_k^\sigma\rangle = \Omega_k|\Theta_k^{(0)}\rangle$

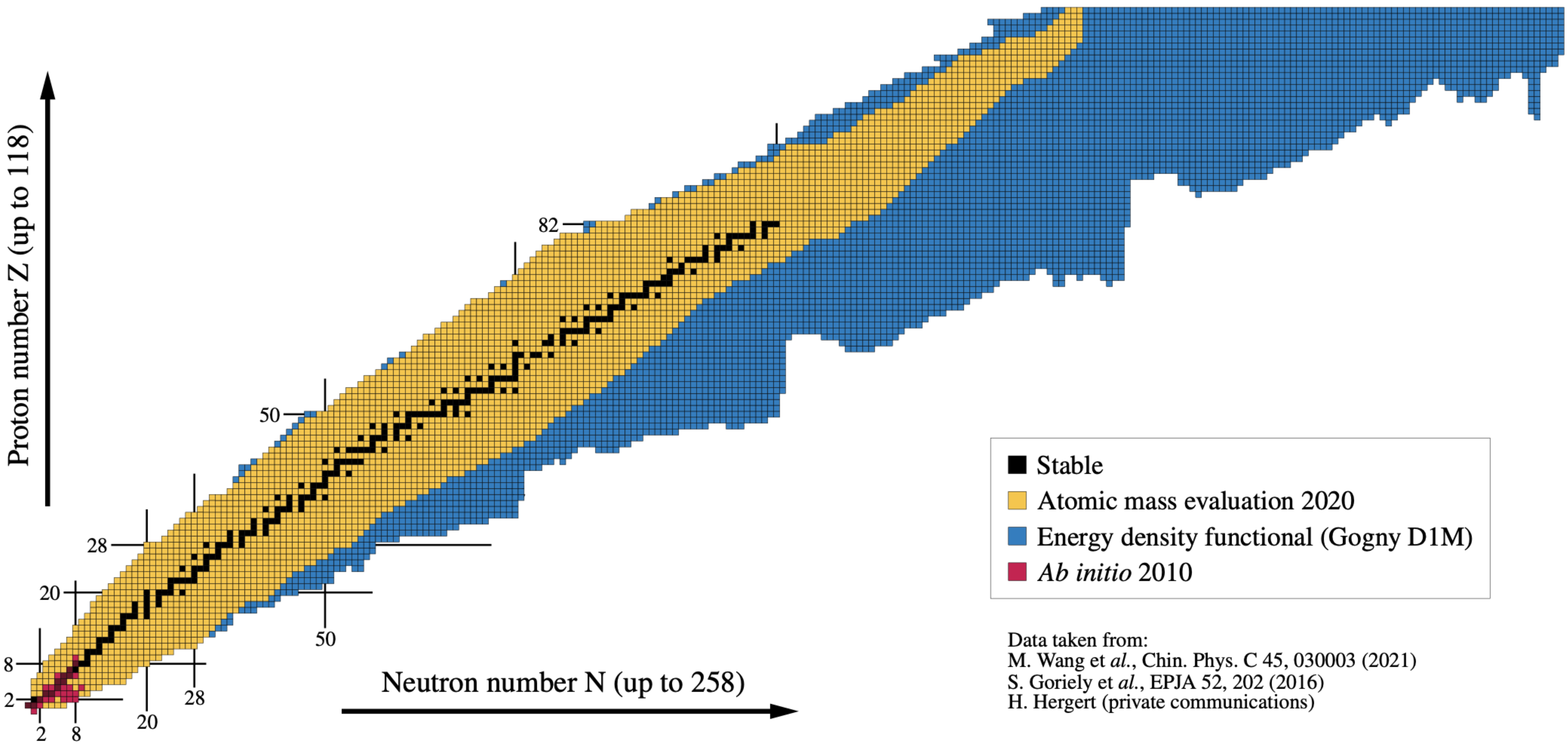
	Doubly closed shell	Singly open shell	Doubly open shell
H_0	$[H_0, R(\theta)] = 0$	$[H_0, e^{i\theta A}] \neq 0$	$[H_0, e^{i\vec\theta\cdot\vec J}] \neq 0$
$\vert\Theta_0^{(0)}\rangle$	sHF	sHFB	dHF(B)
Ω_0	sMBPT sDSCGF sCC sIMSRG	sBMBPT sGSCGF sBCC	dBMBPT dDSCGF dCC

► Numerical results shown in the below

Ground-state *ab initio* nuclear chart… then

Quasi-exact methods (>1990)

Examples: No core shell-model (NCSM)
Green's function monte carlo (GFMC)



2010

[*Figure*: B. Bally]

Ground-state *ab initio* nuclear chart… now!

Single-reference expansion methods (>2010)

Scaling: $\mathcal{O}(A^n)$ → CPU scalable (memory limitations arise)

Hybrid methods for open shell (>2015)

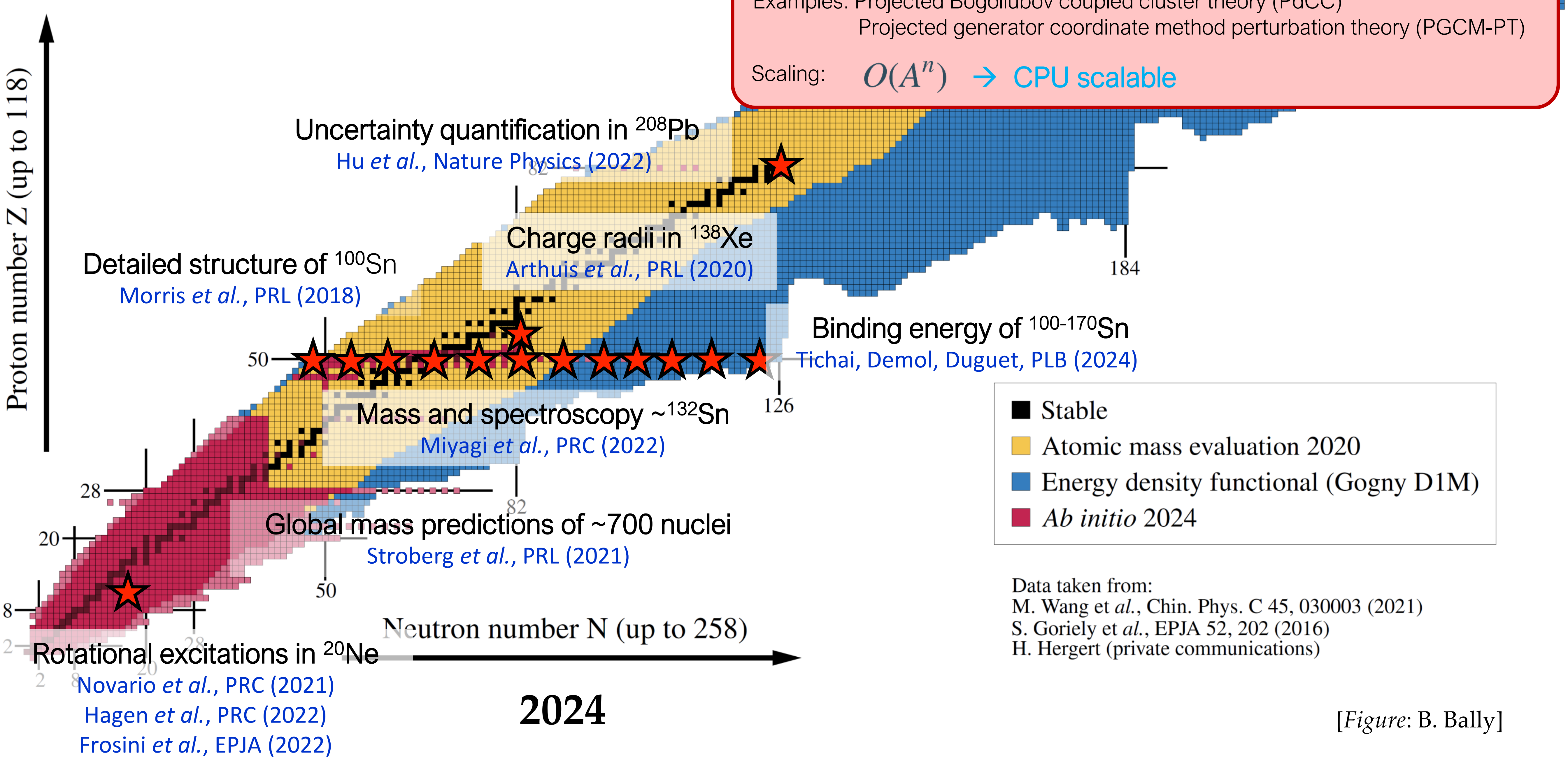
Examples: Valence-space in-medium similarity renormalization group (VS-IMSRG)
Multi-configuration perturbation theory (MCPT)

Scaling: $\mathcal{O}(A^n) + \mathcal{O}(A!)$ → CPU not scalable

SC expansion methods for open shell (>2022)

Examples: Projected Bogoliubov coupled cluster theory (PdCC)
Projected generator coordinate method perturbation theory (PGCM-PT)

Scaling: $\mathcal{O}(A^n)$ → CPU scalable



[*Figure*: B. Bally]

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Numerical applications

Hamiltonian

Empirically optimal for ground-state energies

Not optimal for radii → Use also of $\Delta NNLO_{GO}(394)$ Hamiltonian

Stroberg *et al.*, PRL (2021)

Jiang *et al.*, PRC (2020)

- Chiral-based Hamiltonian EM 1.8/2.0 — Hebeler *et al.*, PRC (2011)
- Three-nucleon interaction rank-reduced to effective two-body interaction — Frosini *et al.*, EPJA (2021)

Systems

Heaviest open-shell nuclei ever computed ab initio so far — Tichai, Demol; Duguet., PLB (2024)

- **Ca** (Z=20) and **Sn** (Z=50) even-even **singly open-shell** isotopes
- **Cr** (Z=24) and Ne (Z=10) even-even **doubly open-shell** isotopes

Model-space parameters

- Spherical harmonic oscillator basis (hw=12)
- $e_{max} \equiv \max(2n + l) = 12$ and $e_{3max} = 18$ (24) in Ca and Cr (Sn) isotopes

Miyagi *et al.*, PRC (2022)

Many-body methods

- sBMBPT(2) — Tichai *et al.*, PLB (2018)
- sBCCSD[T] — Tichai *et al.*, PLB (2024)
- dBMBPT(2) — Frosini *et al.*, EPJA (2021)
- dDSCGF[2] — Scalesi *et al.*, unpublished

► **against sVS-IMSRG(2)** — Stroberg *et al.*, PRL (2021)

Observables

- Absolute binding energy $E(N,Z)$
- Two-neutron separation energy $S_{2n}(N,Z)$
- Two-neutron shell gap $\Delta_{2n}(N,Z)$
- Neutron three-point mass difference $\Delta_n^{(3)}(N,Z)$
- Charge radius R_{ch}
- Neutron skin R_{skin}

Contents

- Ab initio expansion many-body methods for closed- and open-shell nuclei

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    How does the ab initio spherical mean-field looks like along the Ca chain?

    How dynamical correlations improve the ab initio spherical mean-field?

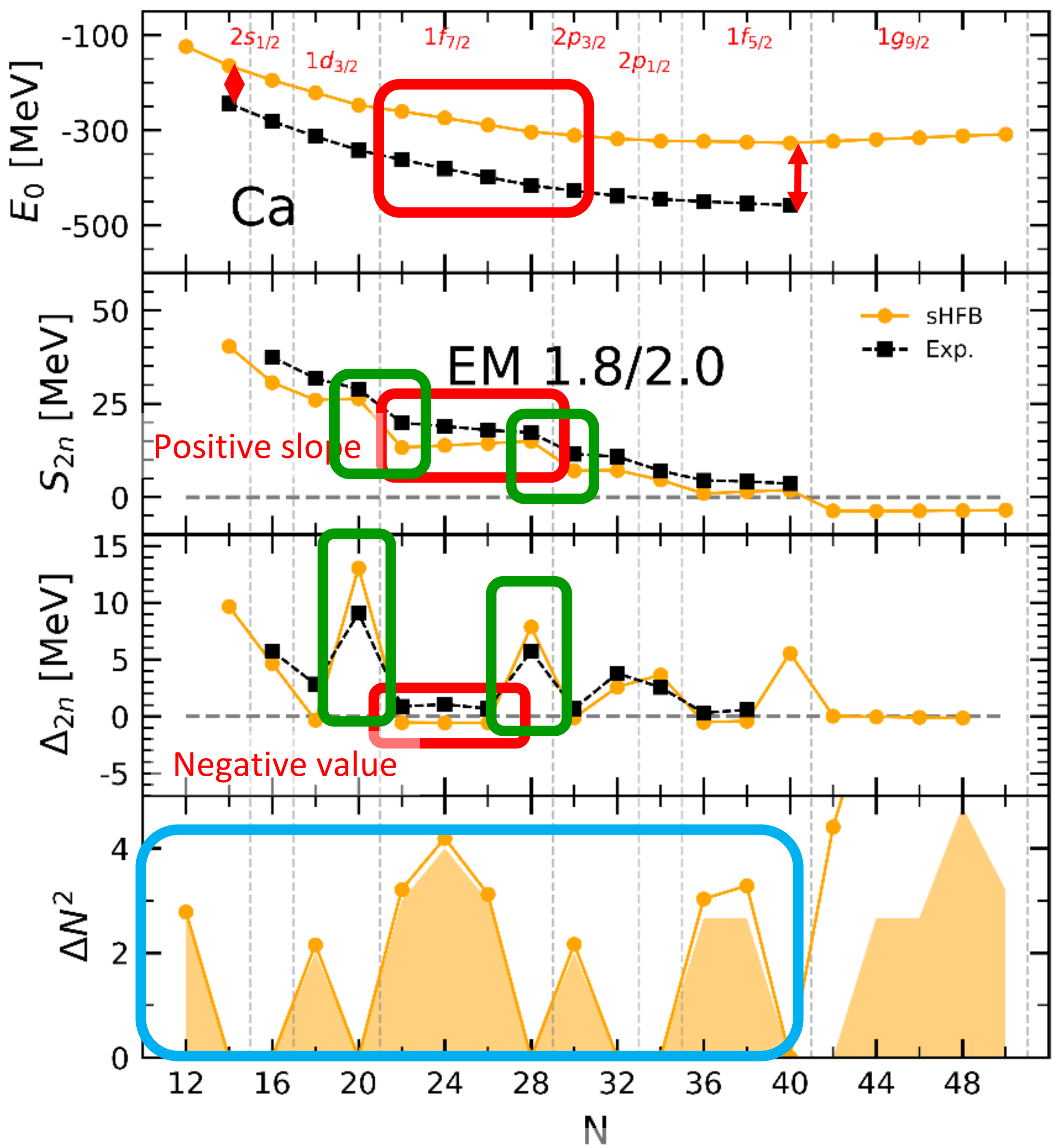
    What happens to the ab initio mean-field when going to the Cr chain?

    Where is the pairing gone?

- Pushing to high accuracy and to heavier open-shell nuclei at polynomial cost

How does the spherical ab initio mean-field looks like?

Scalesi *et al.*, arXiv:2406.03545



ΔN^2 close to « zero-pairing limit of HFB (HFB-ZP) »

Duguet, Bally, Tichai, PRC (2020)

sHFB unbound by [80,130] MeV (account for ~70% of BE)
- → Expected due to missing dynamical correlations
- → Would be more pronounced with a "harder" Hamiltonian
- → Deficit increases with neutron excess

sHFB E(N,Z) wrongly concave throughout open-shells
- → Systematic with (soften) χEFT Hamiltonians

sHFB S_{2n}(N,Z)
- → Too low at the beginning of the shells
- → Exaggerated jumps/magicity at N=20,28

Pairing gap ~20% of exp $\Delta^{(3)}$ at sHFB level
- → Systematic with (soften) χEFT Hamiltonians
- → Despite large $^1S_0$ a_{nn} inducing Cooper pair instability
- → Pairing strictly zero in doubly open-shell mid-mass nuclei

Very different picture from empirical EDF *effective* sHFB
- → m* fitted to be close to empirical value
- → Interaction fitted to match experimental $\Delta^{(3)}$(N,Z)

Superfluidity "fine-tuned" from a many-body standpoint = description at polynomial cost challenging*

*see back up slides

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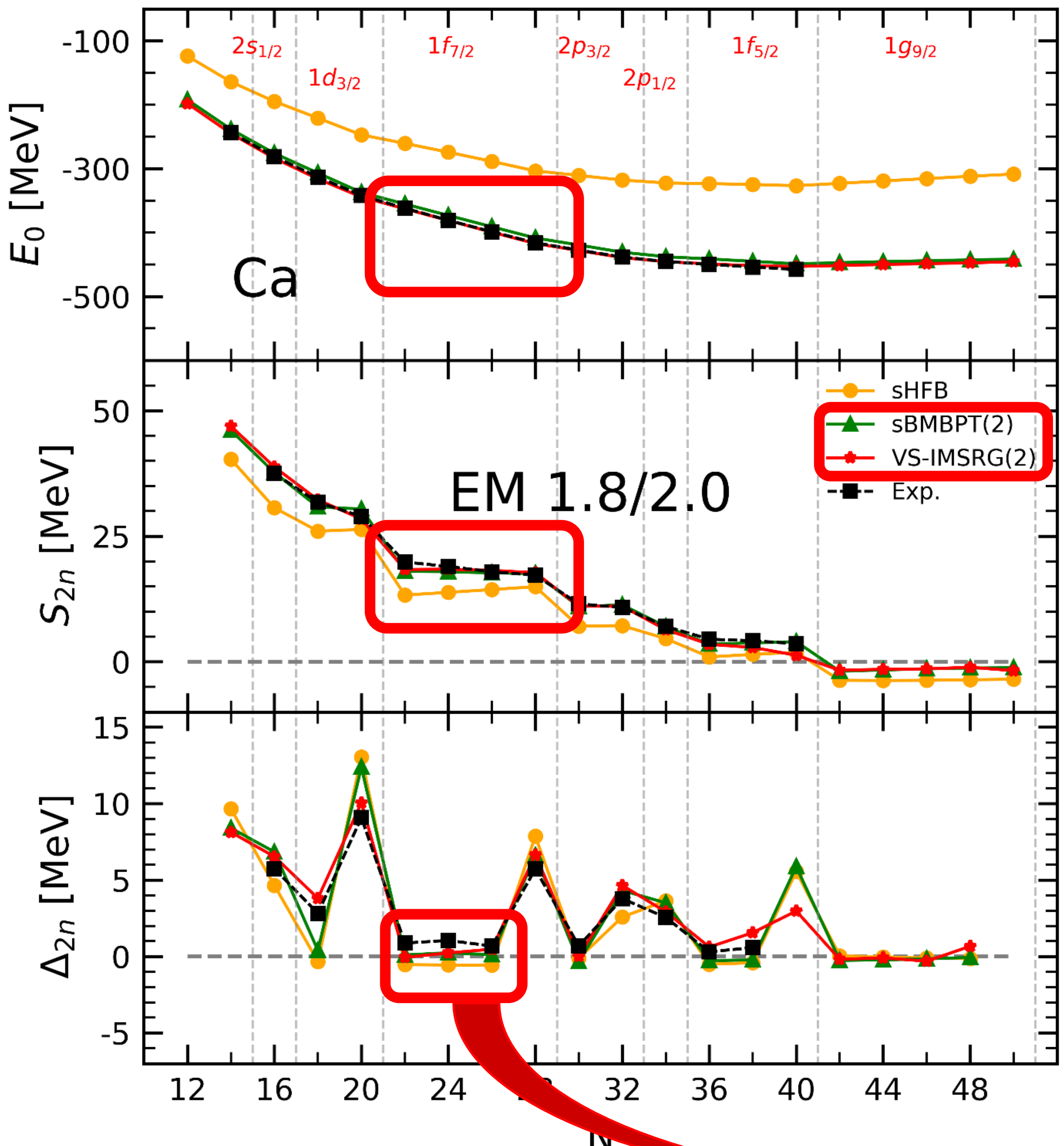
Effect of dynamical correlations in semi-magic nuclei

Scalesi *et al.*, arXiv:2406.03545

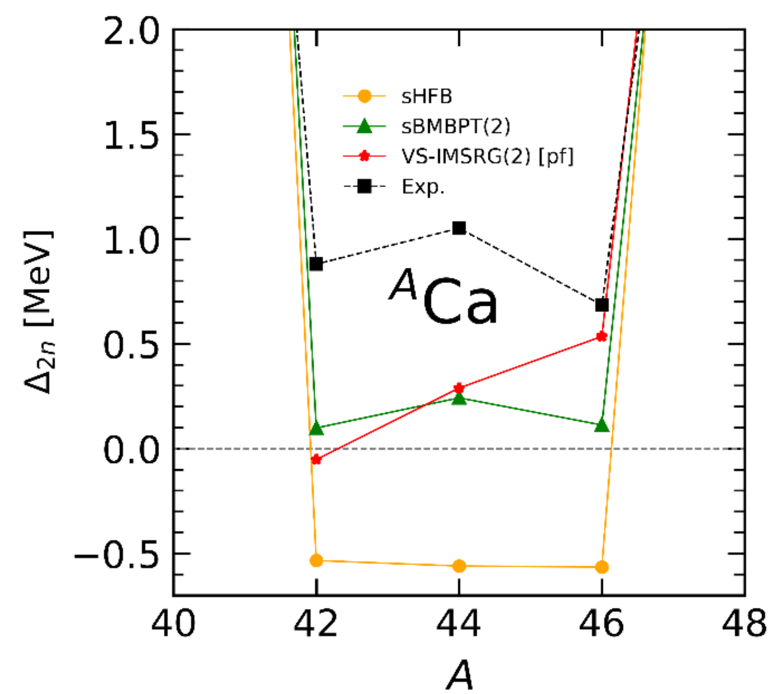


sBMBPT(2) adds [80,130] MeV correlation energy

- → Compensates deficit with neutron excess (a_{sym})
- → rms error to sVS-IMSRG(2) (exp) = 6.9 (7.3) MeV

sBMBPT(2) E(N,Z) correctly convex in open-shells

- → Curvature has correct sign but too small
- → Similar for sVS-IMSRG(2) with ^{40}Ca core



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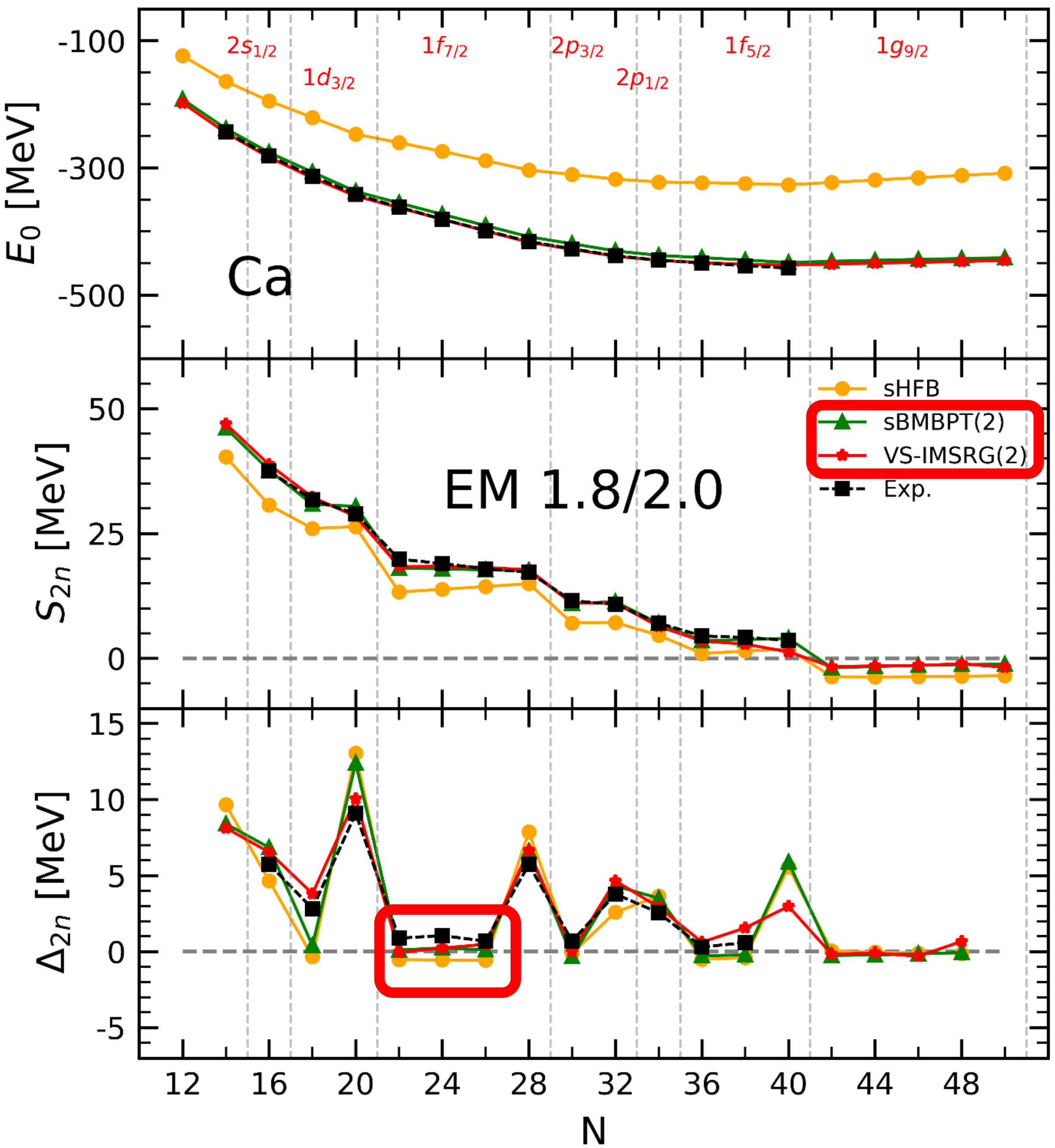

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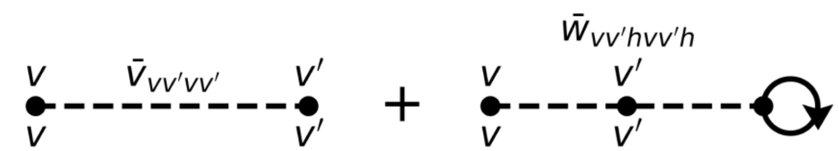
Curvature in sBMBPT(2)

Open shell	$\beta_{\breve{v}}$ (MeV)
$1f_{7/2}$	-0.290
$1g_{9/2}$	-0.270

sHFB (EFA)

$$\beta_{\breve{v}} = \frac{1}{d_v}\sum_{m_{v'}}^{d_v}$$

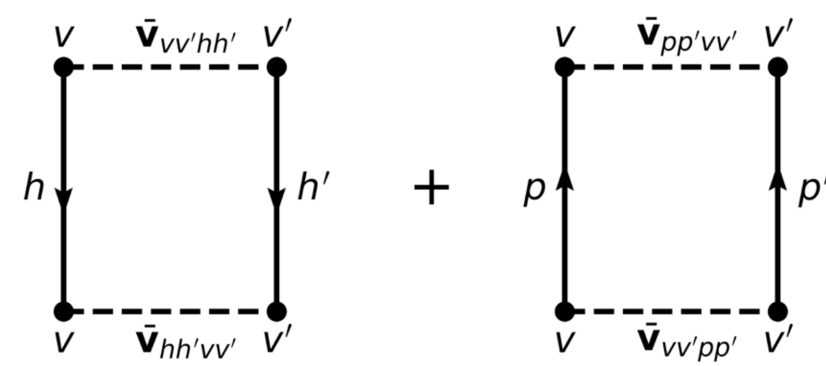


< 0

Monopole valence-shell 2-body matrix element

sBMBPT(2) (EFA)

$$\beta^{(2)}_{\breve{v}} \equiv \frac{1}{d_v}\sum_{m_{v'}}^{d_{\breve{v}}}$$



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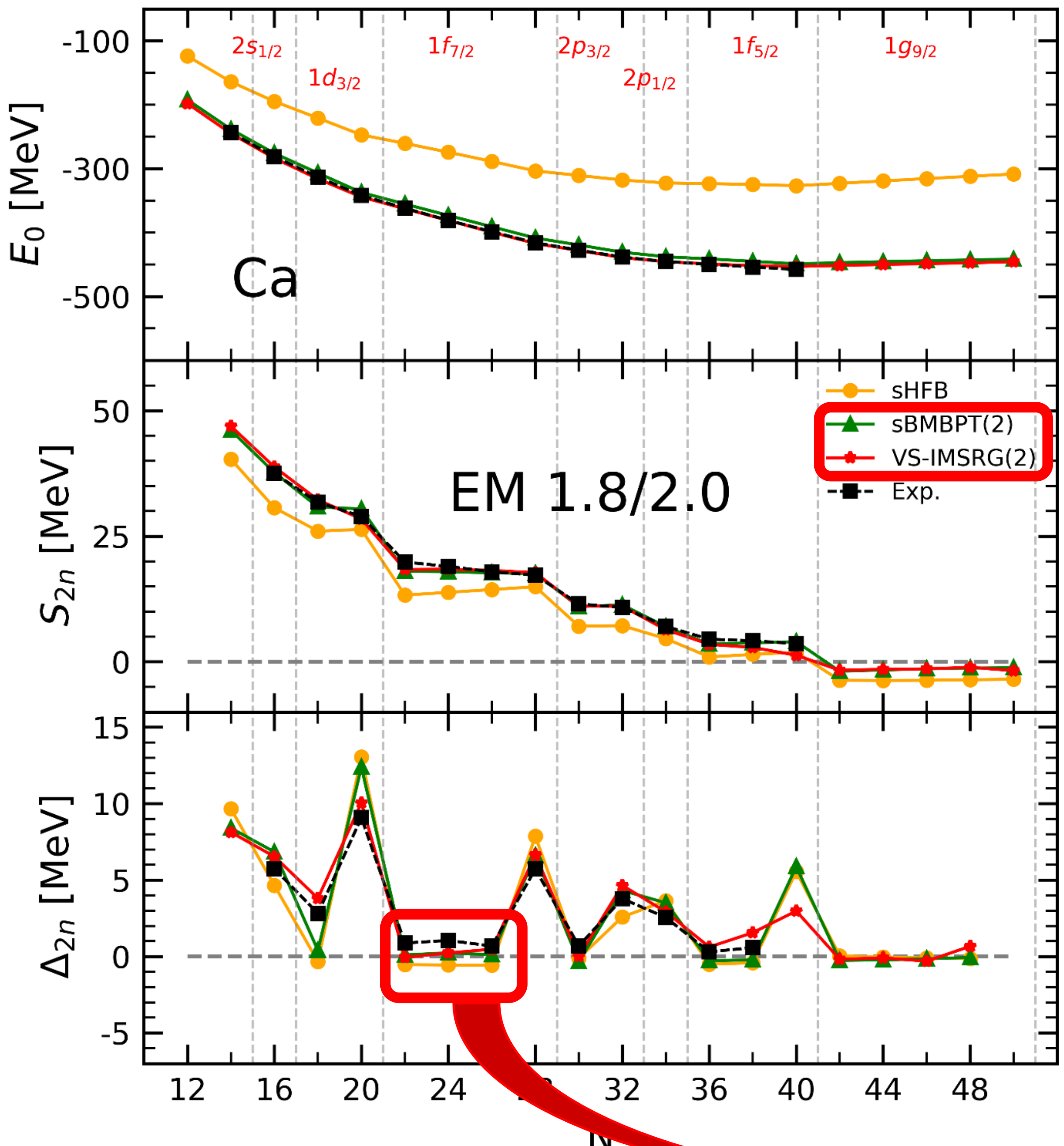
2[nd] order effective valence-shell monopole 2-body matrix element due to 2p and 2h excitations

Effect of dynamical correlations in semi-magic nuclei

Scalesi *et al.*, arXiv:2406.03545



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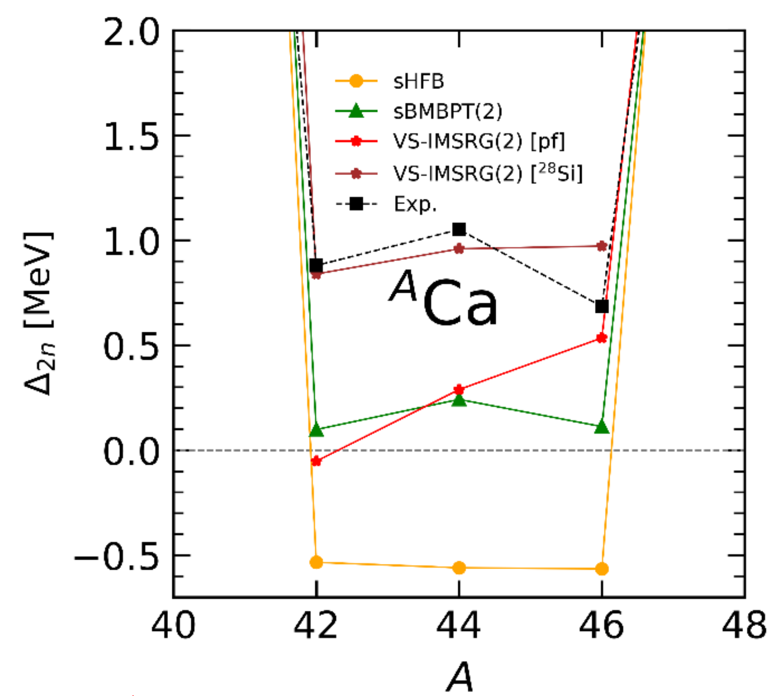


Full diago via sVS-IMSRG(2) not better

Miyagi, Priv. Comm.

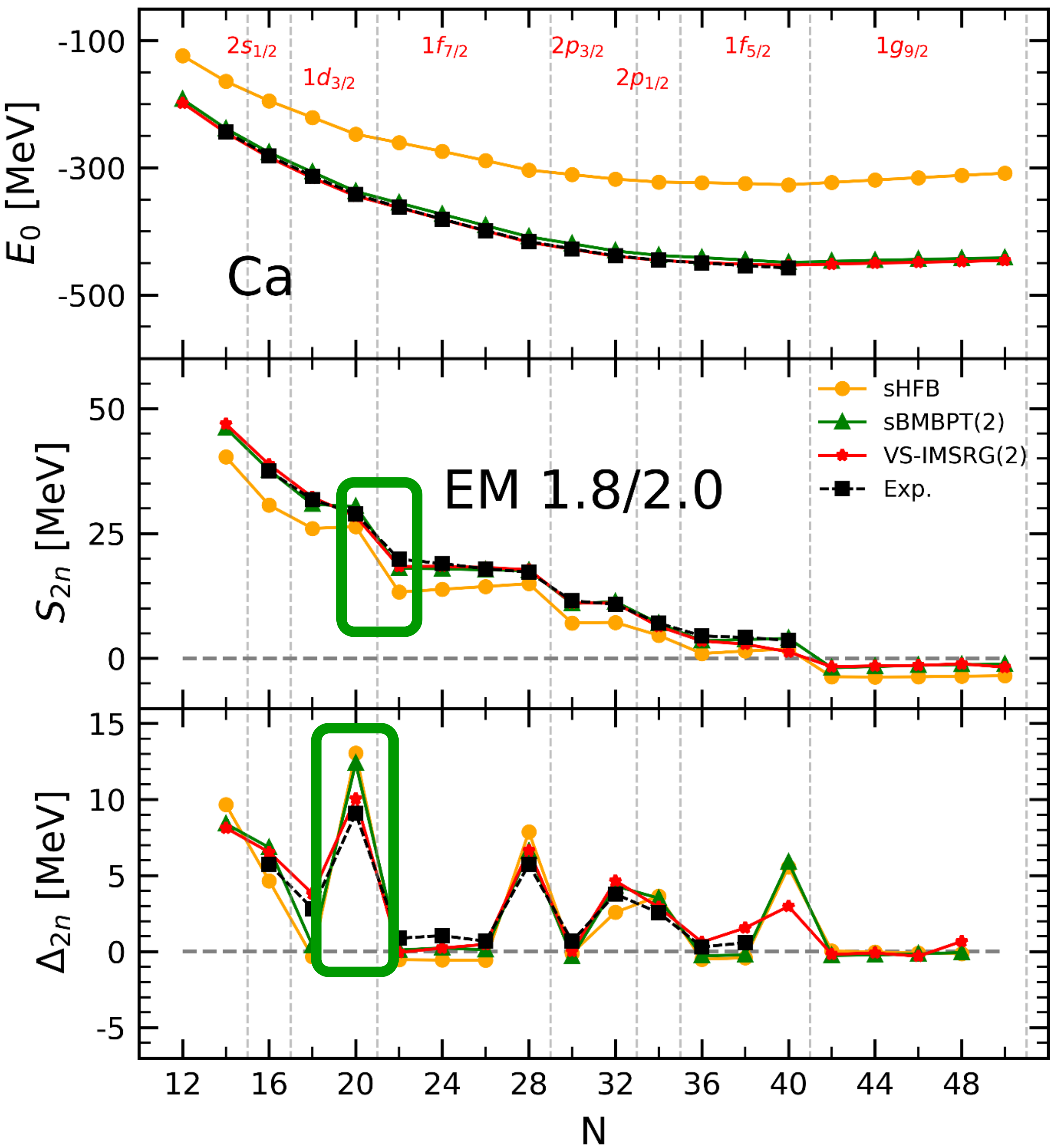
- **sVS-IMSRG(2) with ^{28}Si core gets it right**
  → Collective fluctuations of ^{40}Ca core key
- **Infamous charge radius problem not solved**
  → At variance with Caurier et al., PLB (2001)

Curvature improved by low-order dynamical correlations

Collective fluctuations needed to be quantitative
► At least third order in non-perturbative expansion methods…

Effect of dynamical correlations in semi-magic nuclei

Scalesi *et al.*, arXiv:2406.03545



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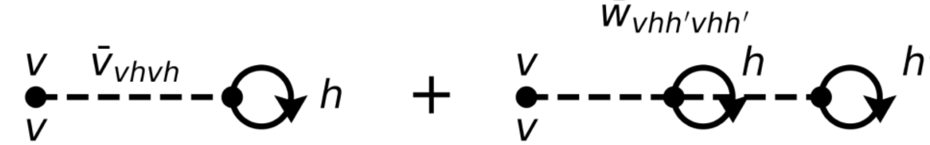
sBMBPT(2) S_{2n}(N,Z)
- → Increases at the beginning of the open shells
- → Exaggerated jump/magicity at N=20 remains

S_{2n} entering open shell in sBMBPT(2) $\qquad S^{(2)}_{2n} = -2\epsilon^{\mathrm{CS}(2)}_{\breve{v}}$

HF-EFA

Mean-field valence shell single-particle energy

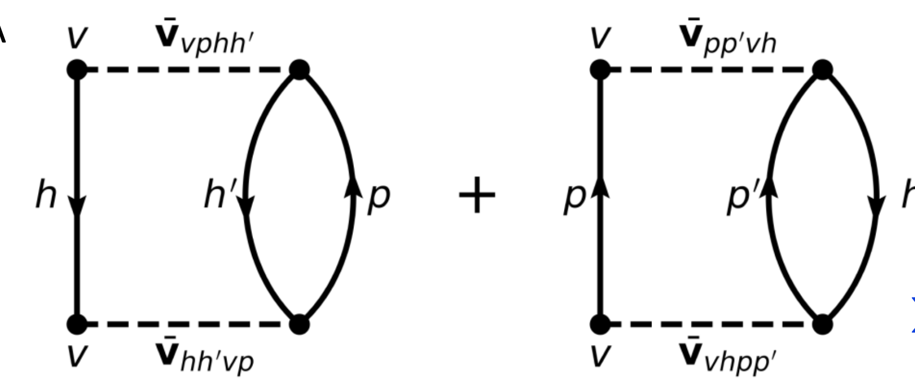
$\epsilon^{\mathrm{CS}}_{\breve{v}} \equiv t_{vv} +$



2^{nd} order self-energy correction due to 2h-1p and 1h-2p excitations

MBPT(2)-EFA

$\Sigma^{(2)}_{\breve{v}}(\epsilon^{\mathrm{CS}}_{\breve{v}}) =$



< 0

$\Sigma^{(2)}{}_{f7/2} = -5$ MeV

Starting S_{2n} ok with low-order dynamical correlations

Not sufficient for Δ_{2n} at N=20

Contents

- Ab initio expansion many-body methods for closed- and open-shell nuclei
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    What happens to the ab initio mean-field when going to the Cr chain?

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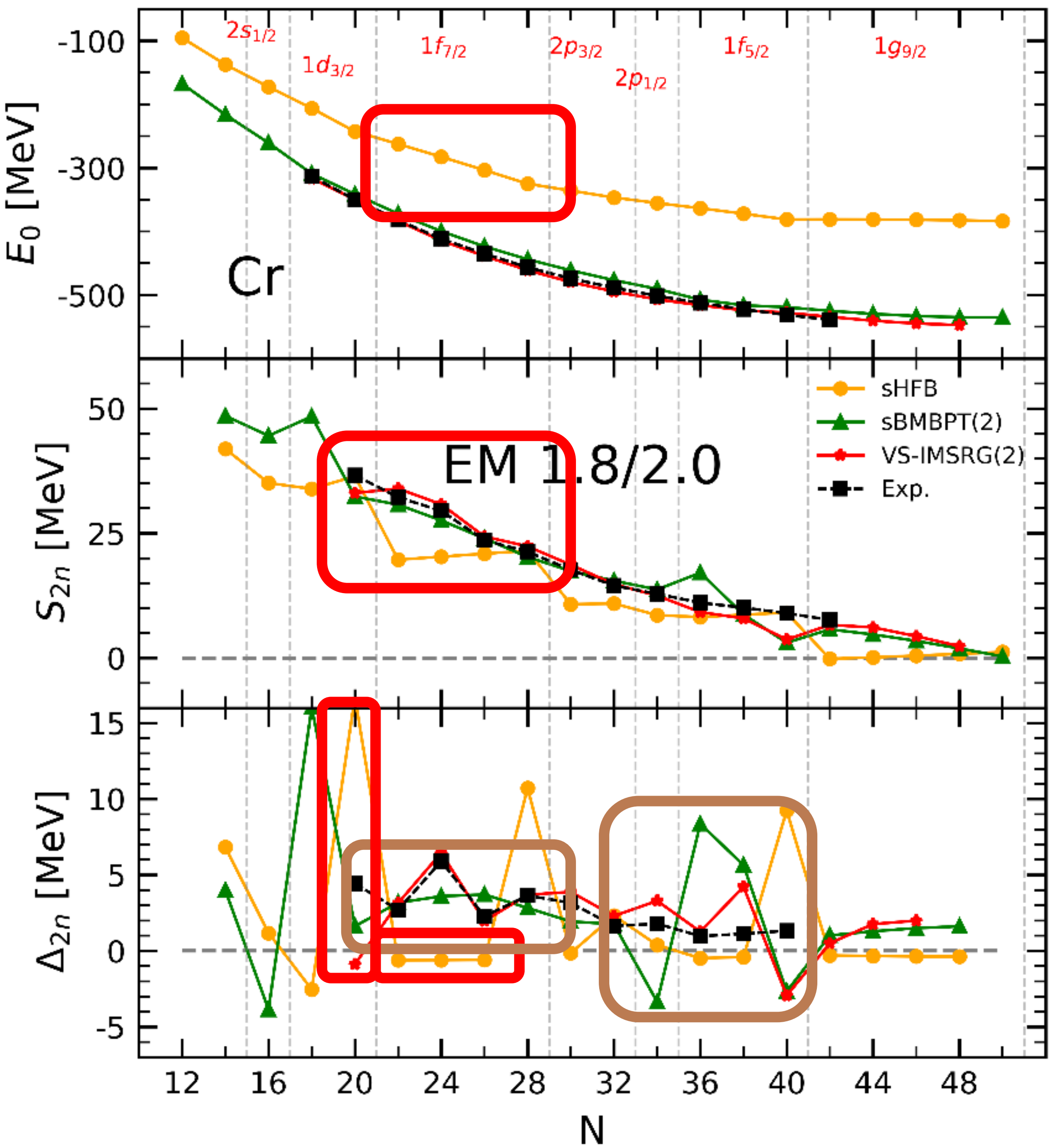
- Pushing to high accuracy and to heavier open-shell nuclei at polynomial cost

What about doubly open-shell nuclei?

Scalesi *et al.*, arXiv:2406.03545



sHFB displays same wrong features

→ Concavity and exaggerated magicity at N=20,28

→ **Magicity signature has disappeared from data**

Dynamical correlations

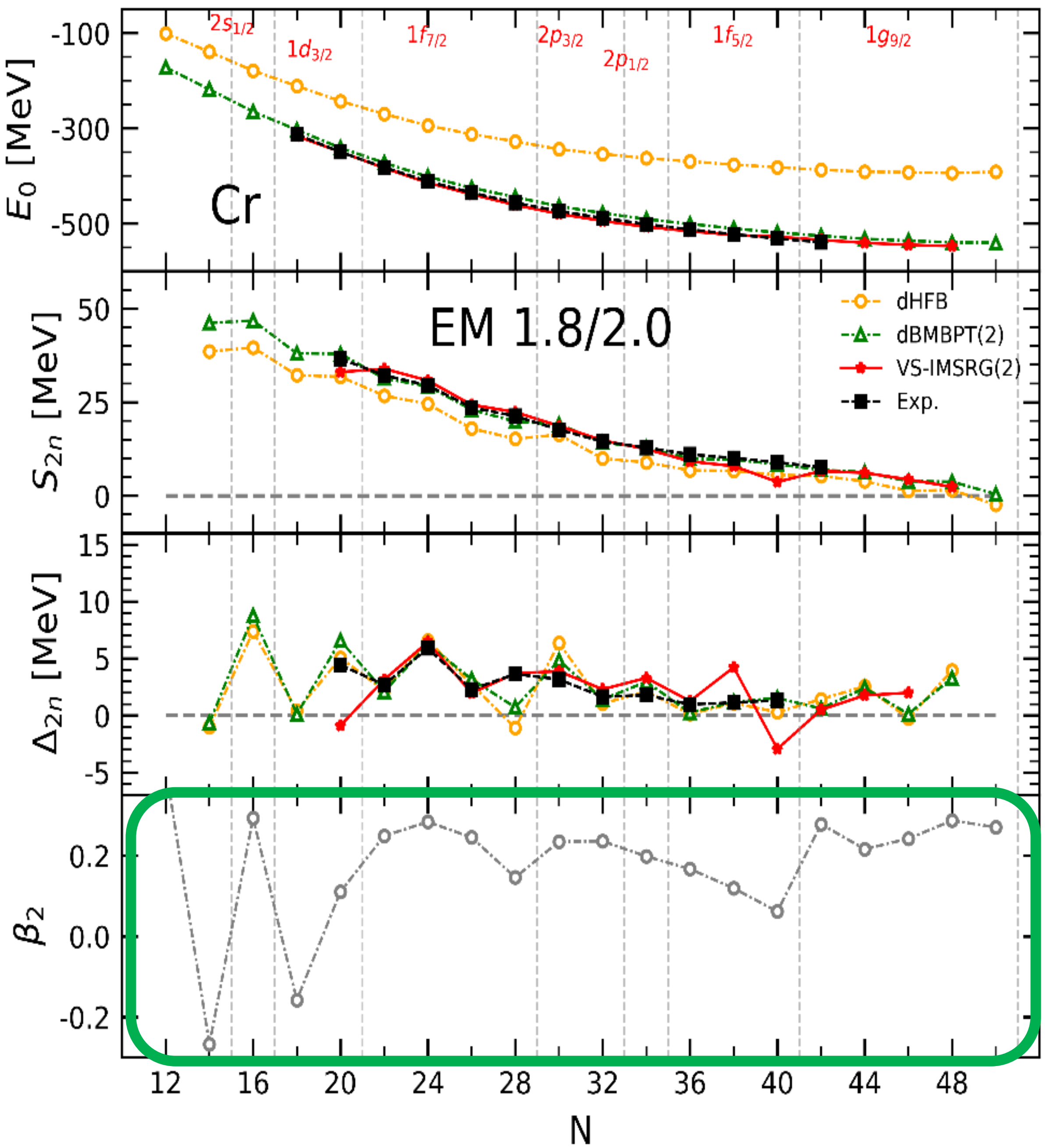
→ sBMBPT(2) remains qualitatively wrong

→ sVS-IMSRG(2) correct via full diagonalization in VS

How to do the same at polynomial cost?

What about doubly open-shell nuclei?

Scalesi *et al.*, arXiv:2406.03545



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Allowing for static deformation via breaking SU(2)

→ dHFB qualitatively correct thanks to static correlations

→ Missing dynamical correlations ok via dBMBPT(2)

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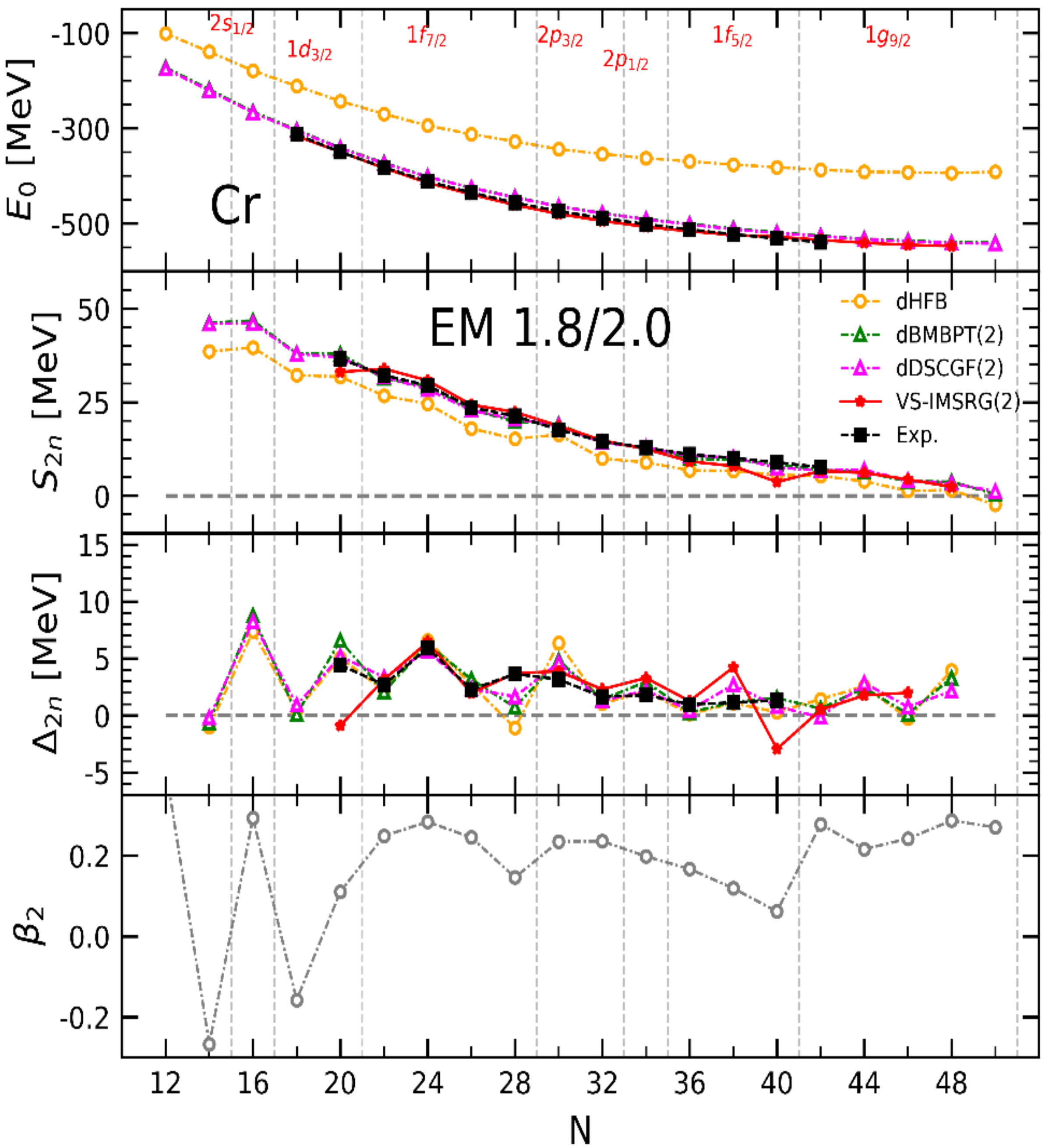

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→ dHFB qualitatively correct thanks to static correlations
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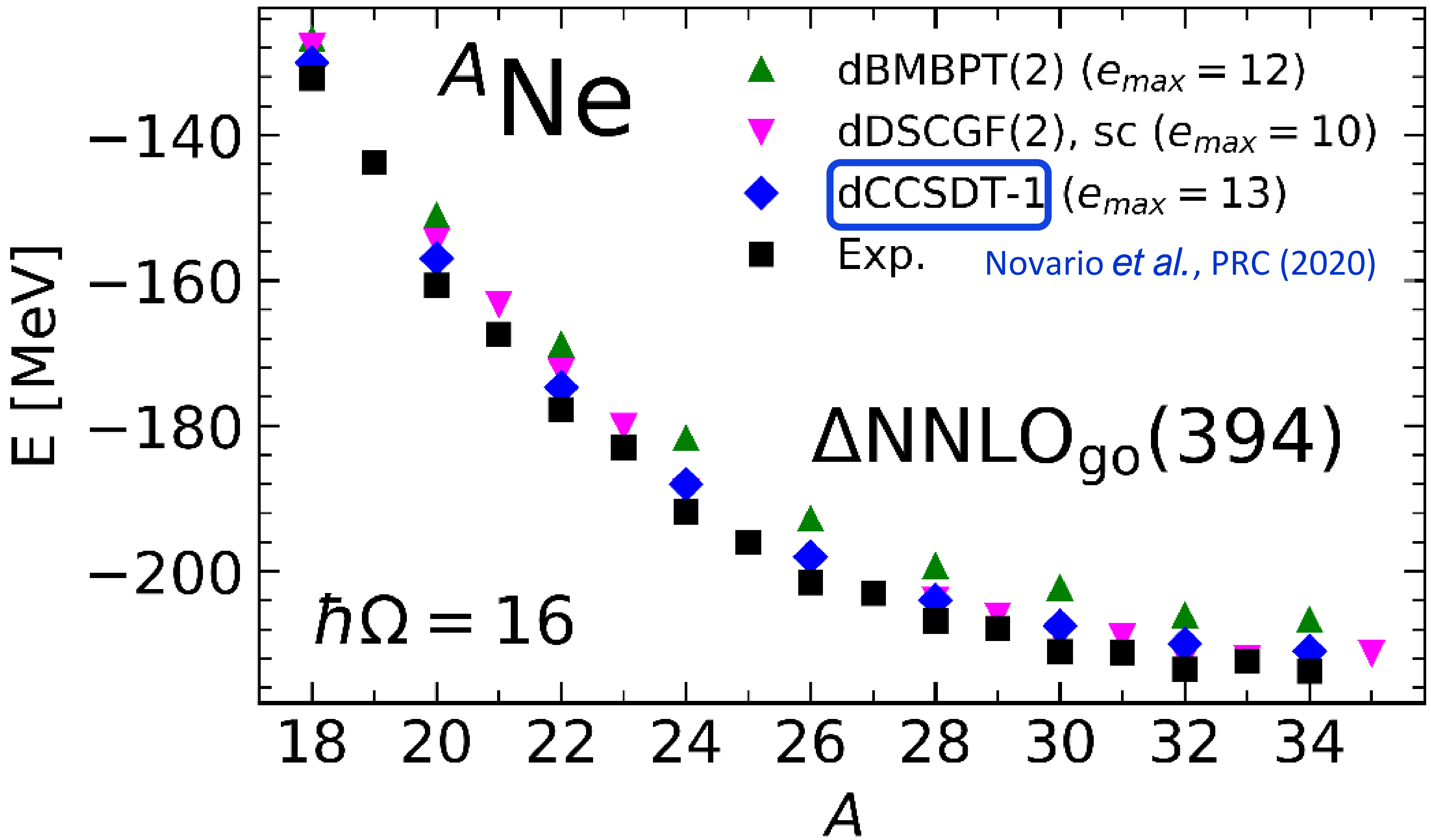
Go *non-perturbative* to be fully quantitative: dDSCGF[2]
→ Consistent with dBMBPT(2) soft Hamiltonian employed

What about doubly open-shell nuclei?

Scalesi *et al.*, unpublished



^{A}Ne	$\sigma_{\text{theo.–exp.}}$
dBMBPT(2)	8.2 MeV
dDSCGF[2]	2.9 MeV
dCCSDT-1	3.2 MeV

Very recent design of *non-perturbative* dDSCGF[2] expansion method

→ +4.2 MeV binding on average compared to dBMBPT(2)

→ Very consistent with dCCSDT-1 but slight trend with neutron excess

→ Access to odd nuclei on the same footing

Allowing for deformation is the key feature to describe doubly open-shell nuclei at polynomial cost

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Where is the pairing gone?© G. Hagen, T. Duguet

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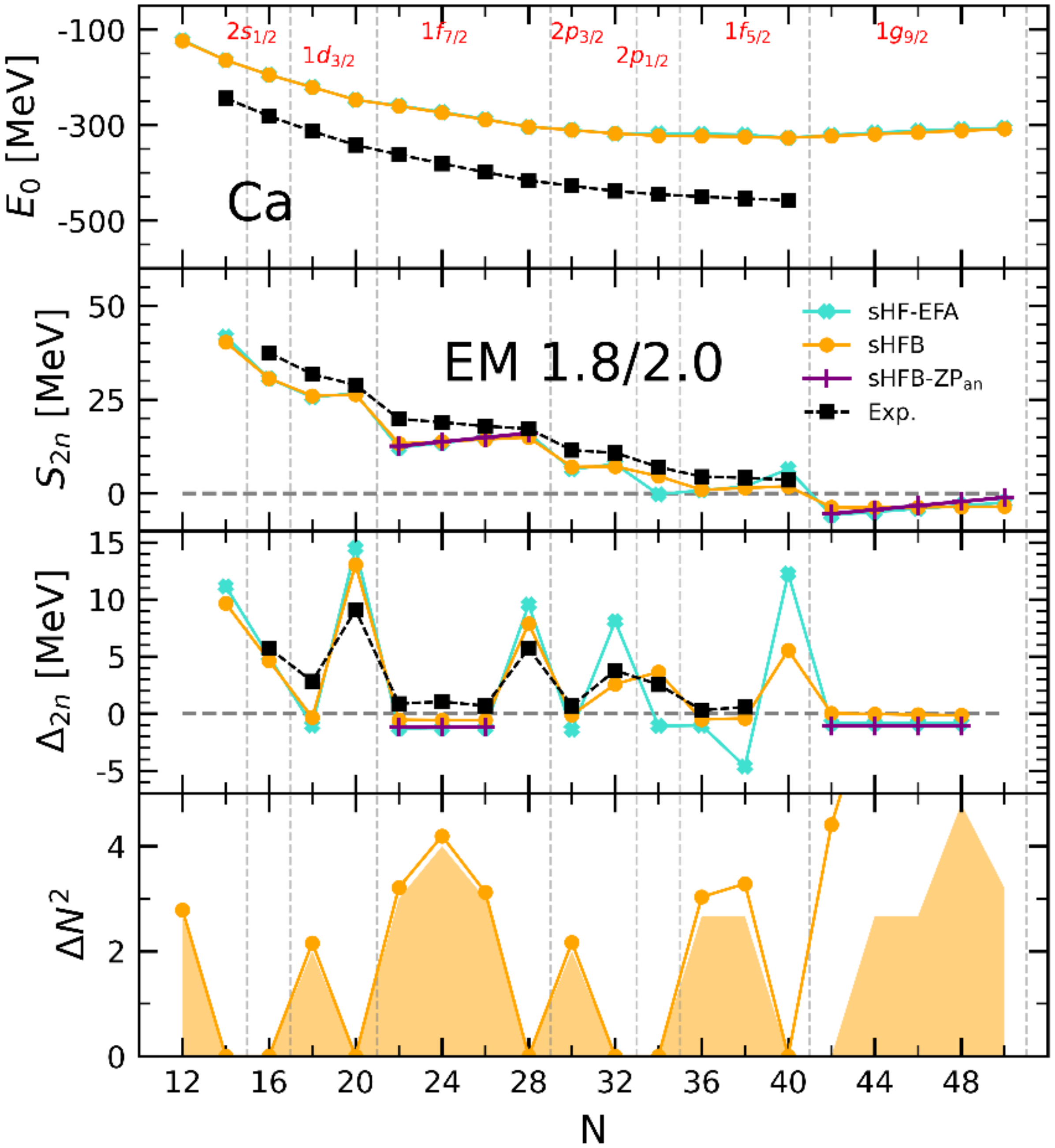

sHFB displays weak pairing

→ S_{2n} and Δ_{2n} very close with HF-EFA and HFB-ZP

→ **Gives ~20% of exp $\Delta^{(3)}$**

→ Too-low effective mass m*

→ **Too weak pairing kernel = bare nn vertex**

Where is the pairing gone?© G. Hagen, T. Duguet

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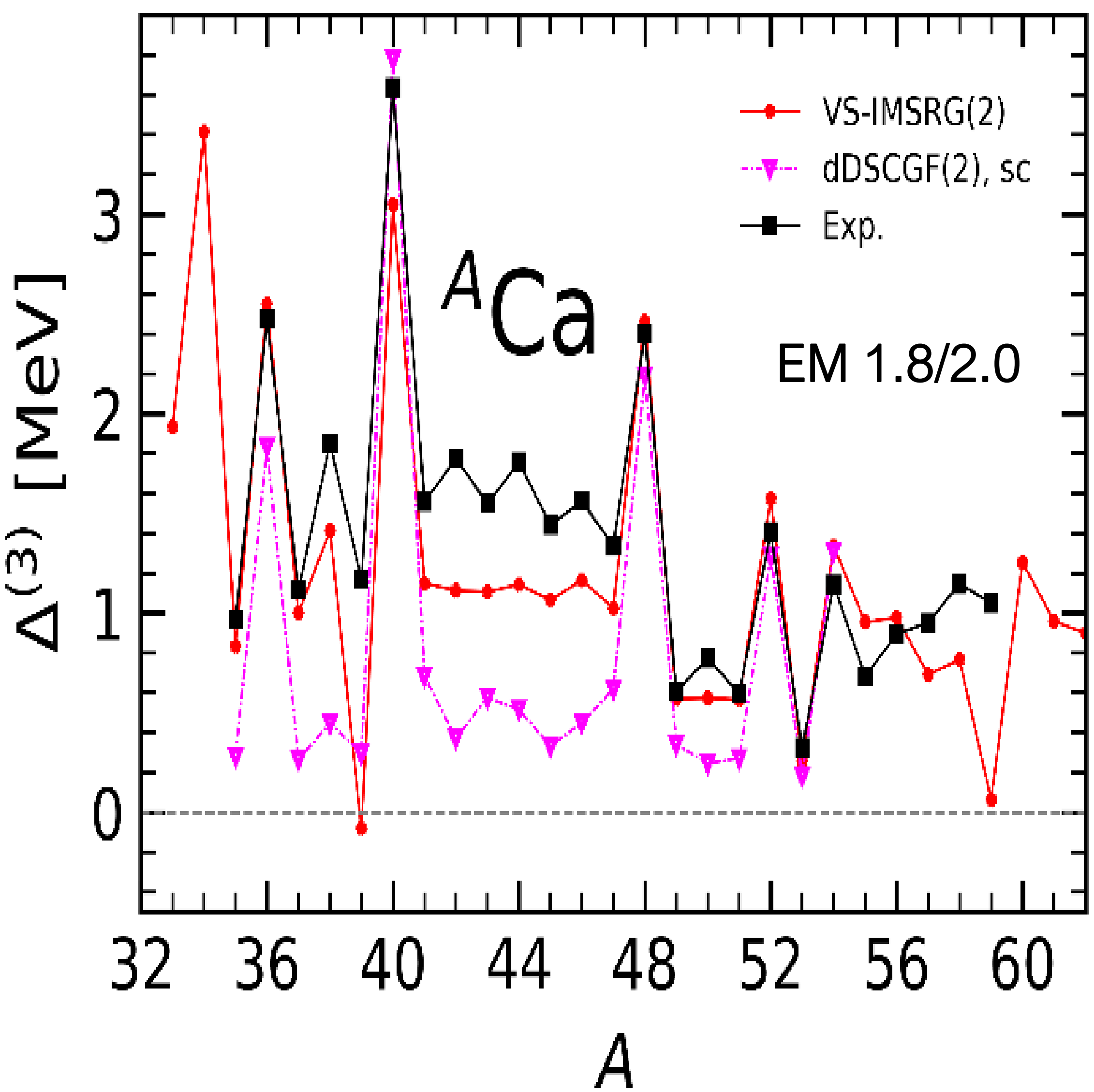

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Dynamical correlations

→ Low-order via sDSCGF(2) **≈ 30% of exp $\Delta^{(3)}$**

→ sVS-IMSRG(2) with ^{40}Ca core **≈ 70% of exp $\Delta^{(3)}$**

→ Higher-order collective process = exchange of vibrations

Barranco *et al.*, JPCS (2011)

Miyagi, Priv. Comm.

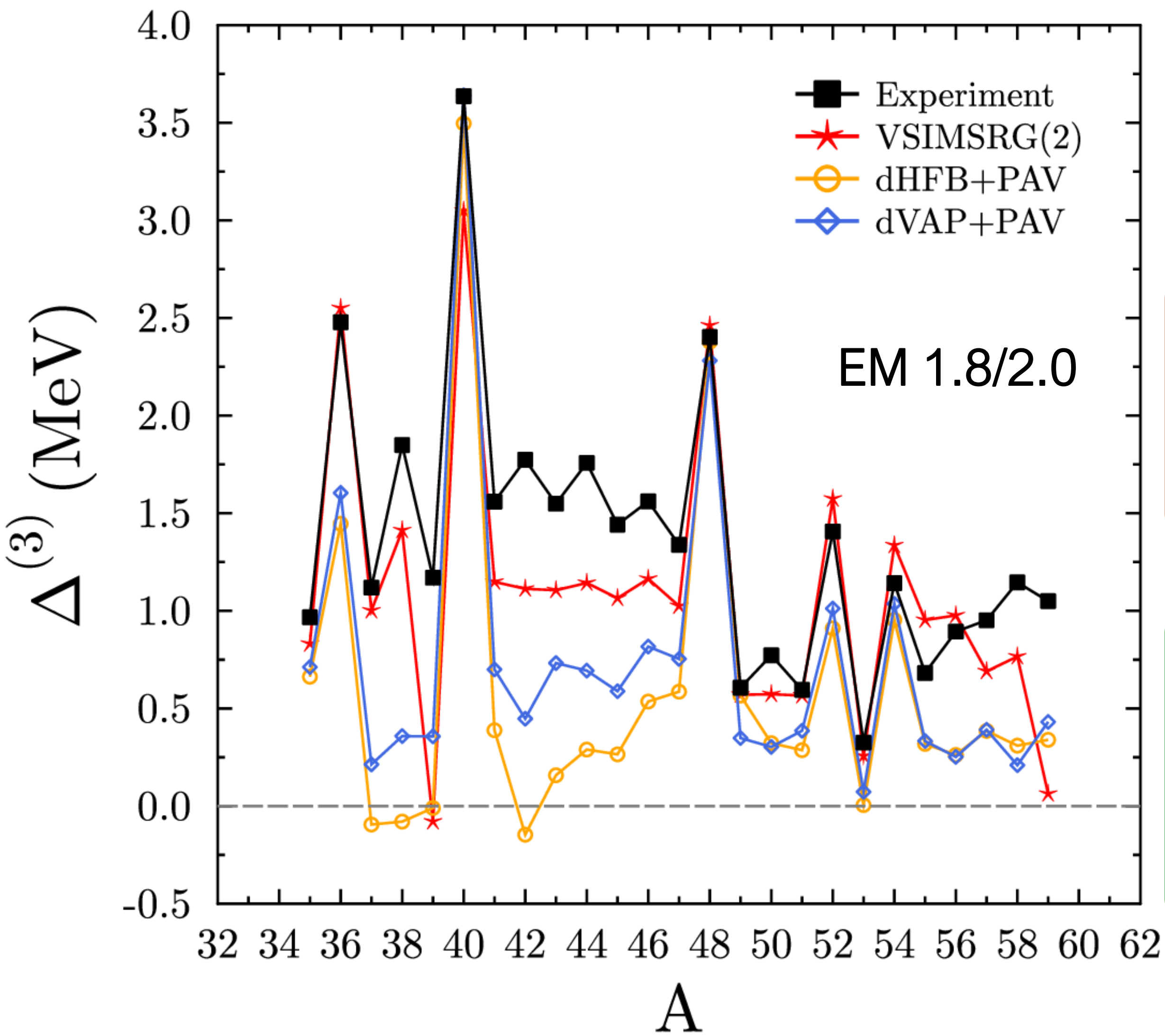
sVS-IMSRG(2) with ^{28}Si core = 100% of exp $\Delta^{(3)}$!

→ Collective fluctuations of ^{40}Ca core does it

At what polynomial cost can this be captured?

Where is the pairing gone?© G. Hagen, T. Duguet

Bally *et al.*, unpublished



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→ Higher-order collective process = exchange of vibrations

Use richer unperturbed state (first step here)

Deformed Bogoliubov with full blocking in odd isotopes

+VAP on N&Z

+PAV on J^{π}

→ **40% of exp $\Delta^{(3)}$: not enough as expected**

Collective vibrations of ^{40}Ca « core » adding GCM

Dynamical correlations on top via PGCM-PT

Frosini *et al.*, EPJA (2022)

Superfluidity "fine-tuned" from a many-body standpoint

►A quantitative ab initio description at polynomial cost is a challenge for the future

Contents

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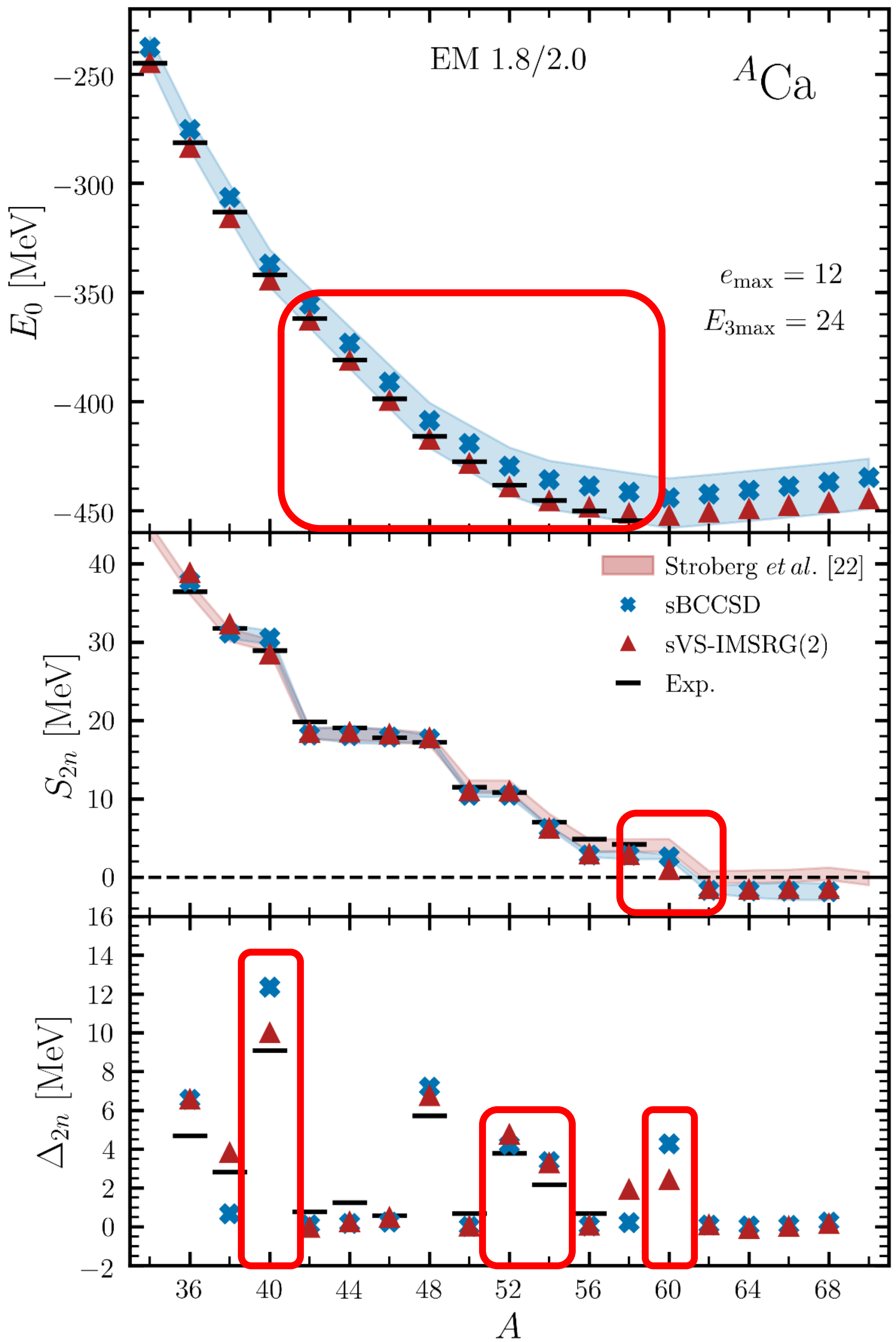
    - BCCSD and BCCSD[T] ground-state energies in Ca and Sn isotopes
    - BCCSD ground-state charge radii and neutron skins in Sn isotopes

Pushing to greater accuracy in open-shell nuclei…

Tichai *et al.*, PLB (2024)



$$\mathcal{T}_{\text{BCCSD}} \equiv \mathcal{T}_1 + \mathcal{T}_2$$

Novel non-perturbative sBCCSD (sBMBPT(3) complete)
$\sigma_{\text{th-exp}}$(E) = 9 MeV (2.3%)
→ 2 MeV for sVS-IMSRG(2)
Exaggerated N=20 magicity / N=28,32,34 magicity ok
Predicted magicity at N=40
→ Exaggerated compared to sVS-IMSRG(2)
Neutron drip-line predicted in ^{60}Ca (closing of $1f_{5/2}$)
→ Consistent with sVS-IMSRG(2)

Many-body uncertainties

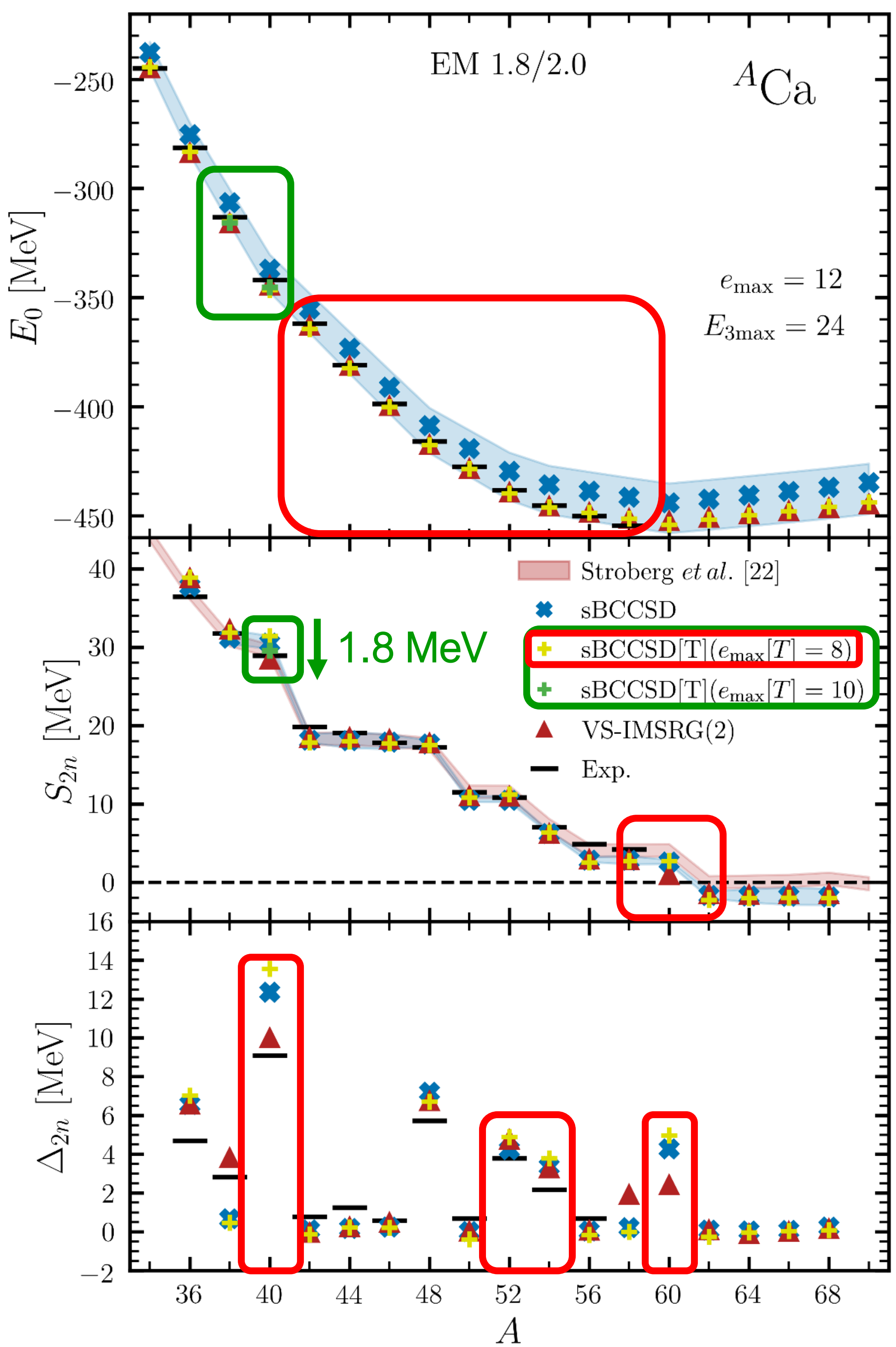
Dominating many-body uncertainty
Can it be removed?

$$\epsilon_{\text{MB}} \equiv \epsilon_{\text{1BB}} + \epsilon_{\text{3BB}} + \epsilon_{\text{NO2B}} + \epsilon_{\text{BCC}} + \epsilon_{\text{PNR}}$$

		^{A}Ca
ϵ_{1BB}	One-body basis (e_{max})	1%
ϵ_{3BB}	Three-body basis ($E_{3\text{max}}$)	Negligible
ϵ_{NO2B}	Normal-order 2B	2%
ϵ_{BCC}	Many-body truncation	8% of ΔE_{BCCSD} 2.5%
ϵ_{PNR}	Particle-number breaking	1 MeV (0.3%)

Pushing to greater accuracy in open-shell nuclei…

Vernik *et al.*, unpublished



$$\mathcal{T}_{BCCSDT} \equiv \mathcal{T}_{BCCSD} + \mathcal{T}_3$$

sBCCSD[T] = adding *perturbative* triples correction
Challenging n_{dim}^7 process
$\sigma_{th\text{-}exp}$(E) = 9 MeV (2.3%) ▶ 2.1 MeV (0.5%)
→ 2 MeV for sVS-IMSRG(2)
Magicity&drip-line essentially unchanged
→ Relative energies not much affected
→ But [T] still moving from e_{max}=8 to e_{max}=10
→ Do we need feedback onto BCCSD (i.e. $\mathcal{T}_1$&$\mathcal{T}_2$) part?
→ Would naively be a n_{dim}^8 process…

Consistent with triples in closed-shell
→ [8.6,10.6]% of ΔE_{BCCSD} along chain

Many-body uncertainties

$$\epsilon_{MB} \equiv \epsilon_{1BB} + \epsilon_{3BB} + \epsilon_{NO2B} + \epsilon_{BCC} + \epsilon_{PNR}$$

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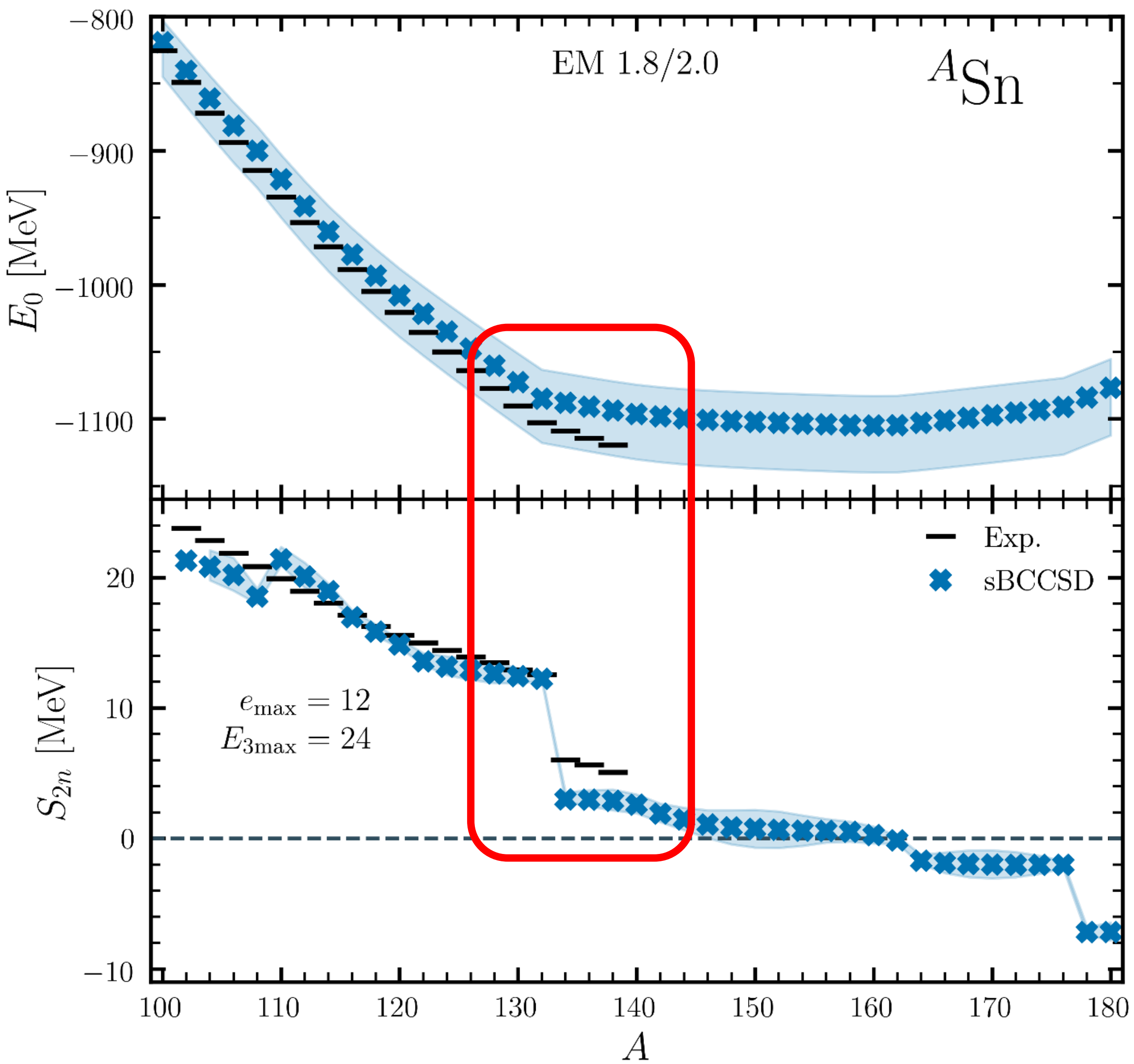
...before pushing to heavier open-shell nuclei

Tichai *et al.*, PLB (2024)

Heaviest open-shell *ab initio* calculation

^{180}Sn



sBCCSD calculations of ^{A}Sn isotopes

Polynomial scaling makes possible to go beyond ^{132}Sn

$\sigma_{\text{th-exp}}$ (E) = 15.4 MeV ~ 1.5%

Exaggerated N=82 magicity

- → Significant lack of binding in $^{132\text{-}138}$Sn
- → Outside many-body uncertainty estimate
- → **Attributable to interaction uncertainty**

...before pushing to heavier open-shell nuclei

Vernik *et al.*, unpublished

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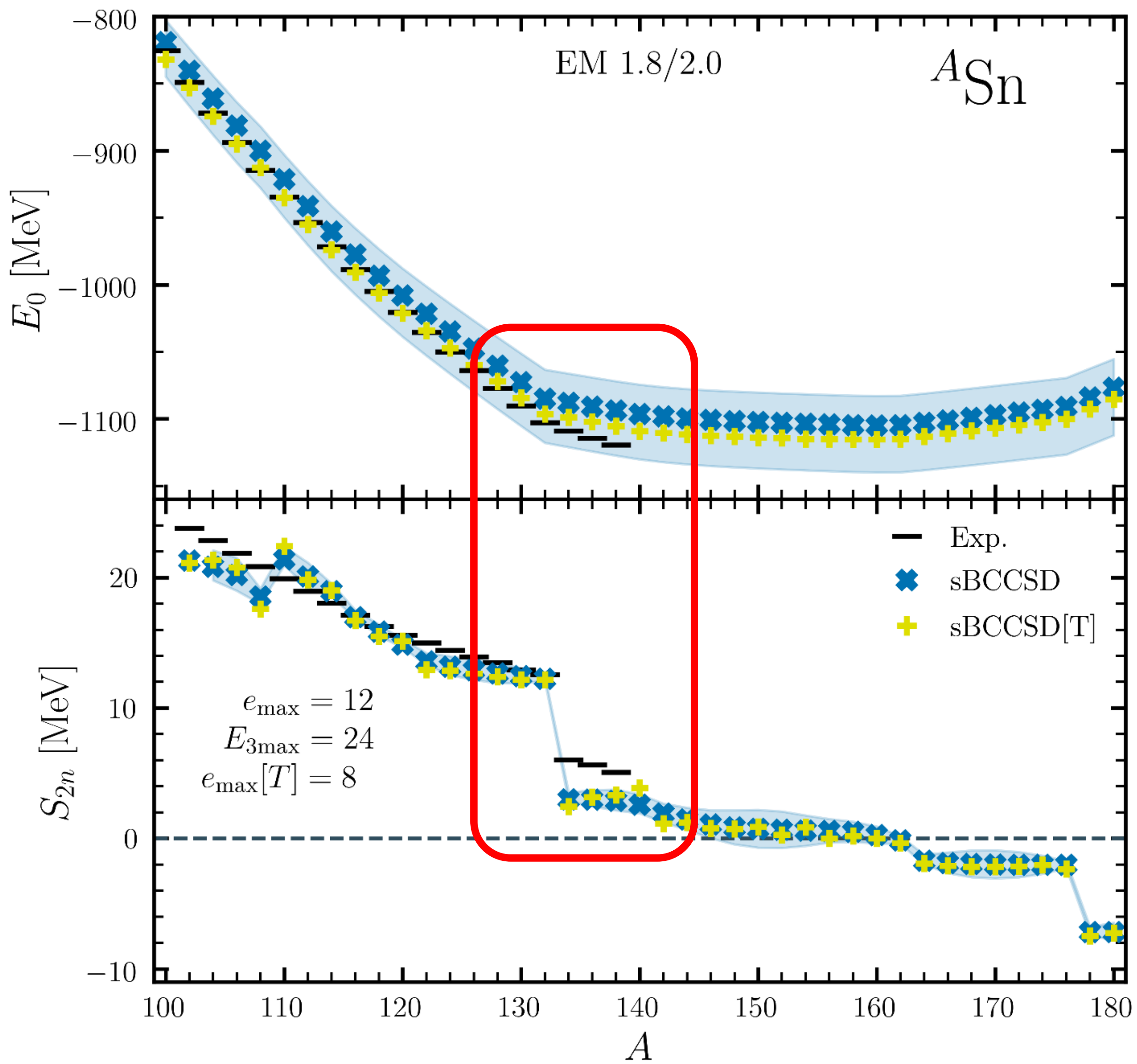

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sBCCSD[T]
$\sigma_{\text{th-exp}}$ (E) = 5.8 MeV ~ 0.5%
Exaggerated N=82 magicity remains
→ Little effect on relative energies as in ^{A}ca
→ **Need to push to $e_{\max}$=10**

...before pushing to heavier open-shell nuclei

Tichai *et al.*, PLB (2024)

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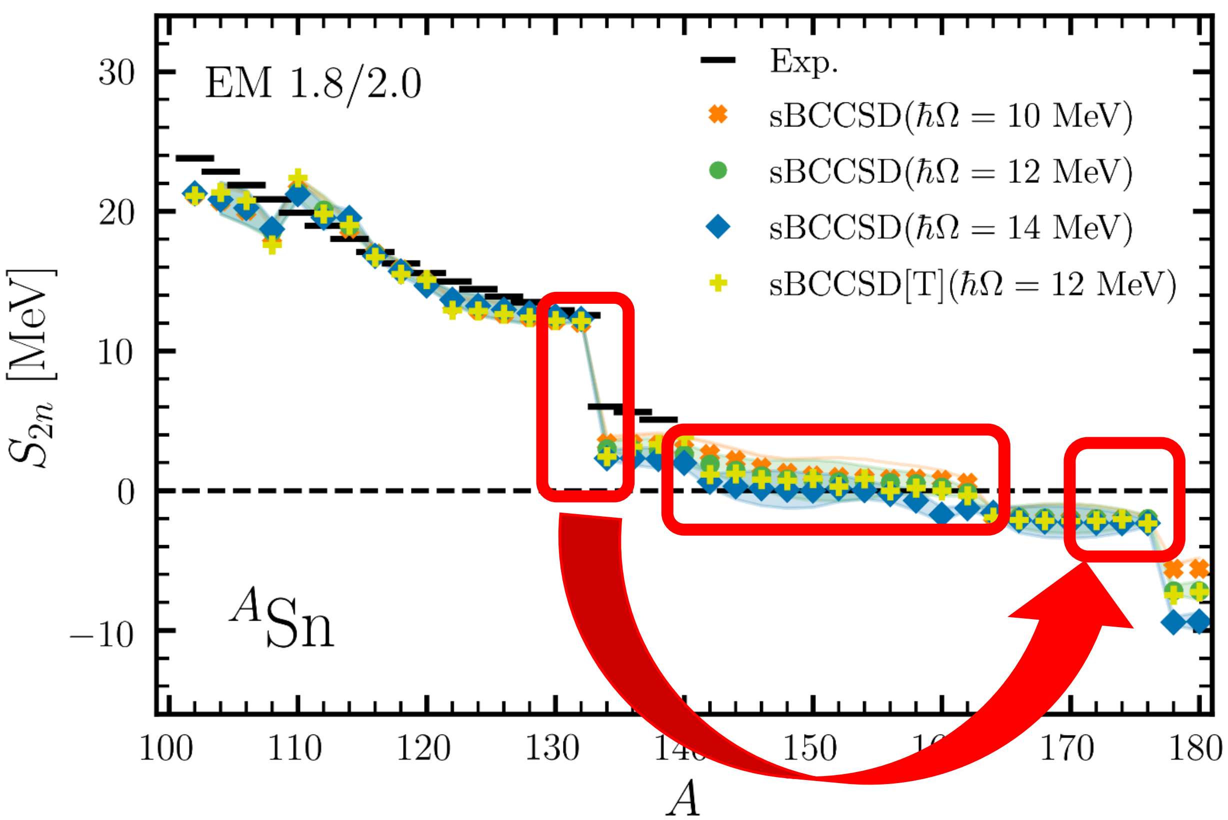

Could be compatible with EDF prediction

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→ **Need to push [T] to e_{max}=10**

Very neutron-rich Sn isotopes

Significant sensitivity to hw value at e_{max} = 12

→ **1BB size uncertainty larger than estimated**

Predicted drip-line location [^{140}Sn, ^{162}Sn]

→ Much affected by 1BB size uncertainty: δN = 22!

→ **Possibly equally affected by interaction uncertainty**

→ **Not affected by (perturbative) [T] at e_{max}=8**

Need to push beyond e_{max} = 12 in heavy neutron-rich open-shell nuclei

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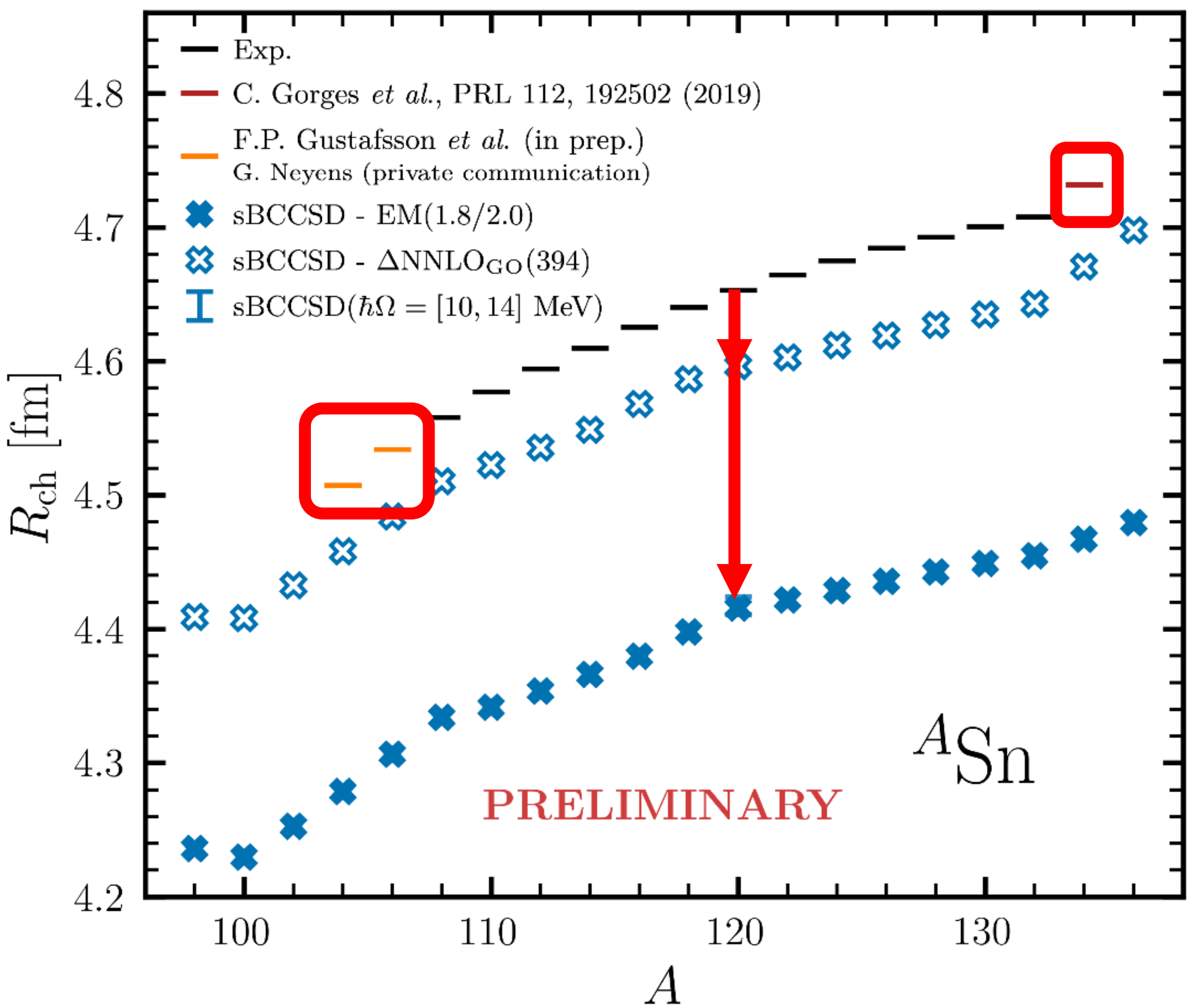
…and beyond energies: charge radii in Sn

Demol *et al.*, unpublished



Absolute radii from sBCCSD

Recent/unpublished new data in ^{134}Sn/$^{104-106}$Sn

Results depend strongly on χEFT-based interaction

→ EM 1.8/2.0 radii too small by 5%

→ ΔNNLOGo underestimates by 1%

→ Variants to be tested

Arthuis *et al.*, arXiv:2401.06675

...and beyond energies: charge radii in Sn

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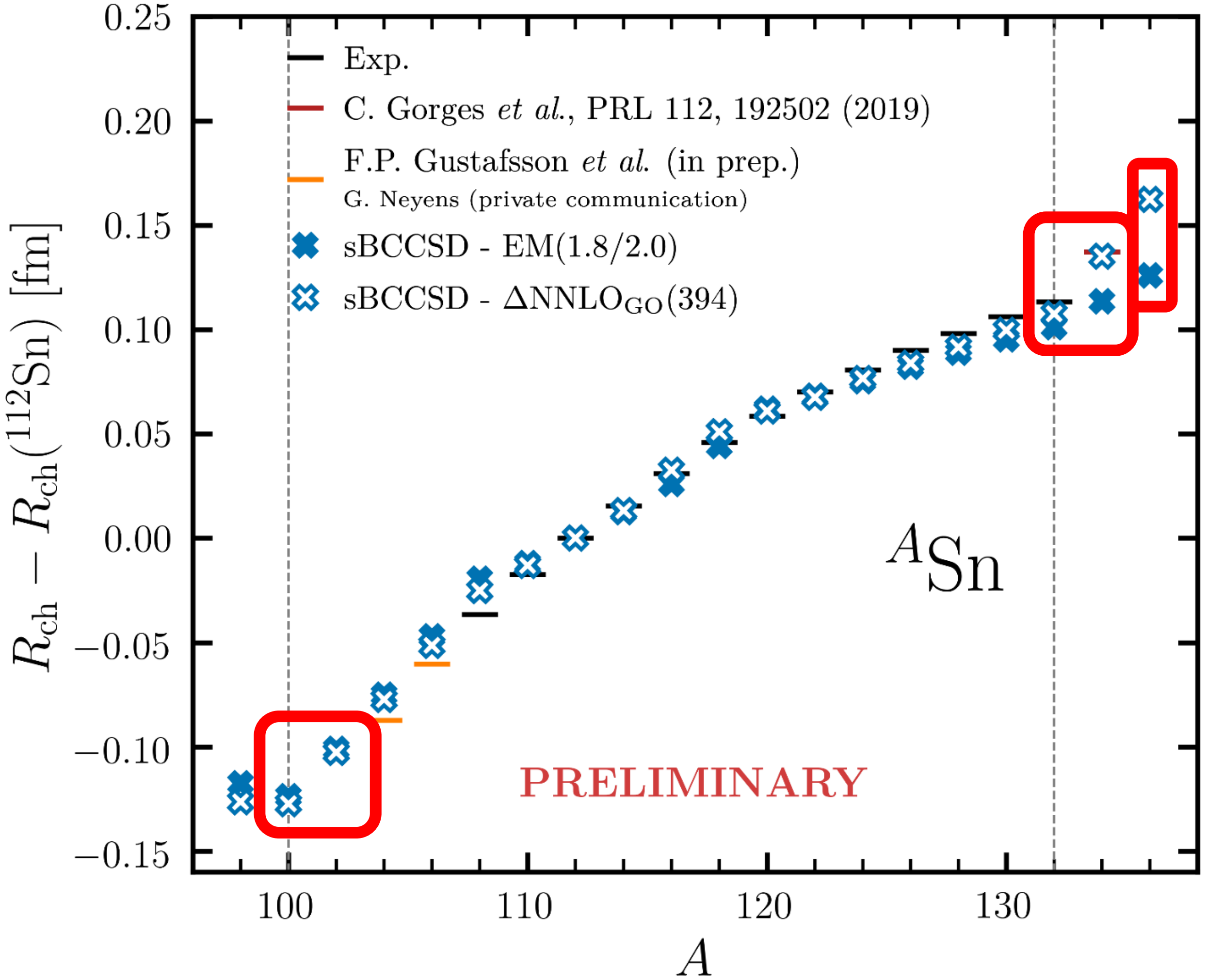

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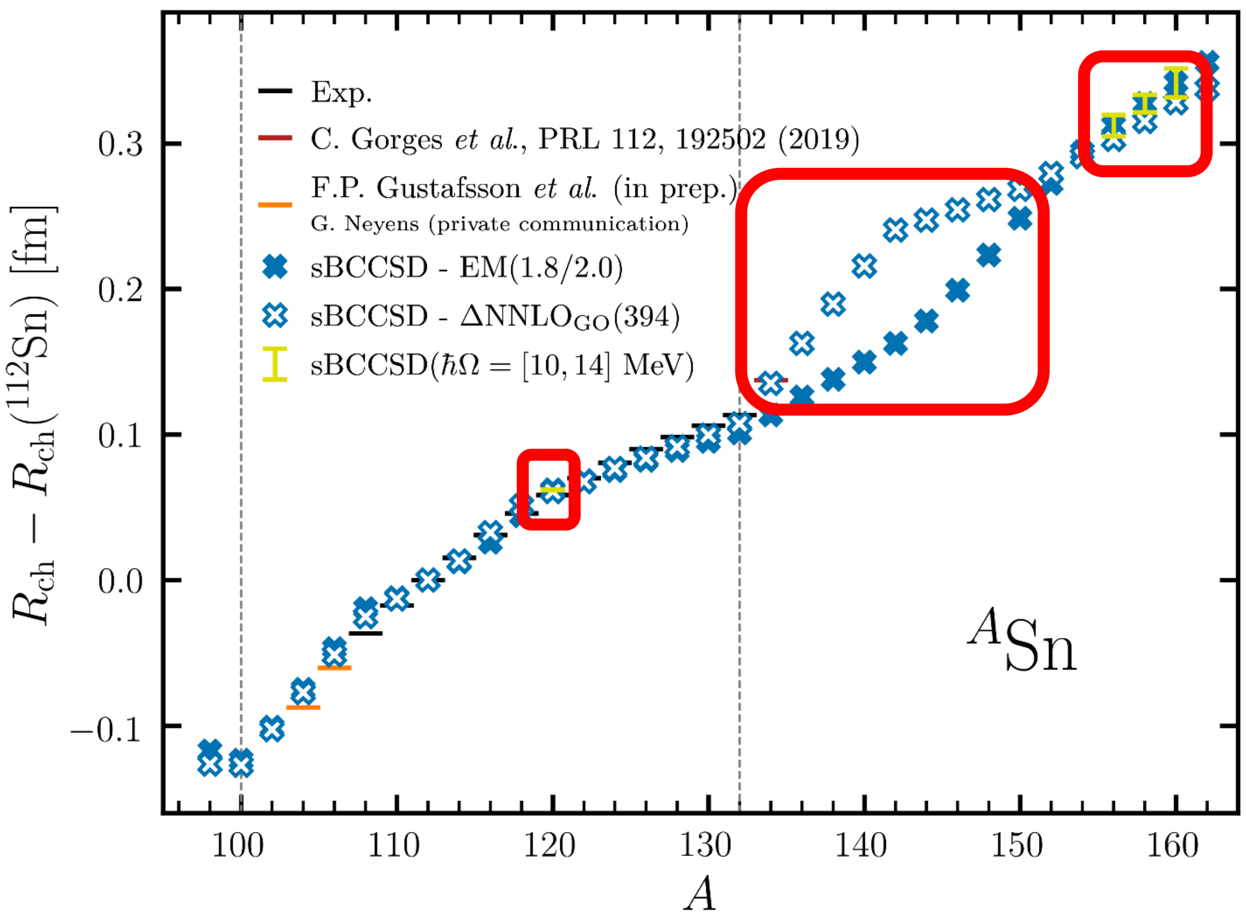
Isotope shifts
sBCCSD in great agreement with data (linear&quad)
Kink at N=82 thanks to recent data in ^{134}Sn
→ EM 1.8/2.0 underestimates it (too large S_{2n} drop)
→ ΔNNLOGo reproduces it (way too large S_{2n} drop) →
Can variant capture it all? — Arthuis *et al.*, arXiv:2401.06675

Going below ^{104}Sn and beyond ^{134}Sn
→ Possible at CRIS@ISOLDE in future with MR-TOF

...and beyond energies: charge radii in Sn

Demol *et al.*, unpublished



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Can variant capture it all? — Arthuis *et al.*, arXiv:2401.06675

Extension to very neutron rich isotopes

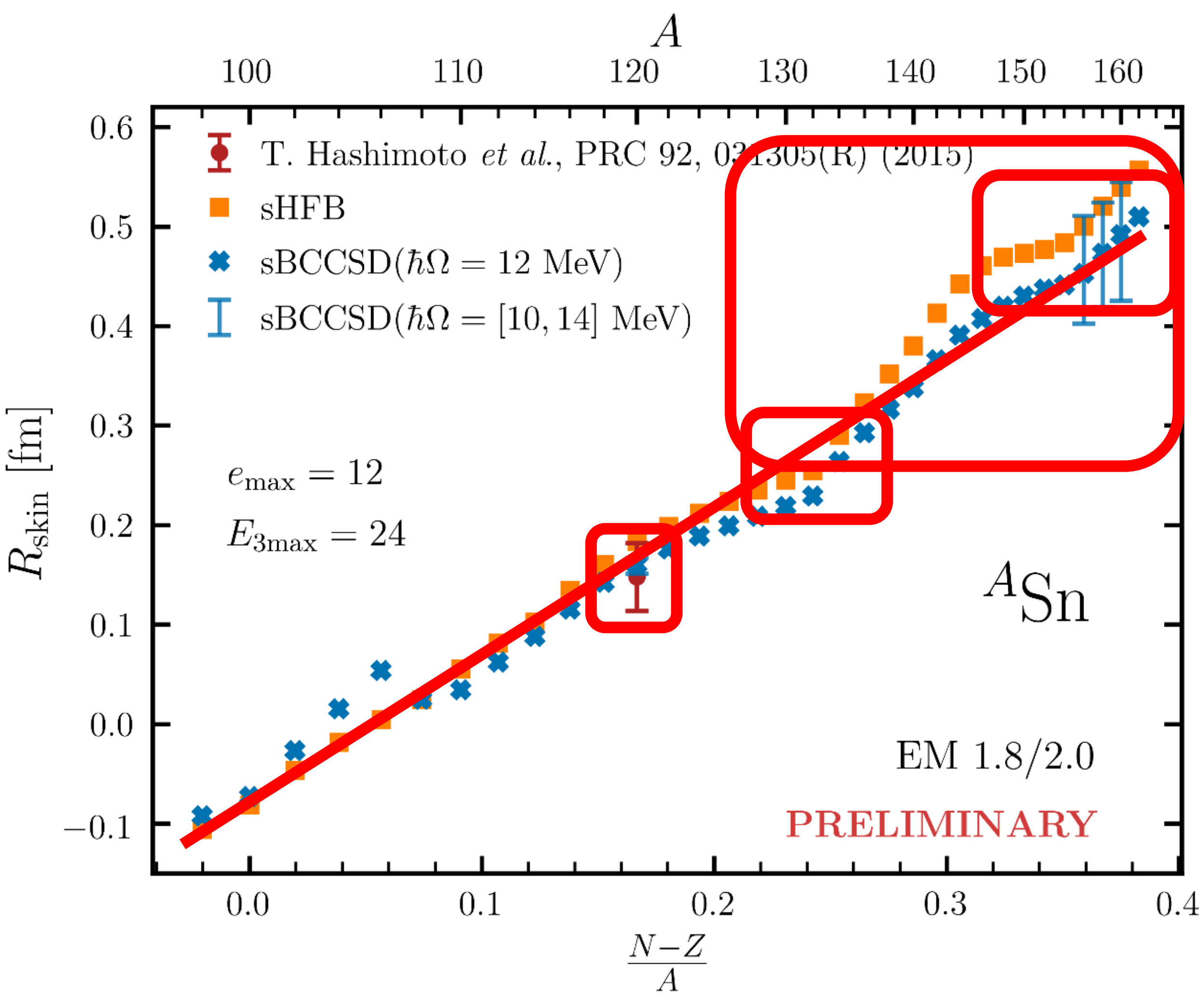
→ Possible thanks to polynomial scaling

→ Increased hw sensitivity at emax=12 with N-Z

→ Need thorough uncertainty quantification

…and beyond energies: neutron skin in Sn

Demol *et al.*, unpublished



Neutron skin thickness
Correlated to the symmetry energy slope L
→ **Key information about the nuclear EOS**
Extracted value in ^{120}Sn from α_D well reproduced

Very neutron rich isotopes
Sensitive to H in CS nuclei Arthuis ***et al.***, arXiv:2401.06675
→ Can be studied systematically here (to be done)
Linear with I=(N-Z)/A in CS nuclei Novario *et al.*, PRL (2023)
→ **Kinks at N=82 and N=104**
→ Driven by neutrons (but underestimated for protons!)
Impact of dynamical correlations (up to 0.05 fm)
→ Triples correction to be evaluated soon
More sensitive to hw value at e_{max} = 12
→ **Uncertainty estimation (to be done)**

Conclusions

- Ask me if not clear