IMSRG CALCULATIONS AND UNCERTAINTY QUANTIFICATION FOR NEUTRON SEPARATION ENERGIES IN MEDIUM-MASS AND HEAVY NUCLEI

Max Cincar

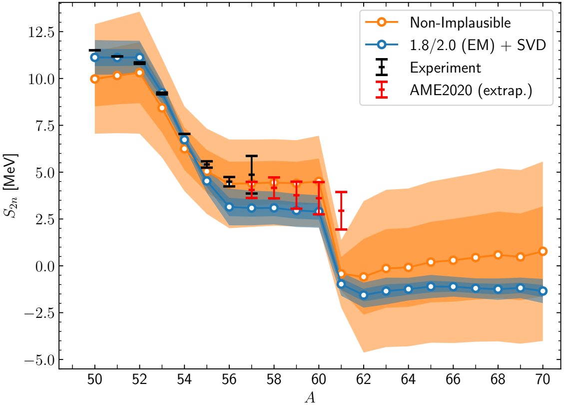
with Zhen Li, Tom Plies, Urban Vernik, Matthias Heinz,

Takayuki Miyagi and Achim Schwenk

Introduction & Motivation

- $S_{xn} = BE(Z, A-x) - BE(Z, A)$
- Nuclear structure of neutron-rich nuclei:
  - Shell closures and shell evolution
  - Neutron dripline
- Experiments provide test for nuclear theory
- S_n for heavy nuclei needed for r-process
  $\rightarrow$ Origin of heavy elements
- Need theory prediction + uncertainty

Example: Ca isotopes



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Nuclear interactions

- Chiral effective field theory (EFT)
  $\rightarrow$ systematic expansion of nuclear Hamiltonian

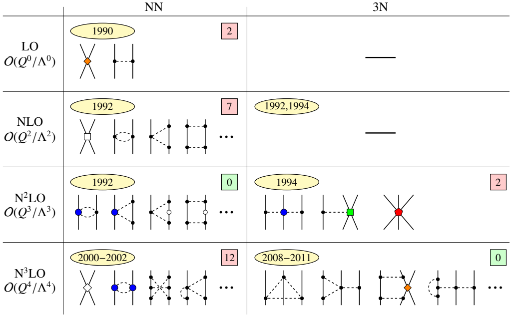
- At a given order of chiral EFT

$$H = H_0 + c_i \sum_i H_i$$

- Distribution of c_i via statistical methods

- Distributions used:
  - 34 Non-implausible (NI) interactions Hu et al., NP (2022)
  - 101 1.8/2.0 (EM) + SVD interactions

    Hebeler et al., PRC (2011), Plies et al., PRC (2026)

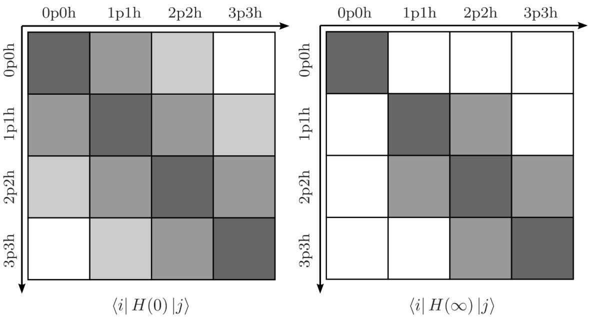


Hebeler et al., PR (2021)

In-Medium Similarity Renormalization Group (IMSRG)

Tsukiyama et al., PRL (2011), Hergert et. al., PR (2016)

- Start from reference state $|\phi\rangle$
- Transform $H(s) = U(s)H(0)U^{\dagger}(s)$
- Differential equation $\frac{dH(s)}{ds} = [\eta(s), H(s)]$
- Expansion in finite harmonic oscillator basis $2n + l \leq \mathbf{e}_{\text{max}}$



- Approximate unitary transformation by truncating operators to two-body rank
  $\rightarrow$ **IMSRG(2)** approximation

Uncertainty model

- Normal distributions to model uncertainties

$$\mathcal{N}(\mu, \Sigma) = \mathcal{N}(\mu_0, \Sigma_0) + \sum_i \mathcal{N}(\Delta\mu_i, \Sigma_i)$$

- Interaction distribution: $\mathcal{N}(\mu_0, \Sigma_0)$

- Vary **e**$_{\max} = 10, 12, 14$ and extrapolate to infinite basis limit: $\mathcal{N}(\mu_{\mathrm{ms}}, \Sigma_{\mathrm{ms}})$
  Furnstahl et al., JPG (2015)

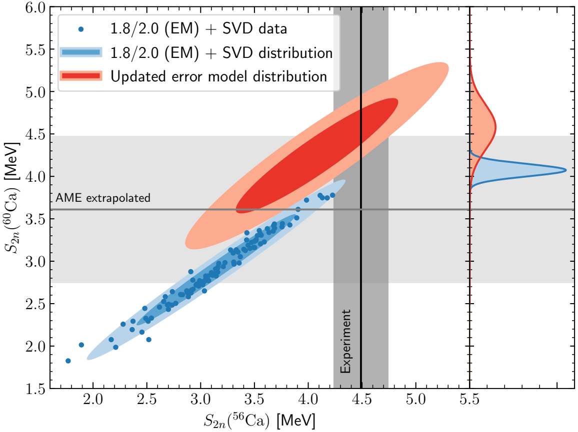
- **IMSRG(3f$_2$)** for leading corrections beyond IMSRG(2): $\mathcal{N}(\mu_{\mathrm{mb}}, \Sigma_{\mathrm{mb}})$
  He et al., PRC (2024)

Correlations among S_{2n}

- Correlations between S_{2n} of ^{56}Ca and ^{60}Ca
- Ab initio correlations + experiment
- Error model gives **updated prediction**
- Agreement with AME 2020 extrapolation

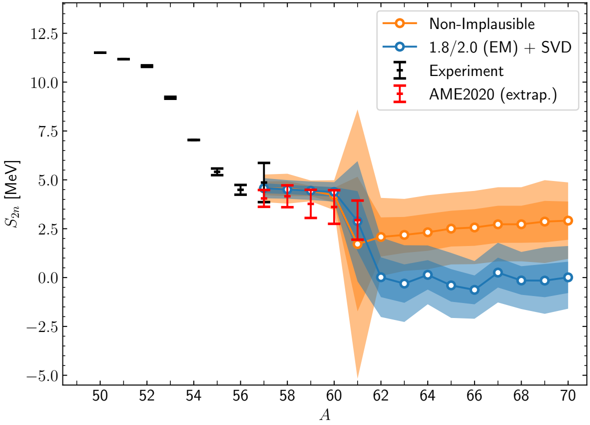
  Meng et al., CPC (2021)

- Uncertainties have statistical interpretation
  $\rightarrow$ Testable prediction



Predictions for Ca isotopic chain

- Use experimental data in ^{50}Ca - ^{56}Ca
- Unambiguous prediction up to ^{60}Ca
- Small tension for $A > 60$
- Measurements to ^{62}Ca can change results
- Interaction uncertainty most important
- Additional $\sim 250 - 350$ keV uncertainty



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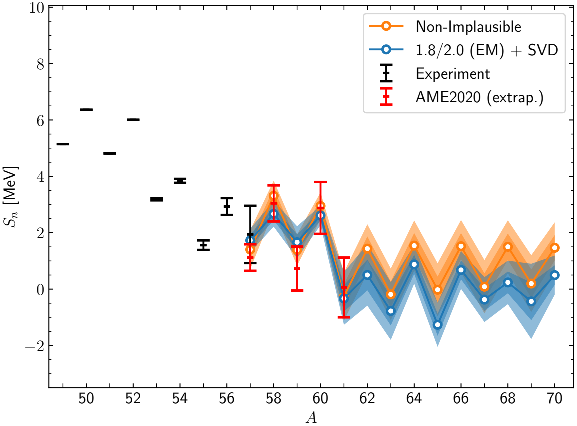


The N=82 region

- Relevant for the astrophysical r-process

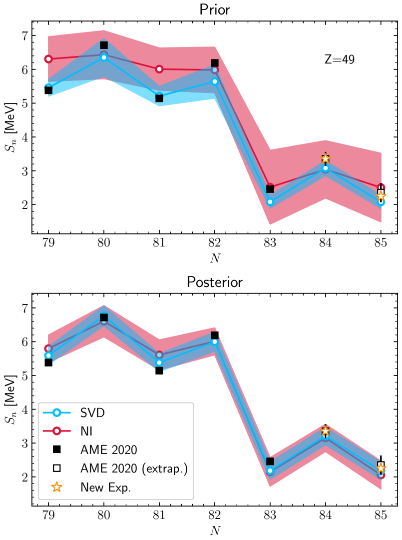
  Kuske et al., PRL (2026)

- Precise data in Sn (Z=50) available
- Shell structure from Sn isotopic chain
- Large computational cost:
  - improve sampling
  - use estimates from Ca
- Controlled extrapolation with uncertainties

^{129}Sn	^{130}Sn	^{131}Sn	^{132}Sn	^{133}Sn	^{134}Sn	^{135}Sn	Experiment
^{128}In	^{129}In	^{130}In	^{131}In	^{132}In	^{133}In	^{134}In	
^{127}Cd	^{128}Cd	^{129}Cd	^{130}Cd	^{131}Cd	^{132}Cd	^{133}Cd	Extrapolate
^{126}Ag	^{127}Ag	^{128}Ag	^{129}Ag	^{130}Ag	^{131}Ag	^{132}Ag	
^{125}Pd	^{126}Pd	^{127}Pd	^{128}Pd	^{129}Pd	^{130}Pd	^{131}Pd	

Results for N=82 region

- Focus on representative In (Z=49) isotopes
- Excellent agreement between distributions
- Good agreement with experiment
- Shell structure and pairing well constrained by data in Sn and ab initio correlations
- Similar results for all nuclei calculated



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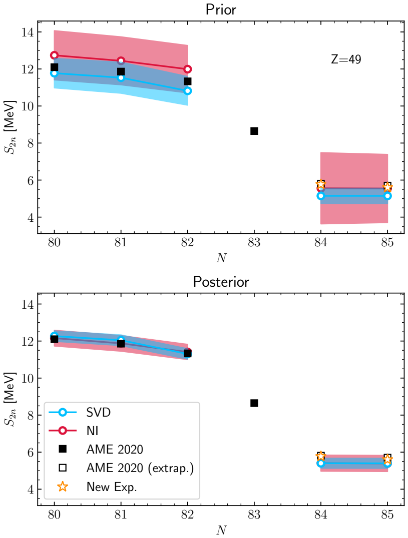
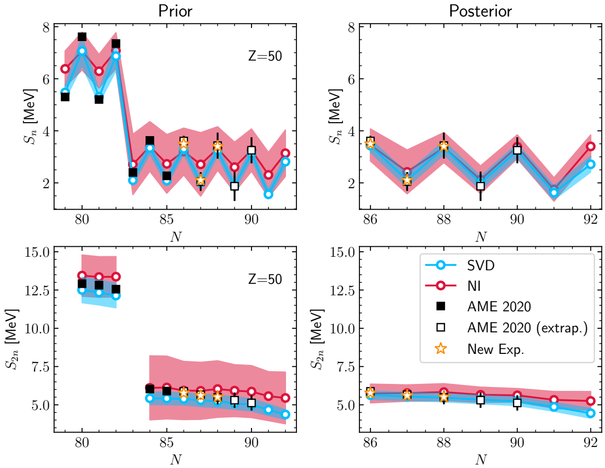


Sn isotopes around N=90

- Apply model to unmeasured Sn isotopes
- Absence of shell closure for N=90
- Agrees with other ab initio calculations

  Vernik et al., arXiv:2607.05086 (2026)

  Bonaiti et al., arXiv:2607.09897 (2026)
- Systematic interaction uncertainties possible up to heavy Sn isotopes



Summary and Outlook

- Uncertainty quantification for S_n and S_{2n} up to heavy neutron-rich nuclei
- Test of modern nuclear interactions + many-body theory
- Application to nuclear astrophysics possible
- Future work:
  - Provide ab initio predictions for most important r-process nuclei
  - Extend framework to more observables
  - Increase precision of calculations