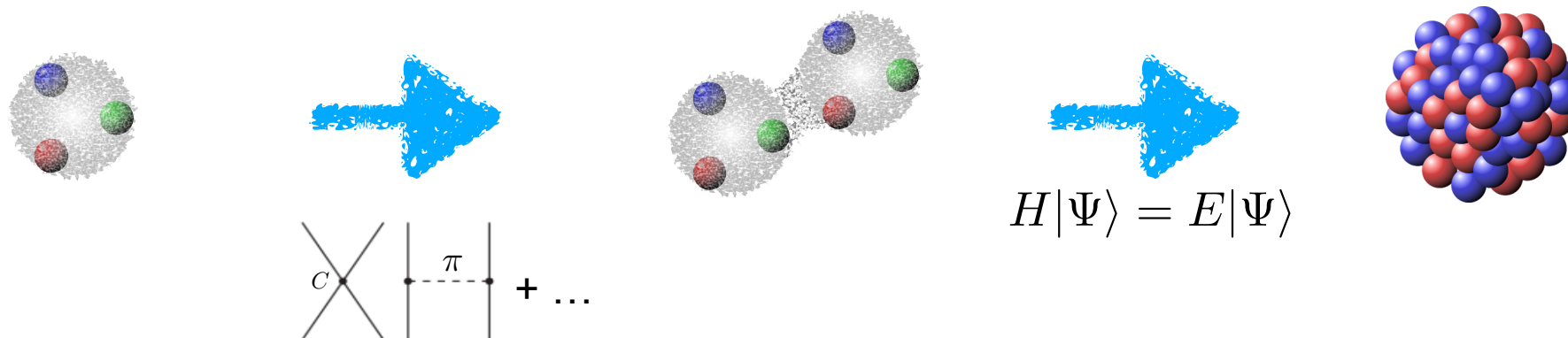


Heavy-mass frontier in nuclear ab initio calculations



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SFB workshop, Darmstadt (October 6, 2022)

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T. Papenbrock (University of Tennessee)

Z. Sun (University of Tennessee)

I. Vernon (University of Durham)

Noritaka Shimizu (University of Tsukuba)

Yusuke Tsunoda (University of Tsukuba)

New 3N matrix element storage

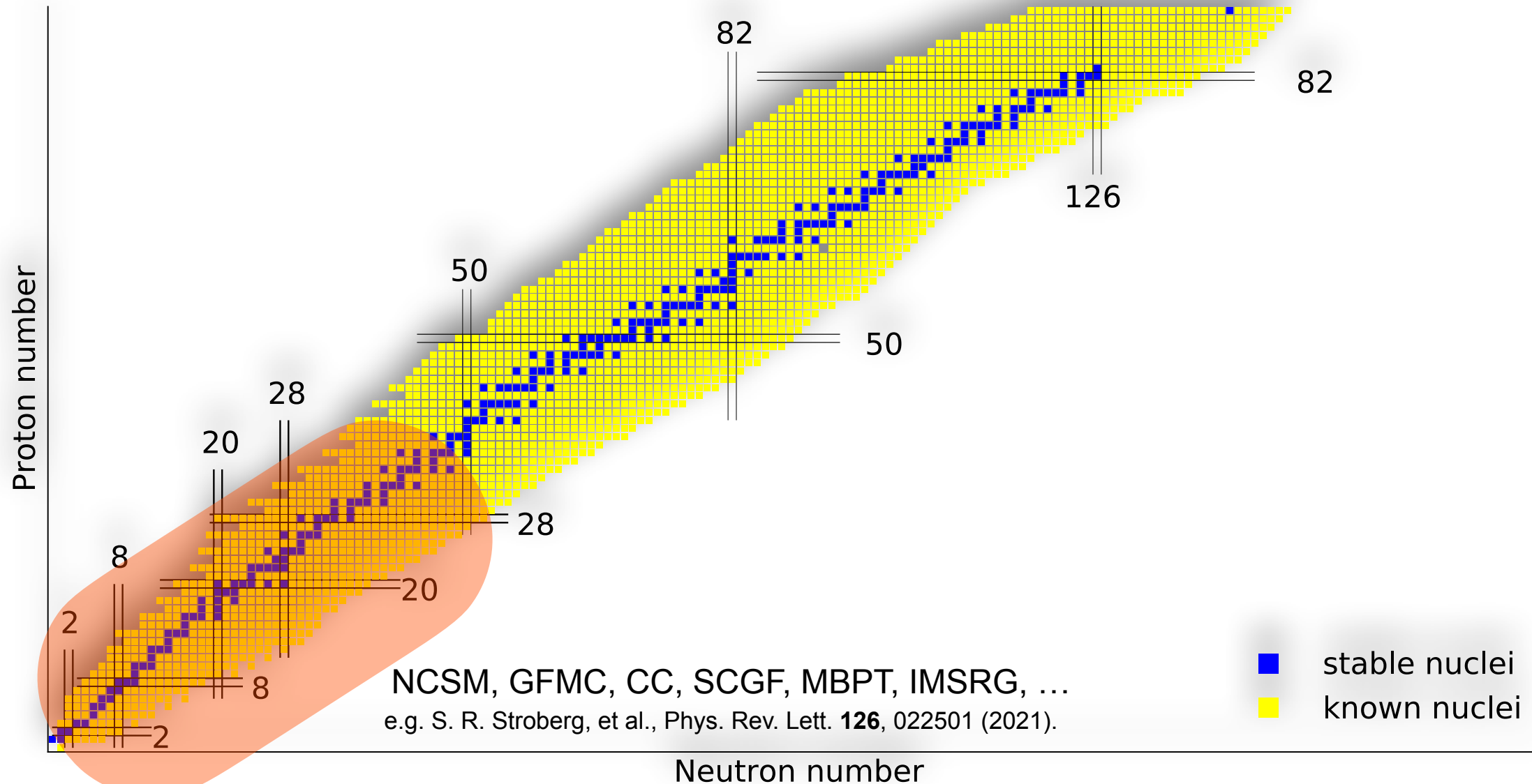
TM et al., Phys. Rev. C 105, 014302 (2022).

Application to ^{208}Pb

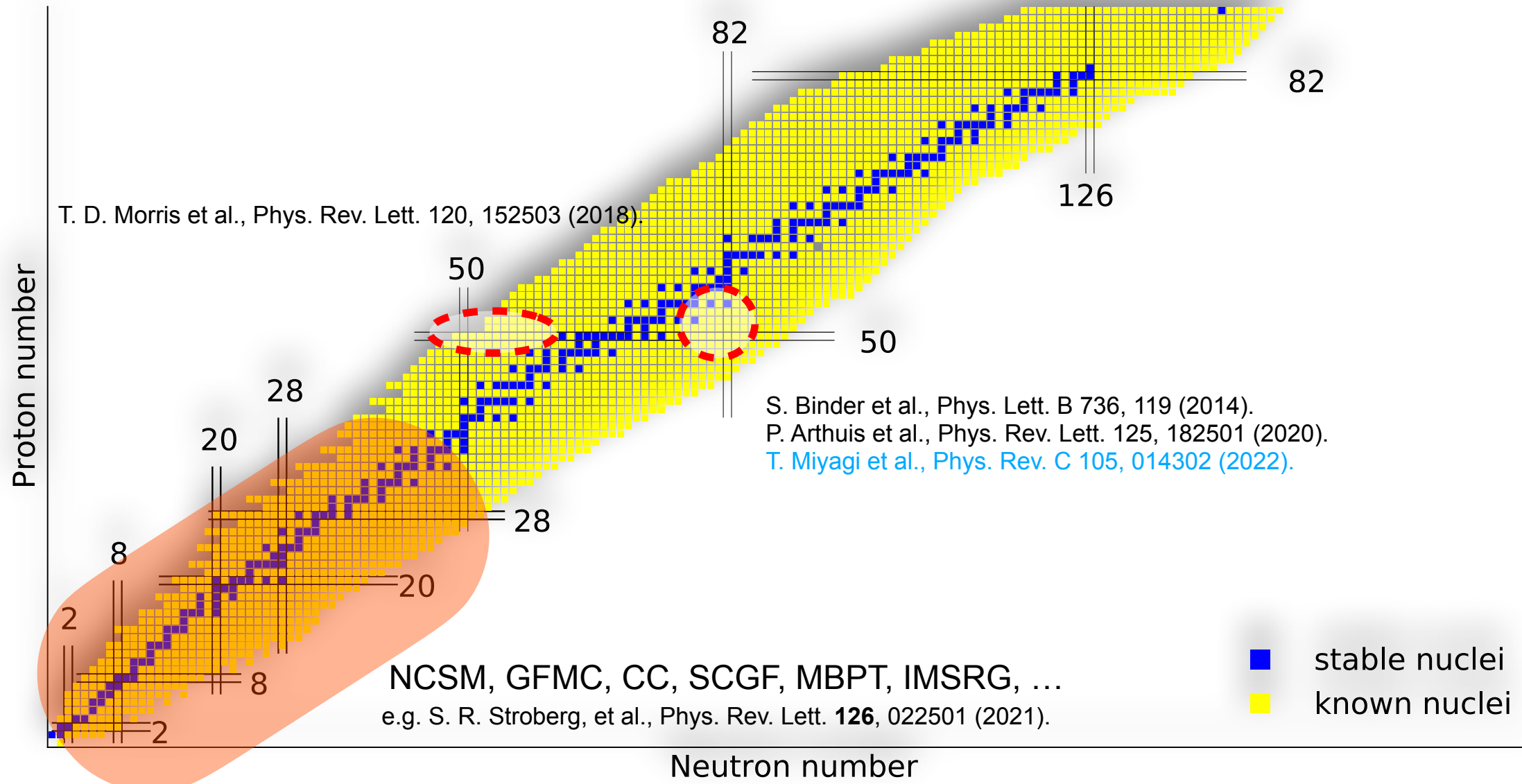
B. Hu et al., Nat. Phys. (2022).

Large valence-space diagonalization

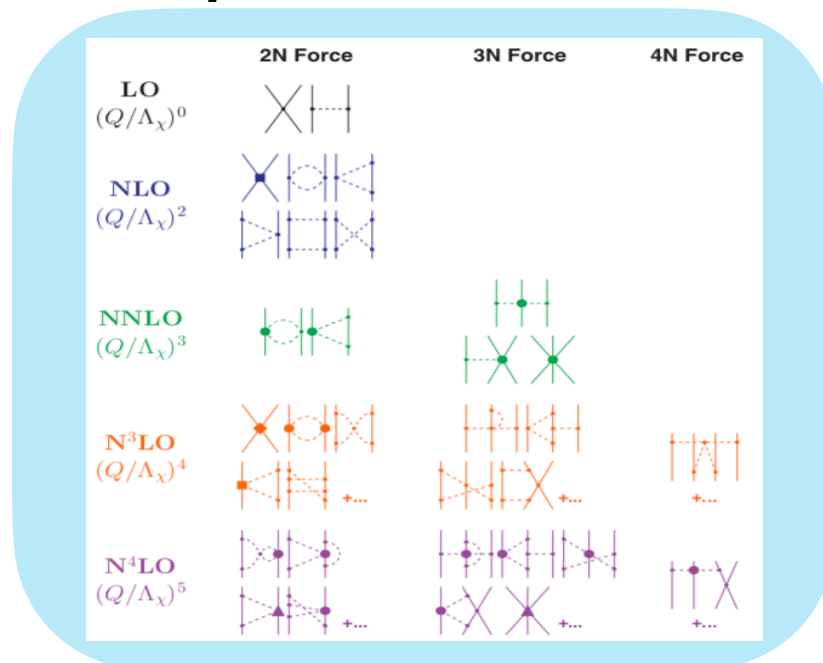
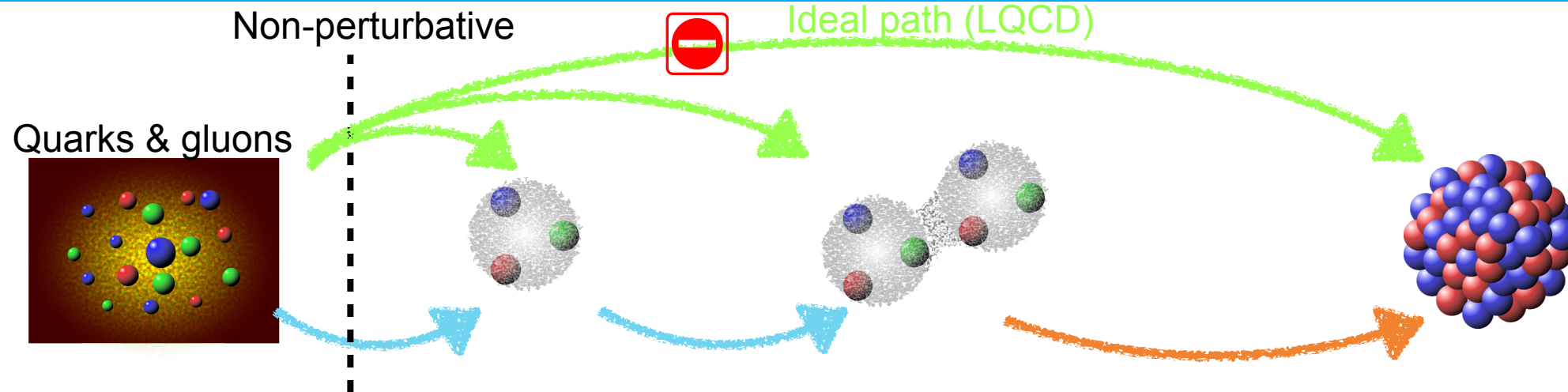
Heavy-mass frontier in ab initio methods



Heavy-mass frontier in ab initio methods



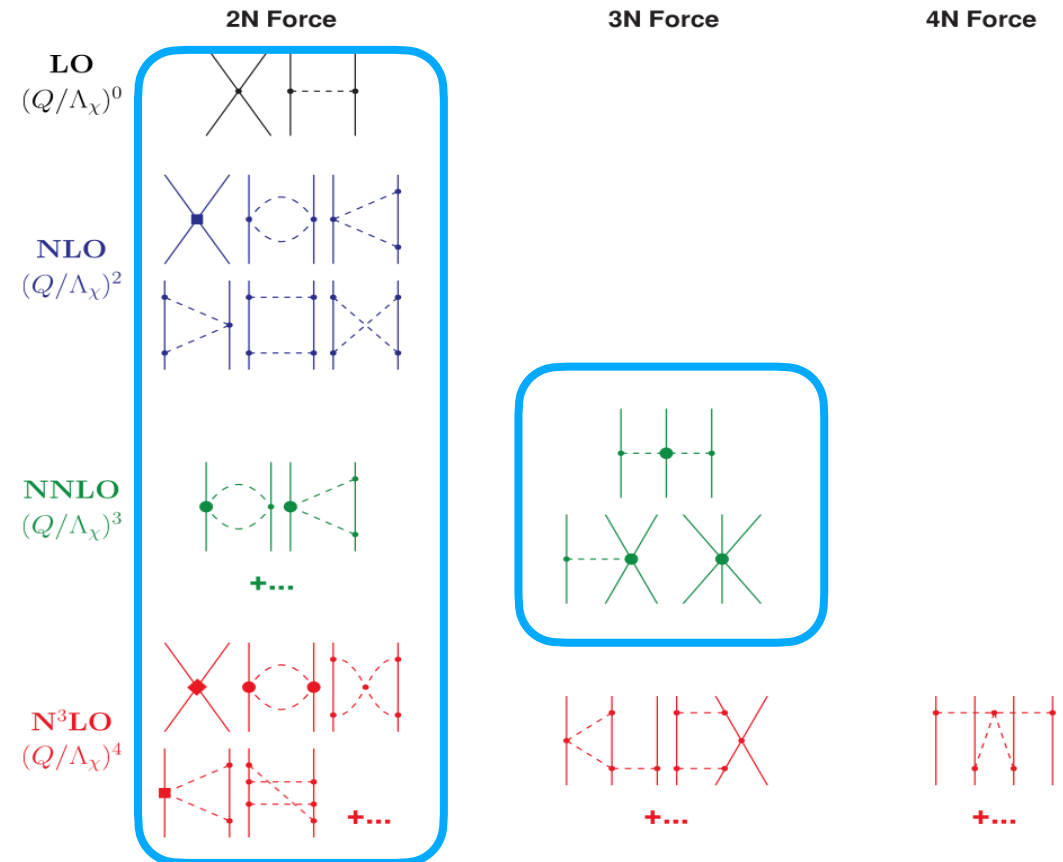
Nuclear ab initio calculation



Nuclear many-body problem

- ◆ Green's function Monte Carlo
- ◆ No-core shell model
- ◆ Nuclear lattice effective field theory
- ◆ Self-consistent Green's function
- ◆ Coupled-cluster
- ◆ In-medium similarity renormalization group
- ◆ Many-body perturbation theory

- Lagrangian construction
 - ◆ Chiral symmetry
 - ◆ Power counting
- Systematic expansion
 - ◆ Unknown LECs
 - ◆ Many-body interactions
 - ◆ Estimation of truncation error

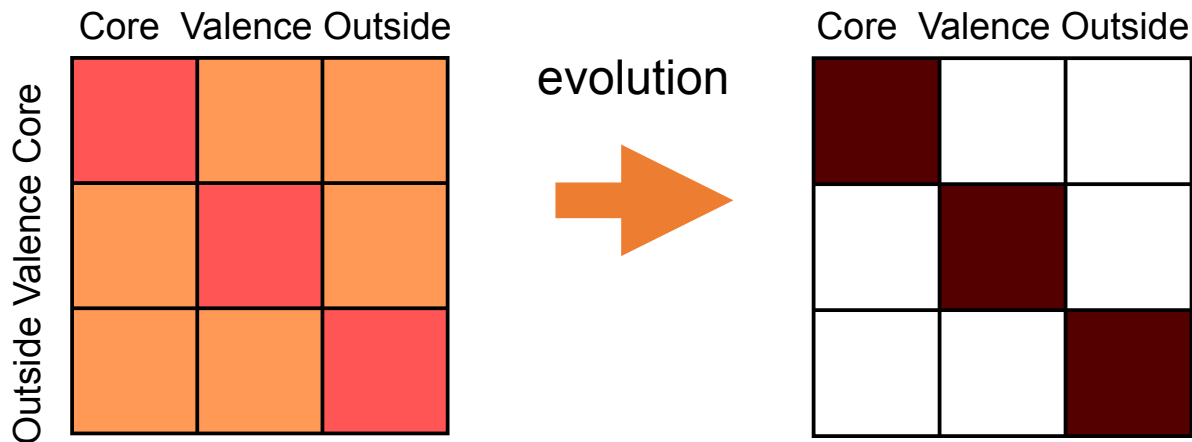


Valence-space in-medium similarity renormalization group



● : frozen core
 — : valence
 - - - : outside

$$\frac{d\Omega}{ds} = \eta(s) - \frac{1}{2}[\Omega(s), \eta(s)] + \dots$$



Similarity transformation

H

$$H(s) = e^{\Omega(s)} H e^{-\Omega(s)}$$

$$H(s) \approx E(s) + \sum_{12} f_{12}(s) \{a_1^\dagger a_2\} + \frac{1}{4} \sum_{1234} \Gamma_{1234}(s) \{a_1^\dagger a_2^\dagger a_4 a_3\}$$

s: flow parameter

$$\eta(s) = \sum_{12} \eta_{12}(s) \{a_1^\dagger a_2\} + \sum_{1234} \eta_{1234}(s) \{a_1^\dagger a_2^\dagger a_4 a_3\}$$

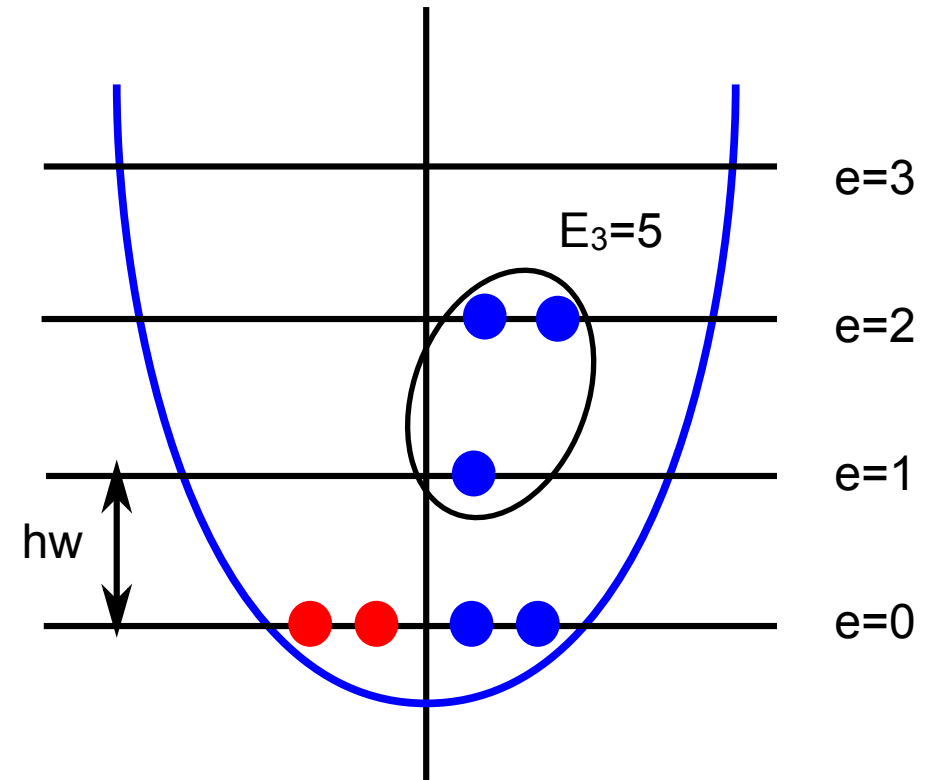
$$\eta_{12} = \frac{1}{2} \arctan \left(\frac{2f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta} \right)$$

$$\eta_{1234} = \frac{1}{2} \arctan \left(\frac{2\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta} \right)$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

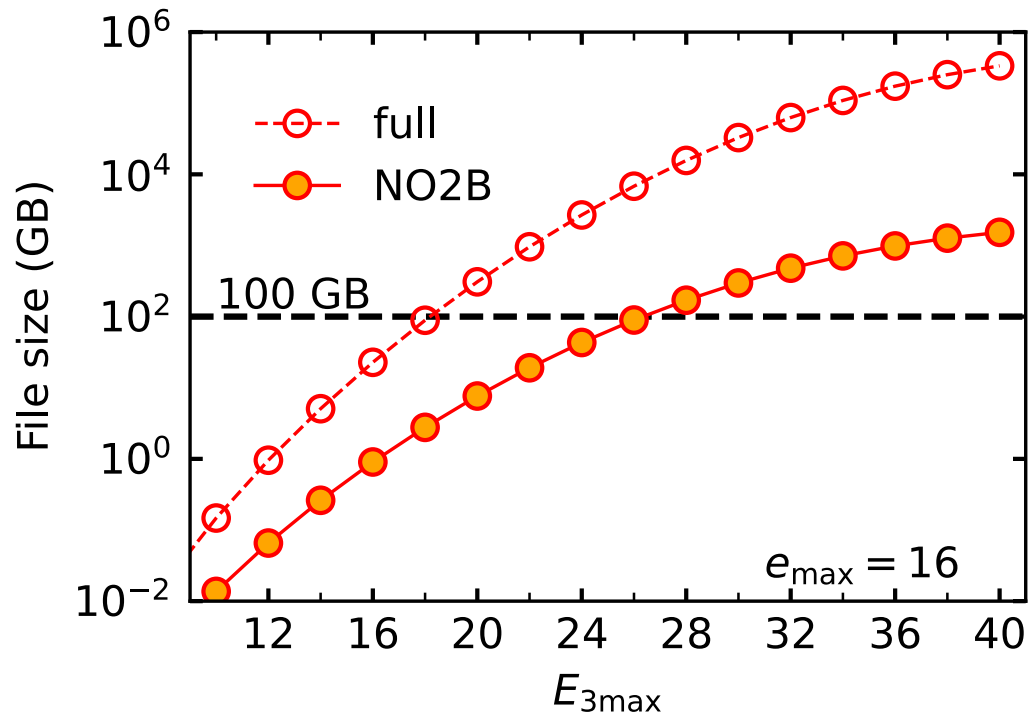
f_{12}, Γ_{1234} : matrix element we want to suppress

- $NN+3N$ Hamiltonian (harmonic oscillator basis)
- Parameters:
 - ◆ hw
 - ◆ $e_{\max} = \max(2n+1)^*$
 - ◆ $E_{3\max} = \max(e_1+e_2+e_3)$.
- As e_{\max} and $E_{3\max}$ increases, the observable should not depend on all the parameters.

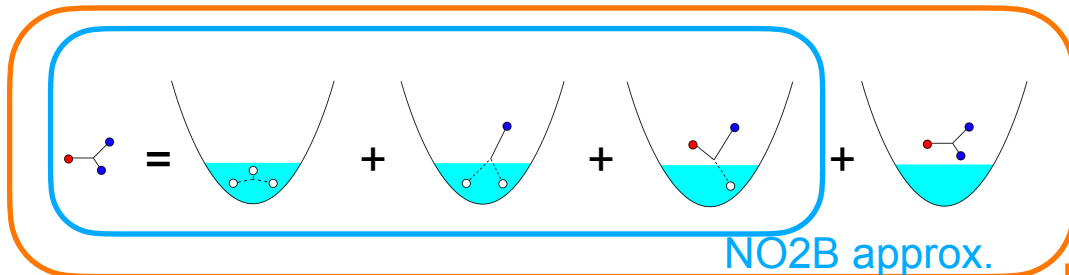
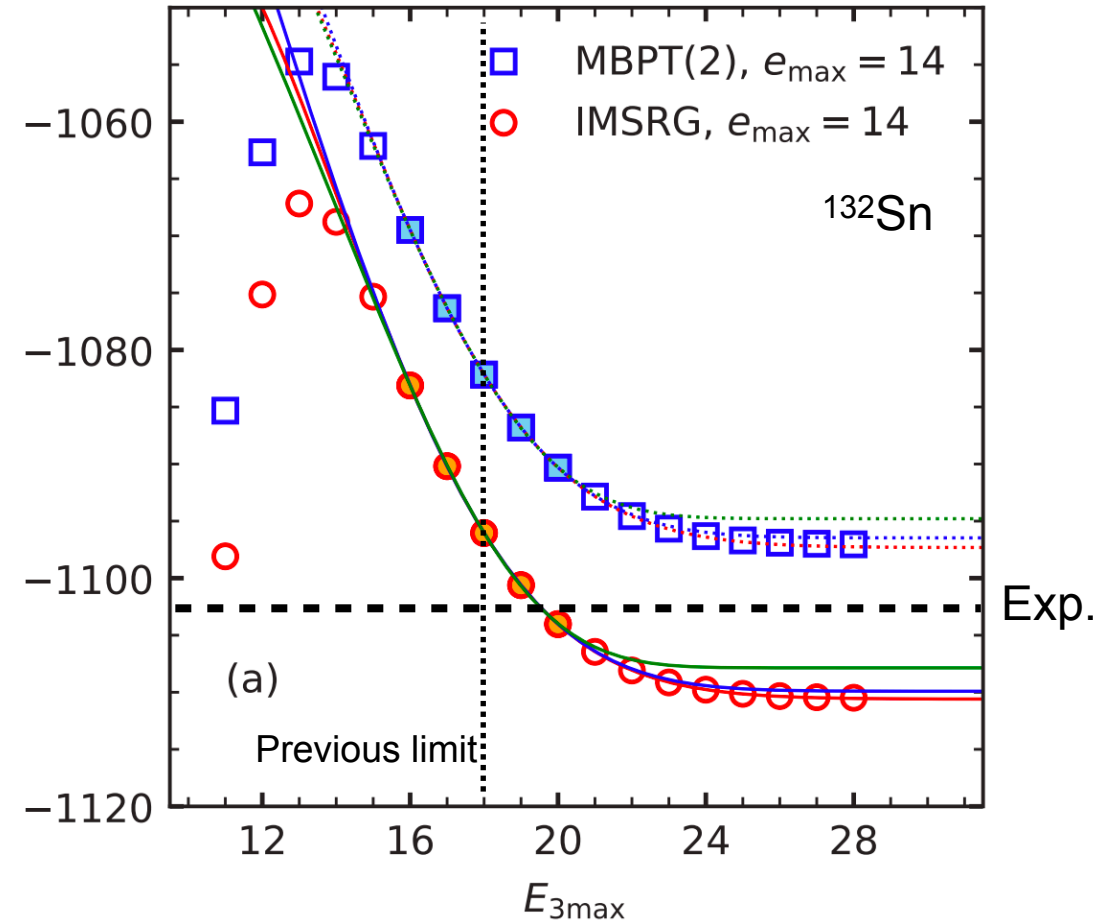


*Equivalent to (number of major shells)+1

$E_{3\max}$ convergence in heavy nuclei



TM, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, Phys. Rev. C 105, 014302 (2022).



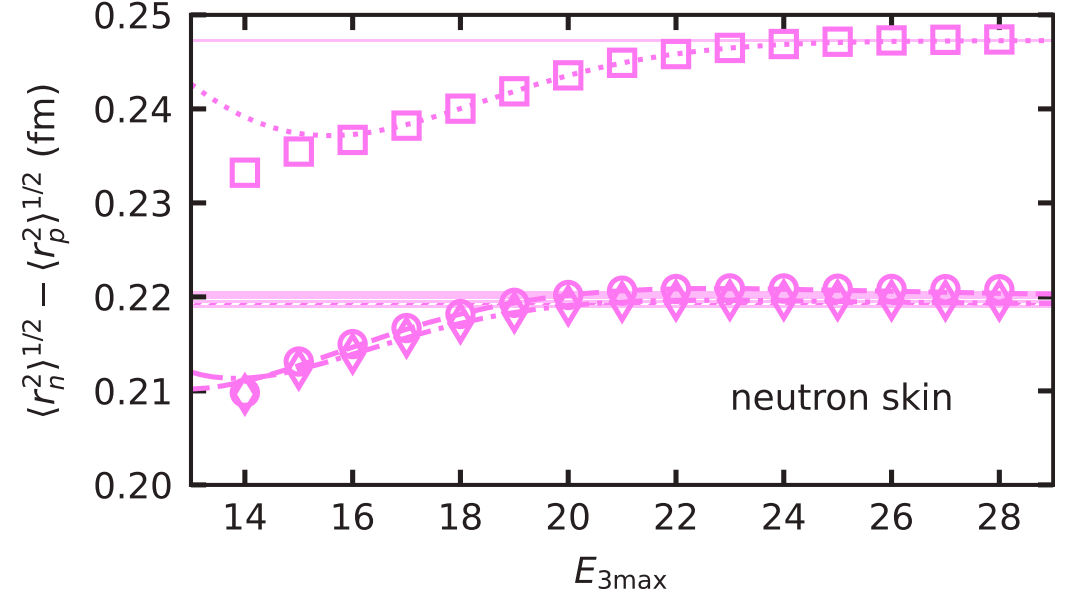
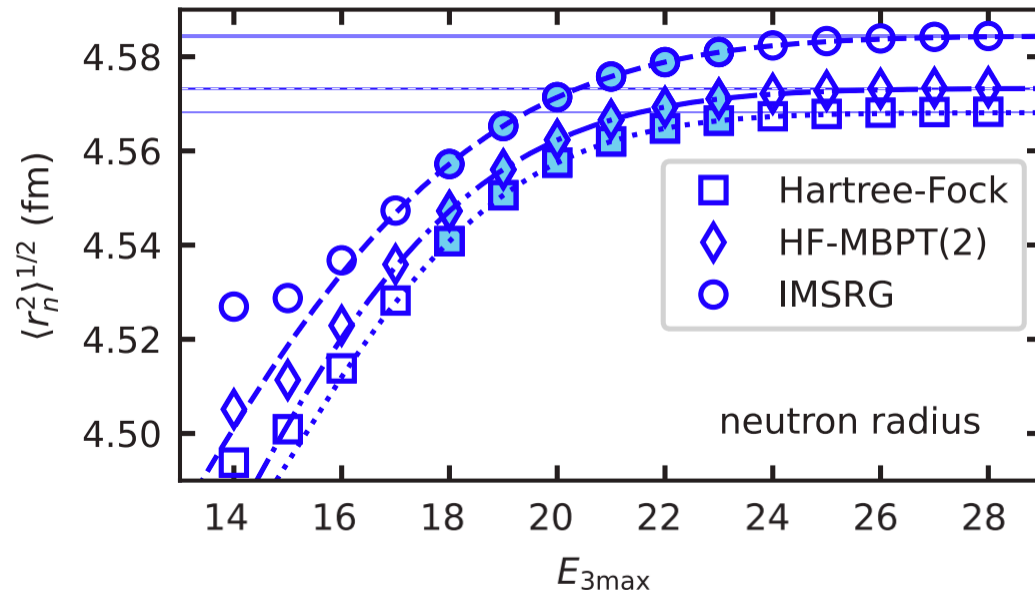
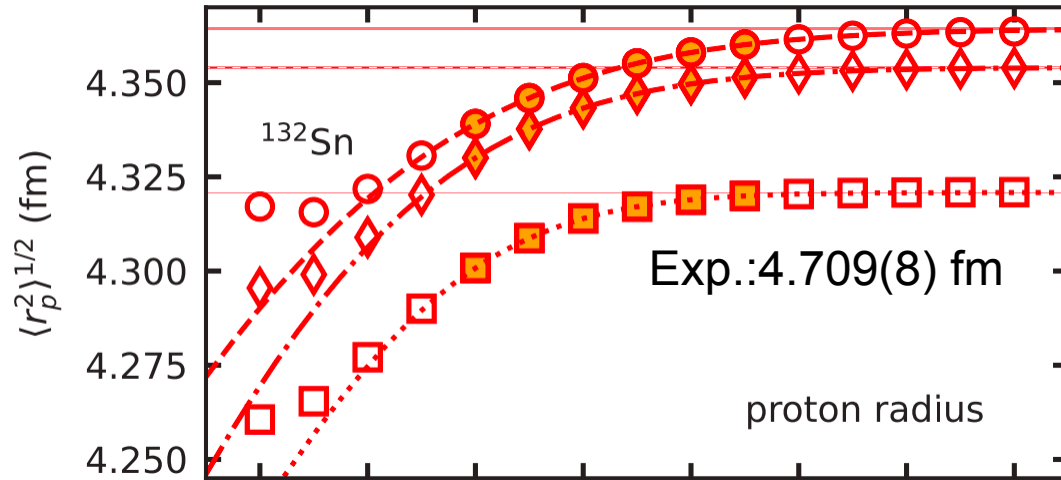
NO2B approximation error ~ a few %
[S. Binder et al., Phys. Rev. C 87, 021303 (2013).]

Full

Asymptotic form: $E \approx A\gamma_{\frac{2}{n}} \left[\left(\frac{E_{3\max} - \mu}{\sigma} \right)^n \right] + E_{\infty}$

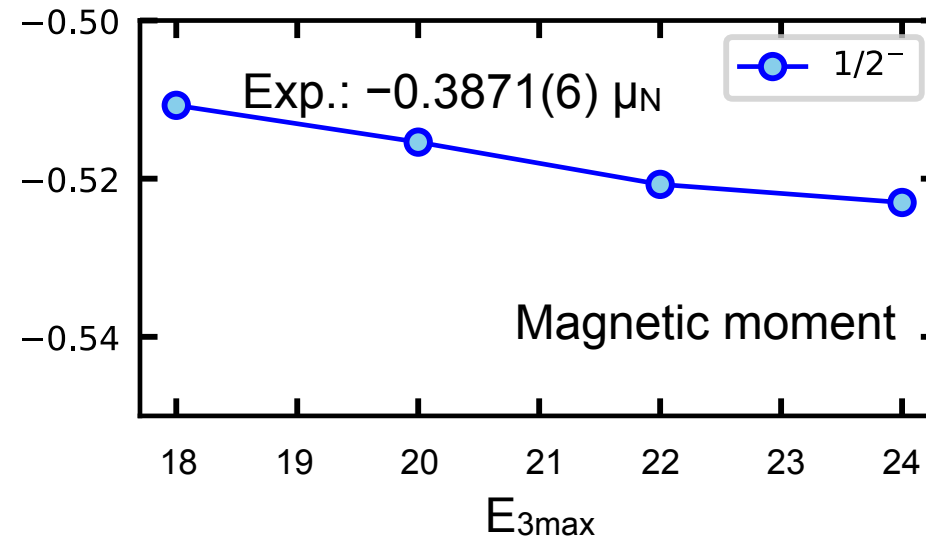
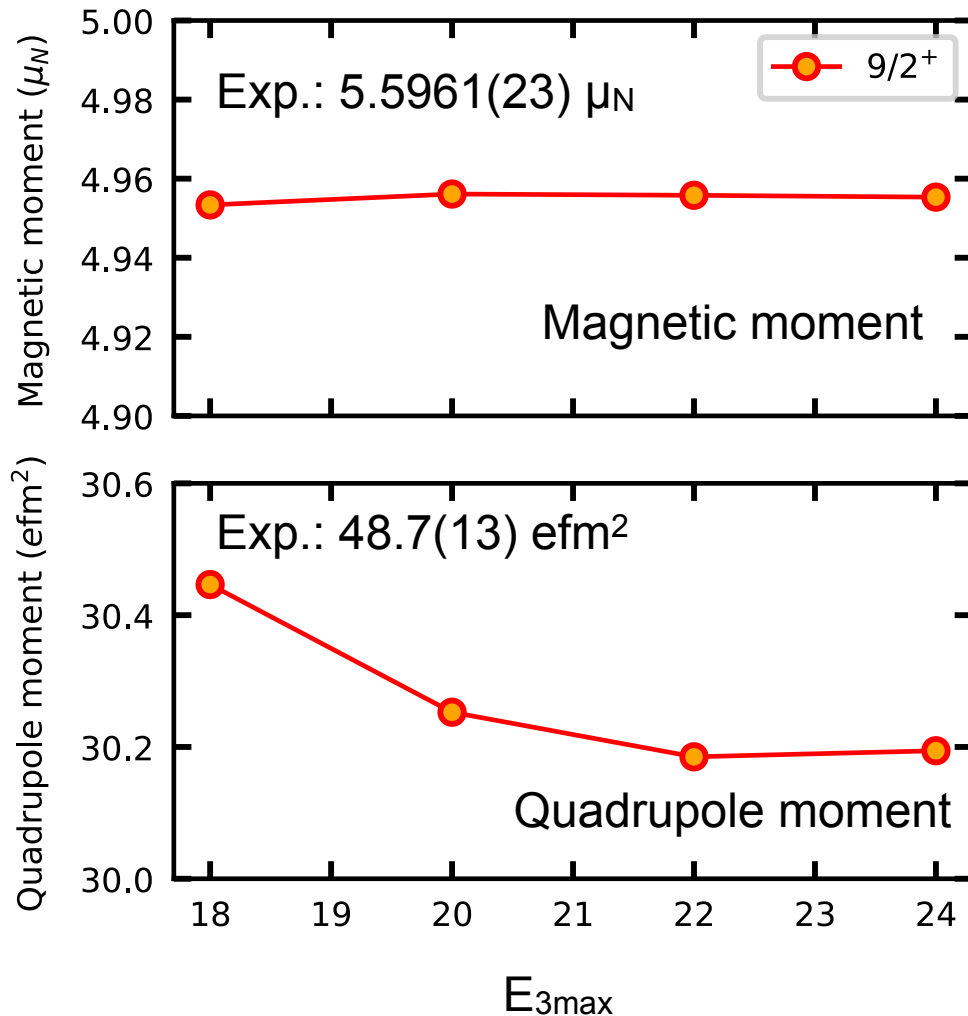
Radii

TM, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, Phys. Rev. C 105, 014302 (2022).



Asymptotic form: $\langle r^2 \rangle \approx A \gamma_{\frac{2}{n}} \left[\left(\frac{E_{3\max} - \mu}{\sigma} \right)^n \right] + \langle r^2 \rangle_{\infty}$

^{129}In , VS-IMSRG, 1.8/2.0 (EM), $e_{\text{max}}=12$



Convergence is OK.

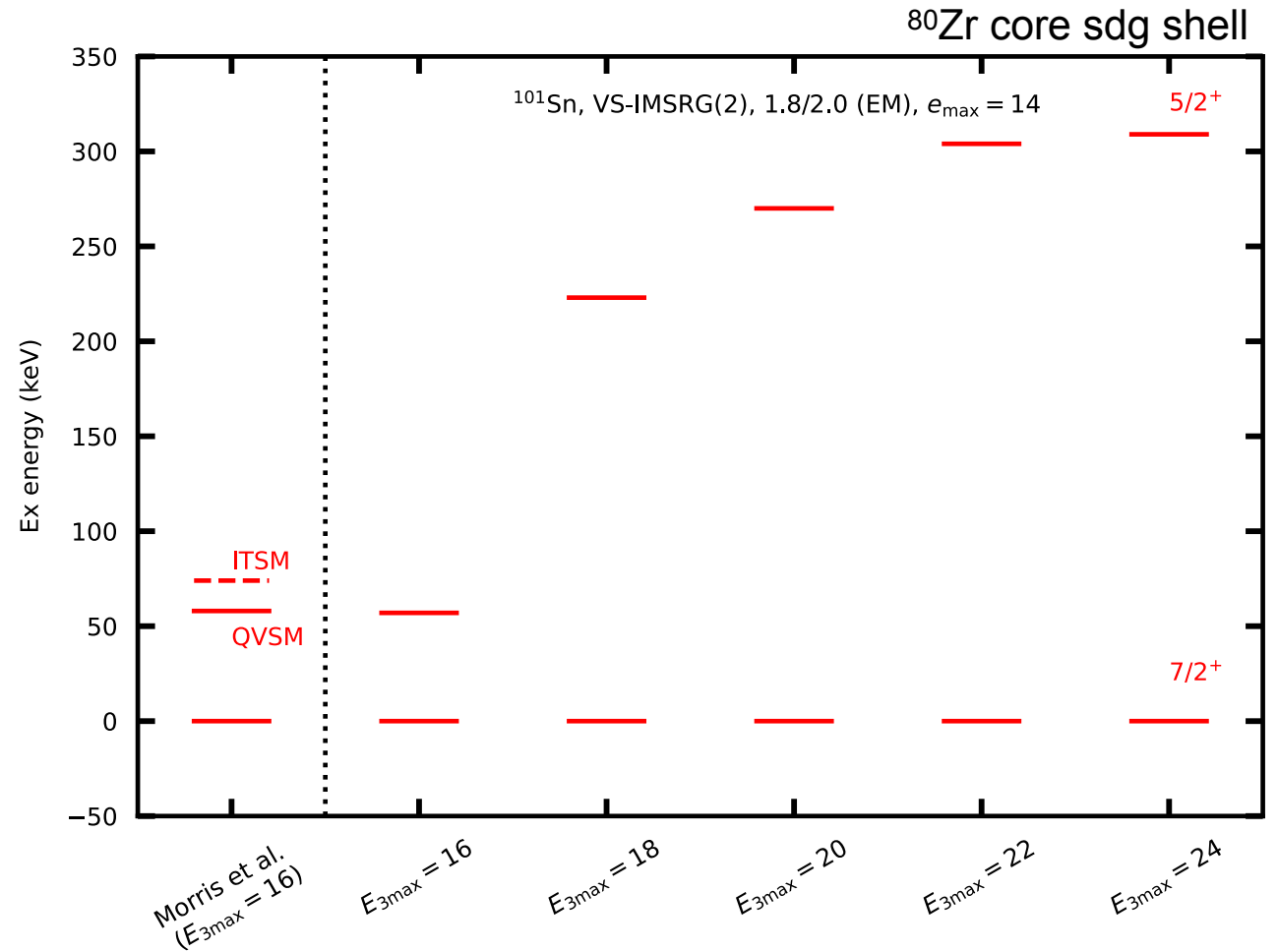
Disagreement with the experiment

Nuclear Hamiltonian

Many-body approximation

Higher order EM current

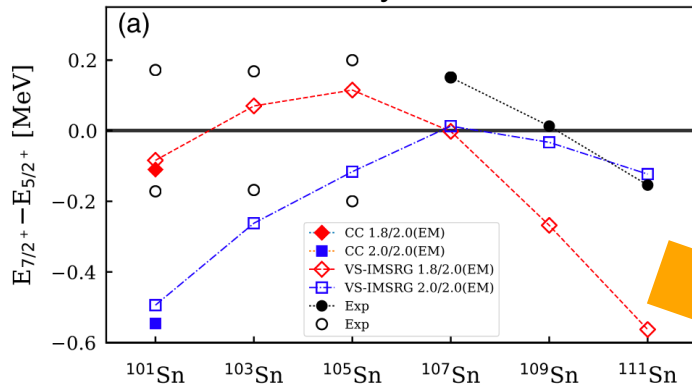
- Near degenerate single-particle structure
- Valence-space IMSRG approach
- The valence-space dimension $> \sim 10^{13}$
 - ◆ Exact diagonalization is impossible
- Quasi-particle vacuum shell model (QVSM)
N. Shimizu et al., Phys. Rev. C 103, 014312 (2021).
- Error of QVSM is the order of 10 keV



T. D. Morris et al., Phys. Rev. Lett. 120, 152503 (2018).

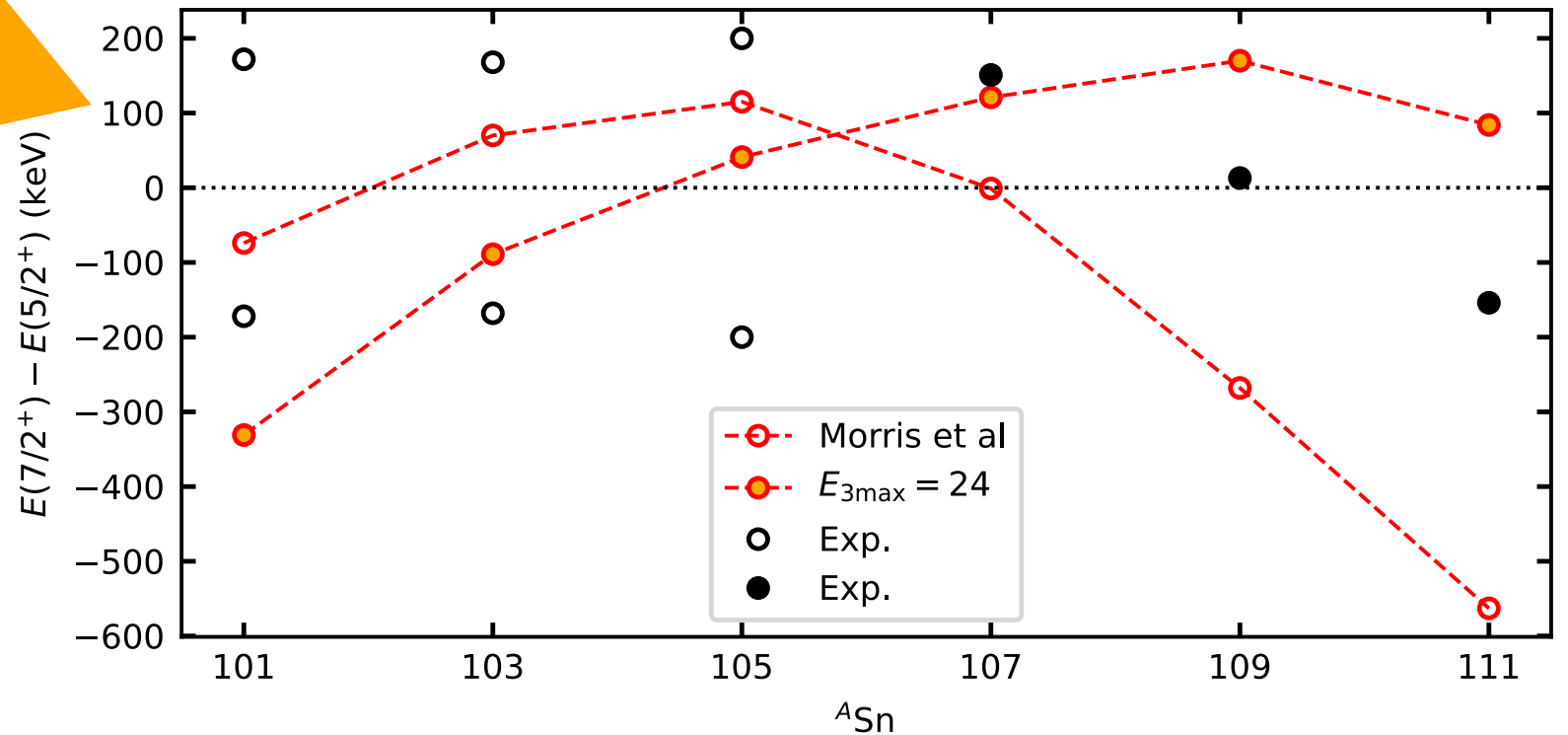
Light tin isotopes

T. D. Morris et al., Phys. Rev. Lett. 120, 152503 (2018).



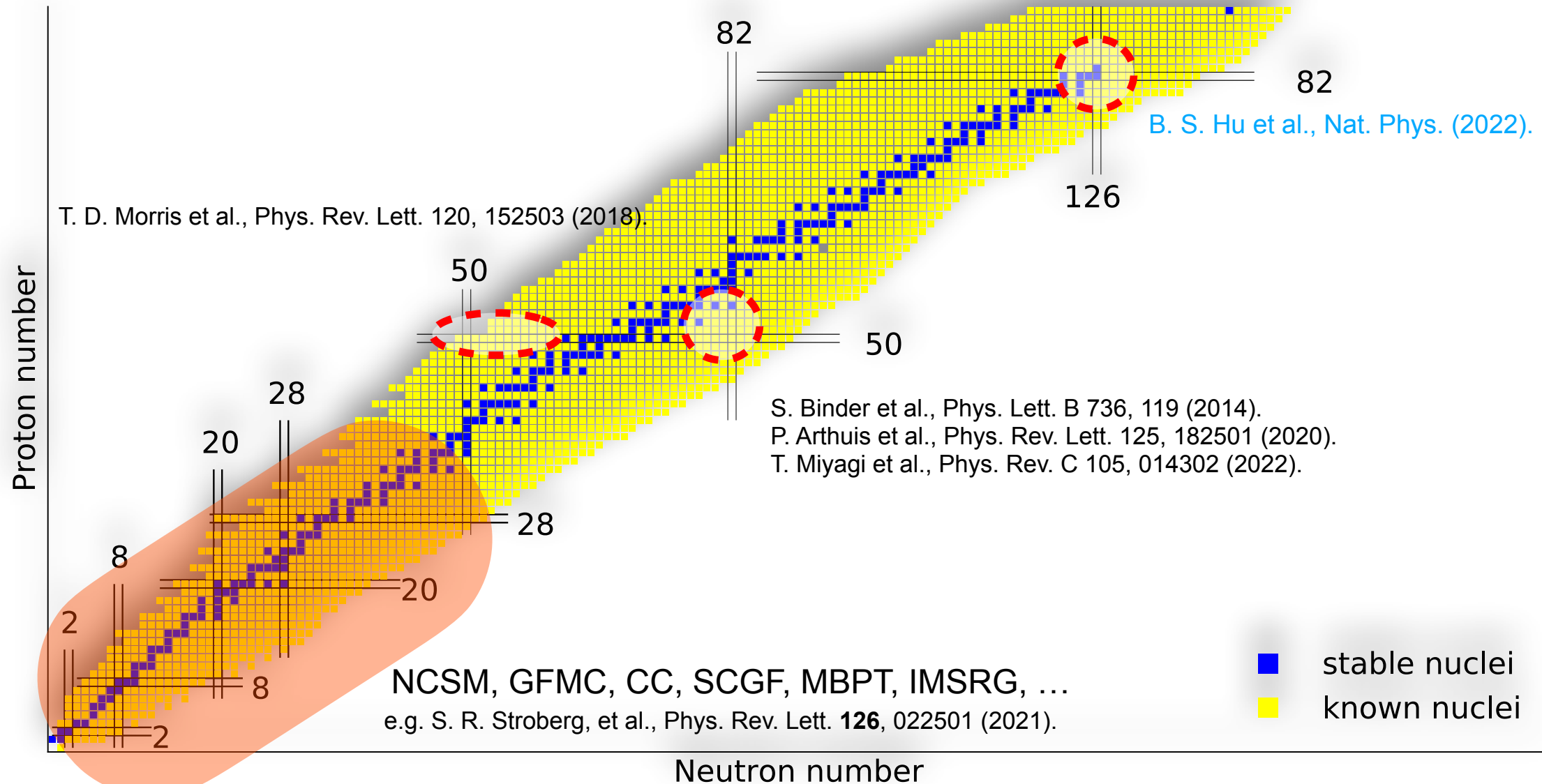
Update

QVSM by N. Shimizu and Y. Tsunoda

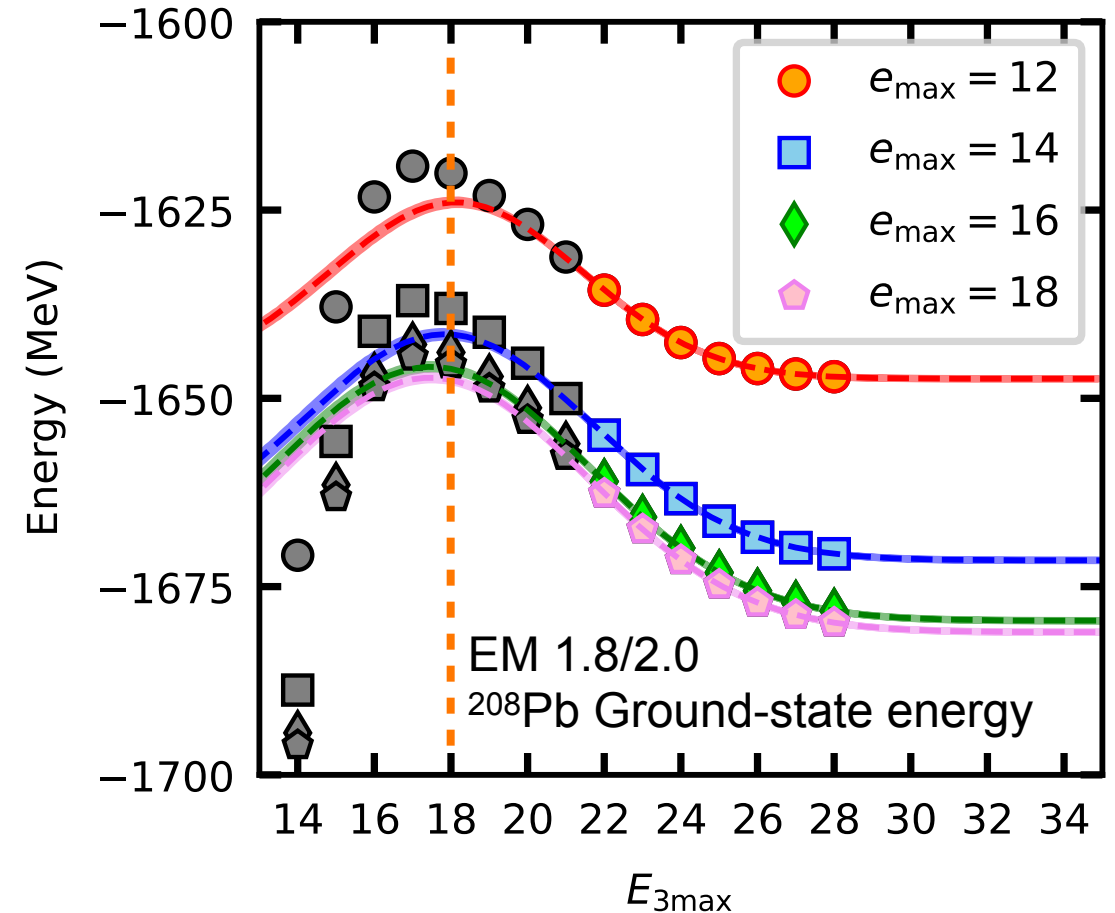
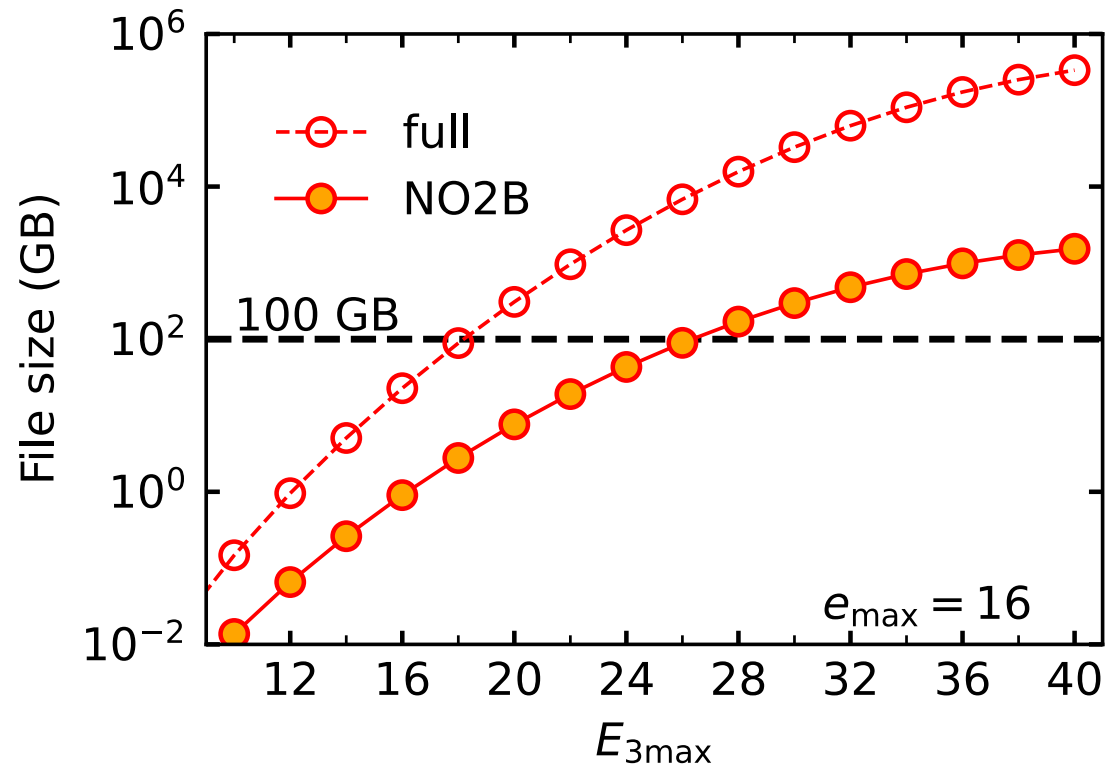


Still difficult to draw a conclusion, but large $E_{3\text{max}}$ calculations are needed.

Towards ^{208}Pb

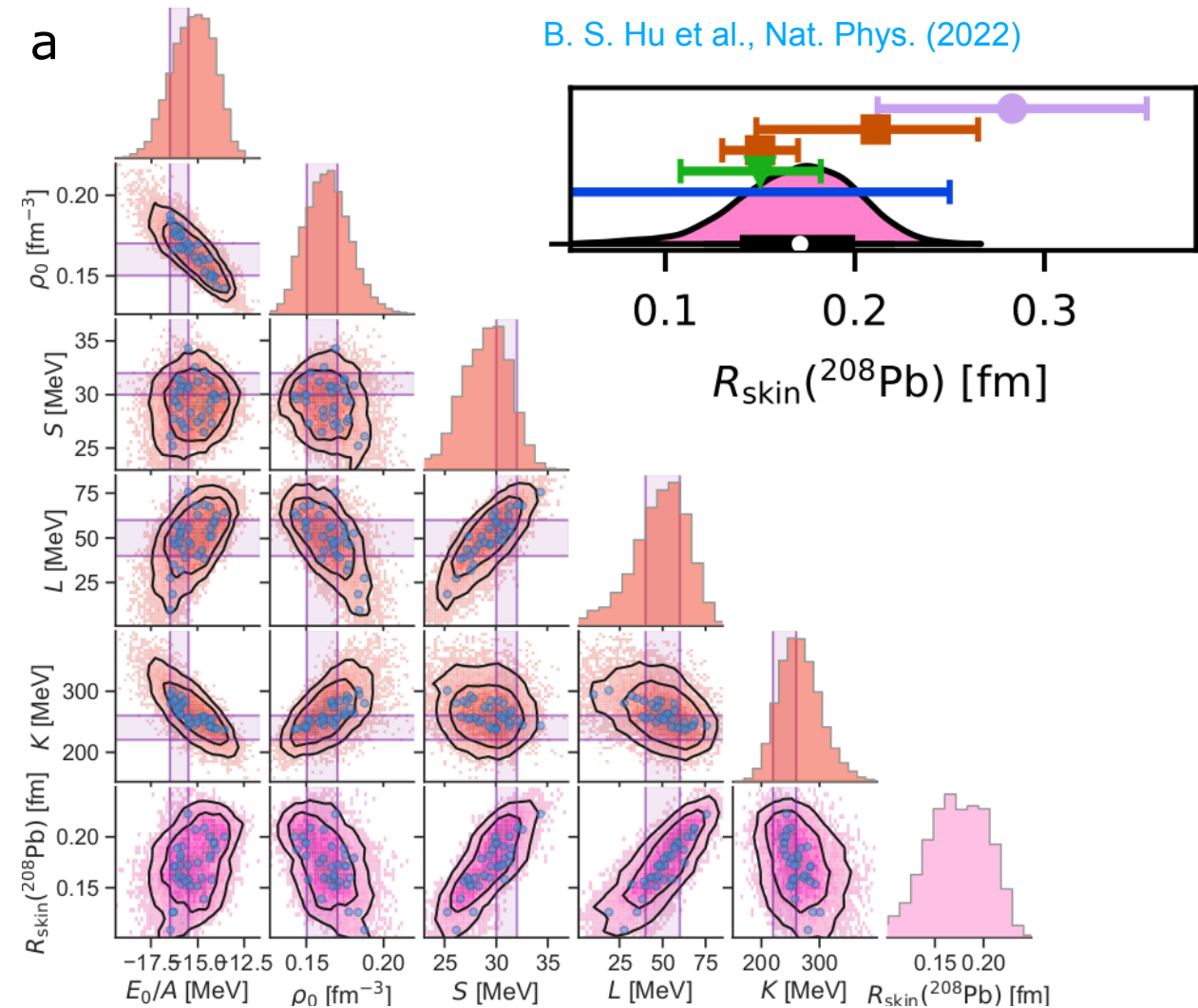


^{208}Pb with the new 3N storage scheme



Neutron skin of ^{208}Pb and EoS parameters

- ^{208}Pb can connect Finite and infinite systems
 - ◆ Neutron skin and nuclear EoS parameter
- Delta-full EFT up to N²LO
- 34 NI interactions consistent with few-body and ^{16}O data
- Posterior predictive distribution
 - ◆ Calibrated by ^{48}Ca data
 - ◆ $0.14 < R_{\text{skin}}(^{208}\text{Pb}) < 0.20$



See Christian Forssen's talk.

- Newly introduced 3N storage scheme [TM et al., Phys. Rev. C 105, 014302 (2022)].
- $A > 100$ region is becoming accessible.
- Neutron skin prediction for ^{208}Pb [B. S. Hu et al., Nat. Phys. (2022)].
- Many possible applications:
 - ◆ Energies, radii, EM moments and transitions for $A > 100$ systems.
 - ◆ 0vbb-decay NMEs [A. Belley et al., Phys. Rev. Lett. 126, 042502 (2021)]
 - ◆