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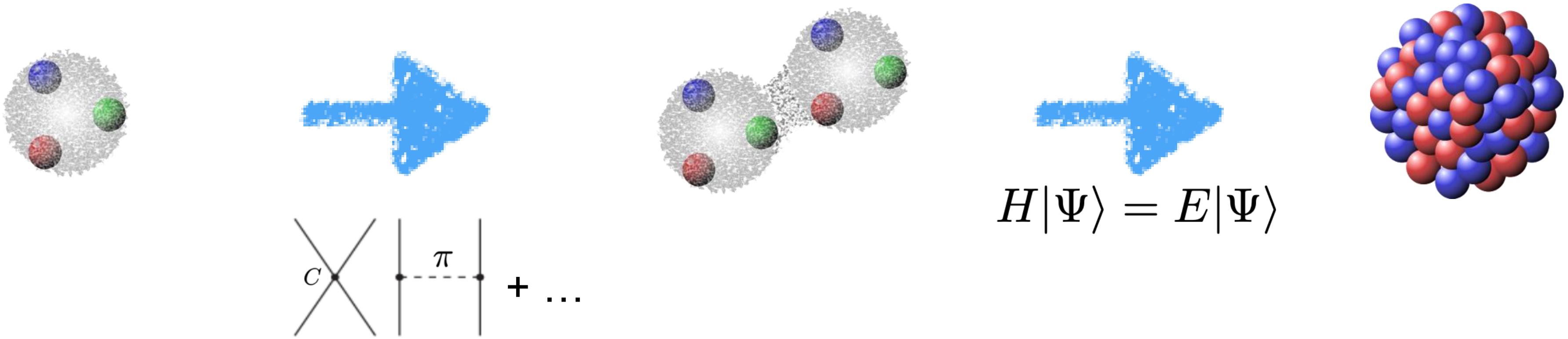
Center for Computational Sciences

Recent advances in ab initio calculaitons of electromagnetic observables



Takayuki Miyagi (University of Tsukuba, Japan)

The 29th International Nuclear Physics Conference @Daejeon, Korea, May 26, 2025

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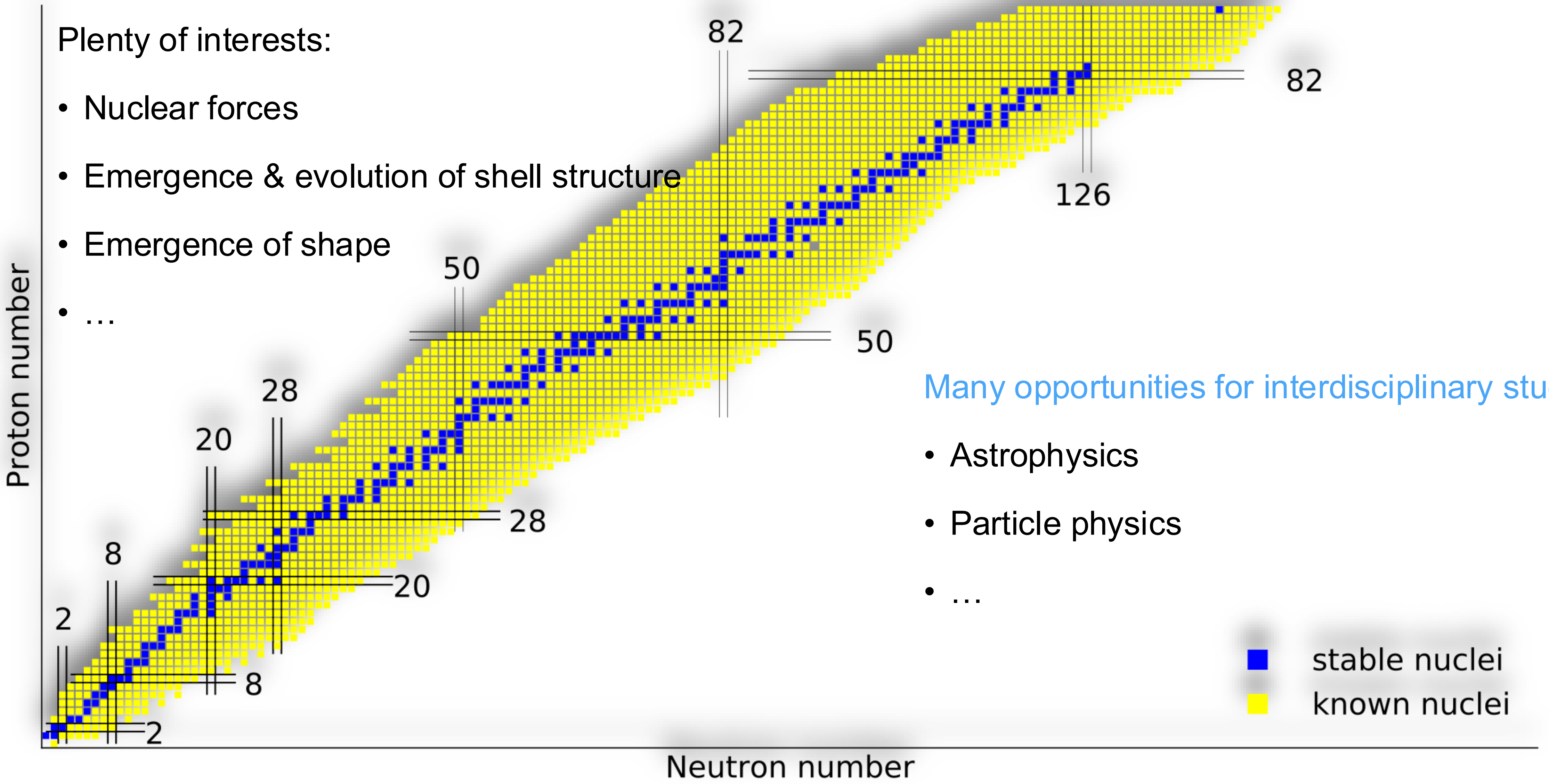
Motivations

Plenty of interests:

- Nuclear forces
- Emergence & evolution of shell structure
- Emergence of shape
- …

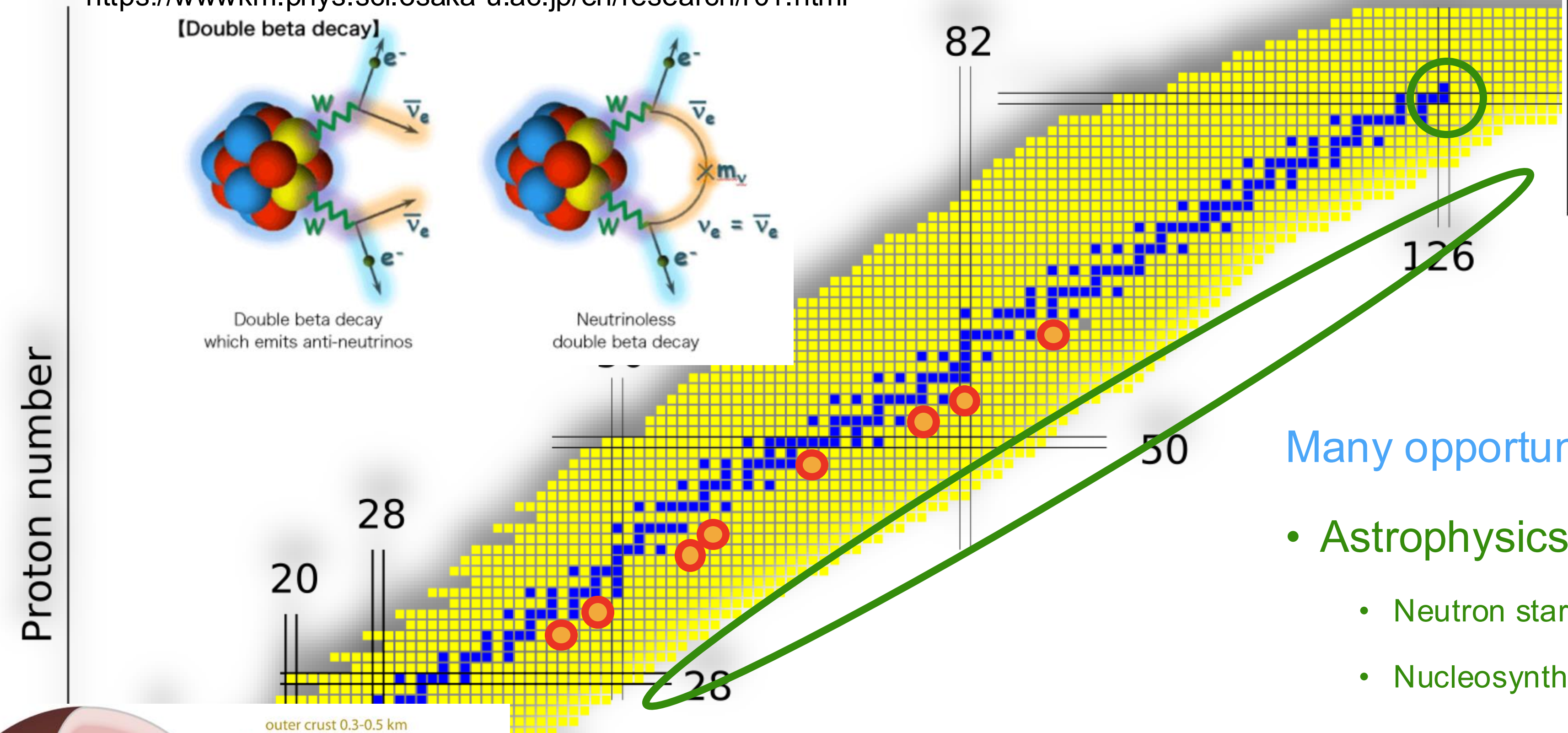


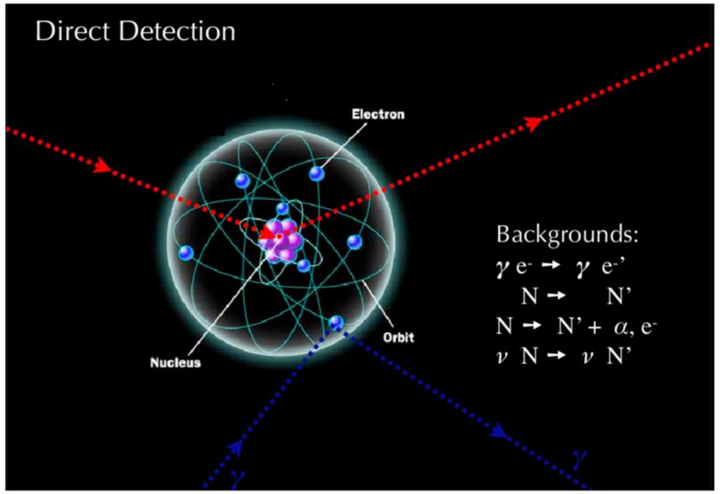
Many opportunities for interdisciplinary studies!

- Astrophysics
- Particle physics
- …

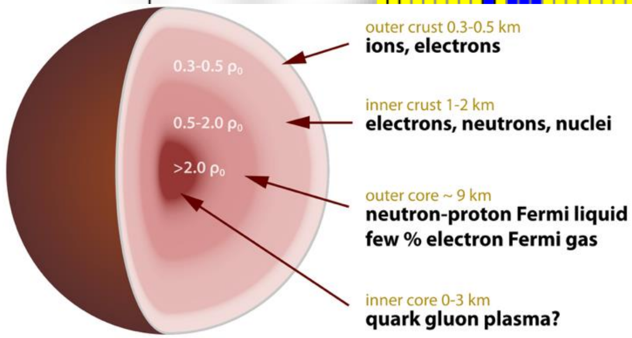
Motivations

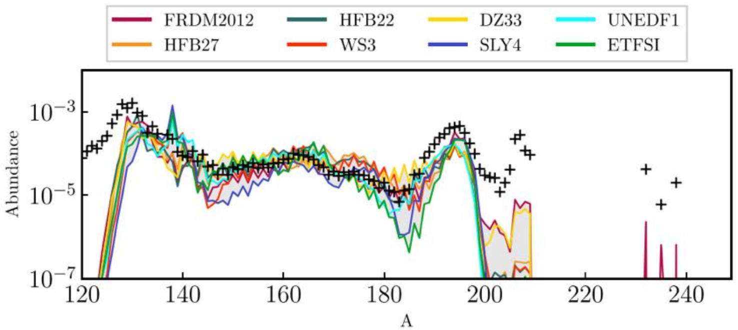
https://wwwkm.phys.sci.osaka-u.ac.jp/en/research/r01.html





F. S. Queiroz, arXiv:1605.08788.





Many opportunities for interdisciplinary studies!

- Astrophysics
  - Neutron star
  - Nucleosynthesis
  - ….
- Particle physics
  - Neutrinoless double-beta decay
  - WIMP neutrino-nucleus scattering
  - …

Motivations

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- EM observables can be used
  - to investigate nuclear structure (shell structure, shape, …)
  - to test nuclear ab initio calculations
- To test ab initio calculations we need:
  - (precise) experimental data
  - reasonable starting nuclear Hamiltonian(s)
  - controllable many-body method(s)
  - higher-order contribution of EM operators

$$H|\Psi\rangle = E|\Psi\rangle$$

$$O_{\mathrm{EM}}^{\mathrm{exp.}} \sim \langle\Psi|\mathcal{O}_{\mathrm{EM}}|\Psi\rangle$$

- Once the methods are tested, making predictions for the unknown are more convincing.

Nuclear ab initio calculations

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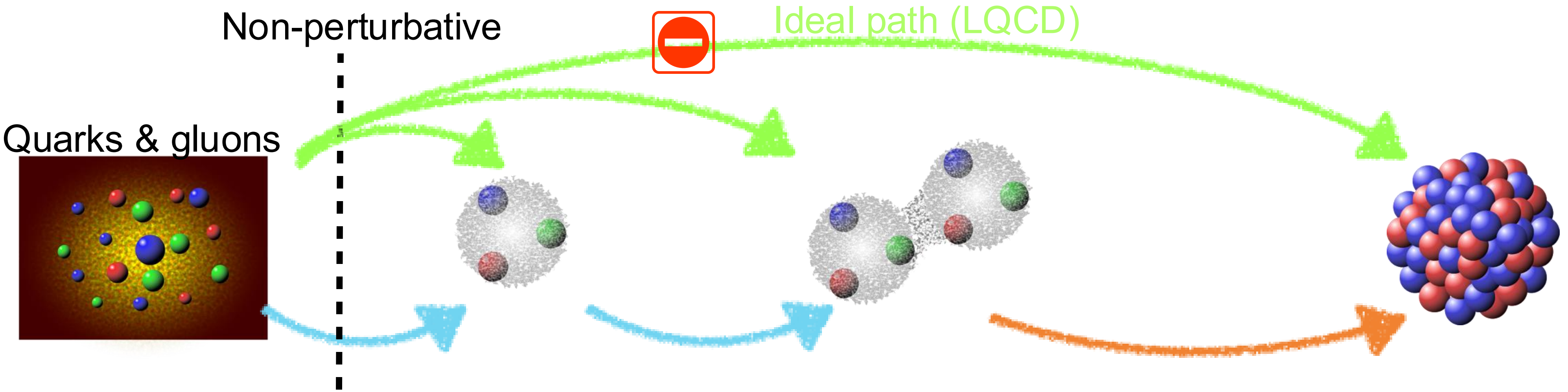
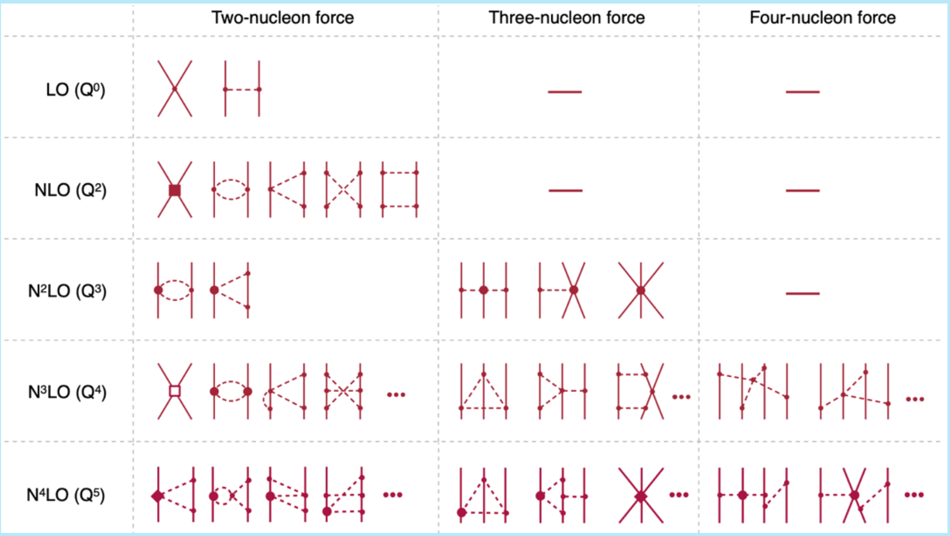




Nuclear many-body problem

- 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
- …

Chiral Effective Field Theory

Weinberg, van Kolck, Kaiser, Epelbaum, Glöckle, Meißner, Entem, Machleidt, …

- Lagrangian construction
  - Chiral symmetry
  - Power counting
- Systematic expansion
  - Unknown LECs
  - Many-body interactions
  - Uncertainty estimation

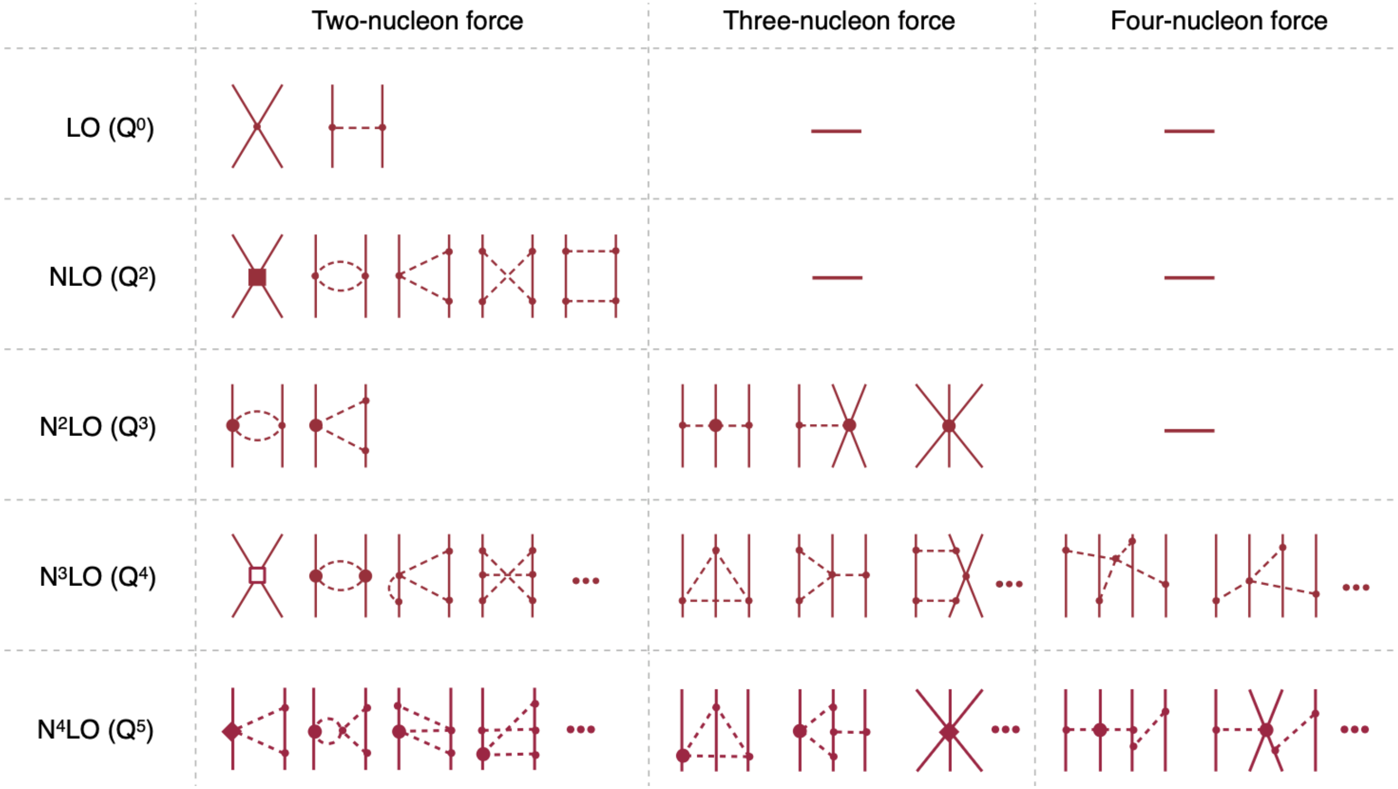
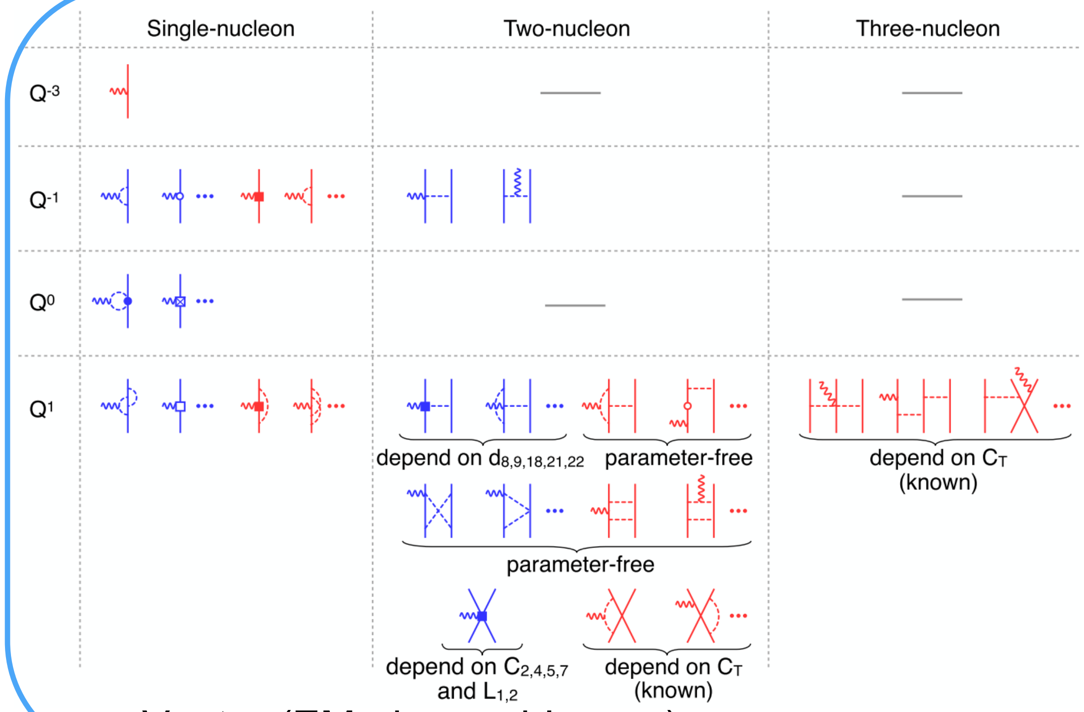


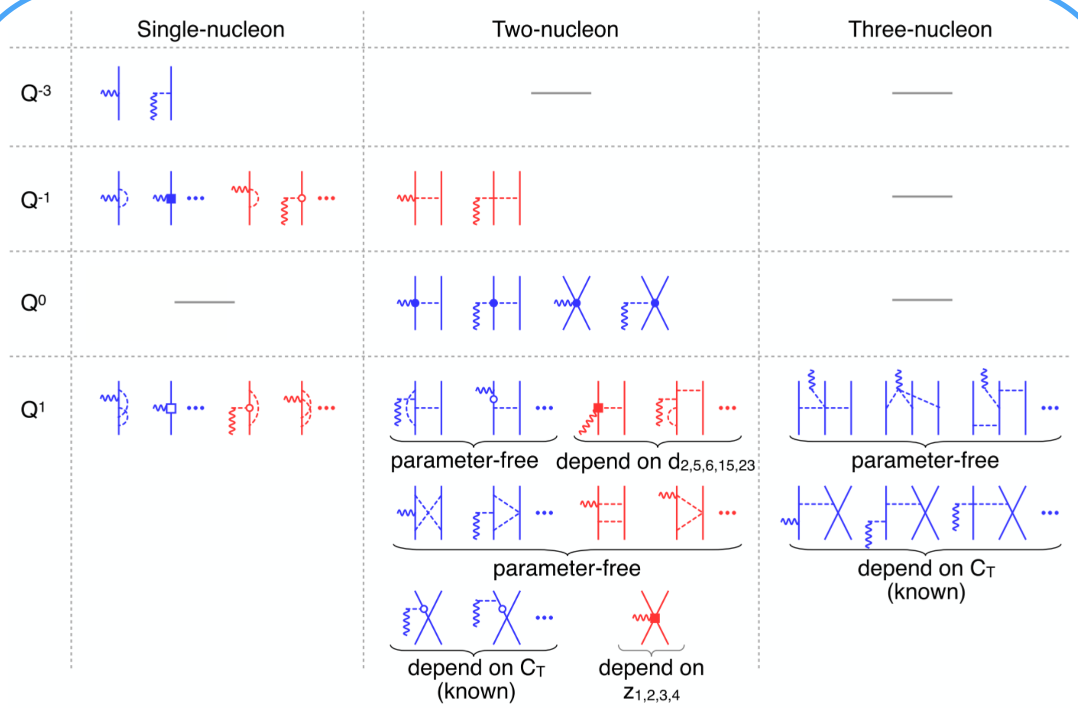
Figure is from E. Epelbaum, arXiv: 1510.07036

Nuclear currents from ChEFT

- Electroweak properties are related to current operators.
- Chiral EFT allows us a systematic expansion for charge and current operators.



Vector (EM observables, …)

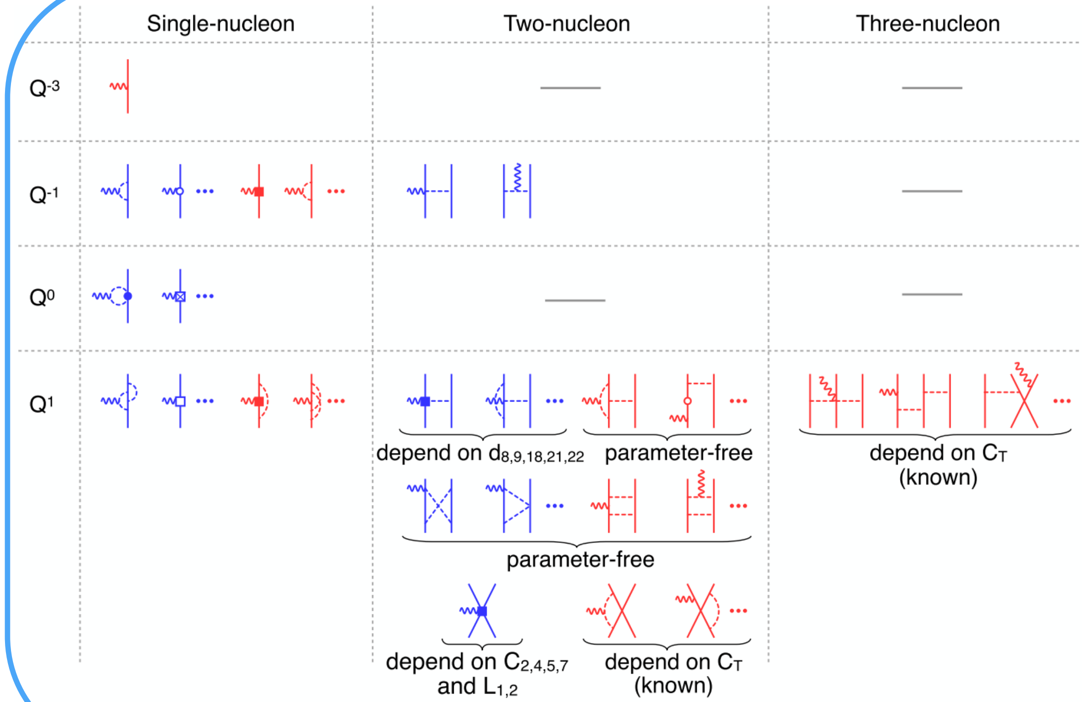


Axial vector (GT transition, …)

E. Epelbaum, arXiv:1908.09349.

Nuclear currents from ChEFT

- Electroweak properties are related to current operators.
- Chiral EFT allows us a systematic expansion for charge and current operators.



Vector (EM observables, …)

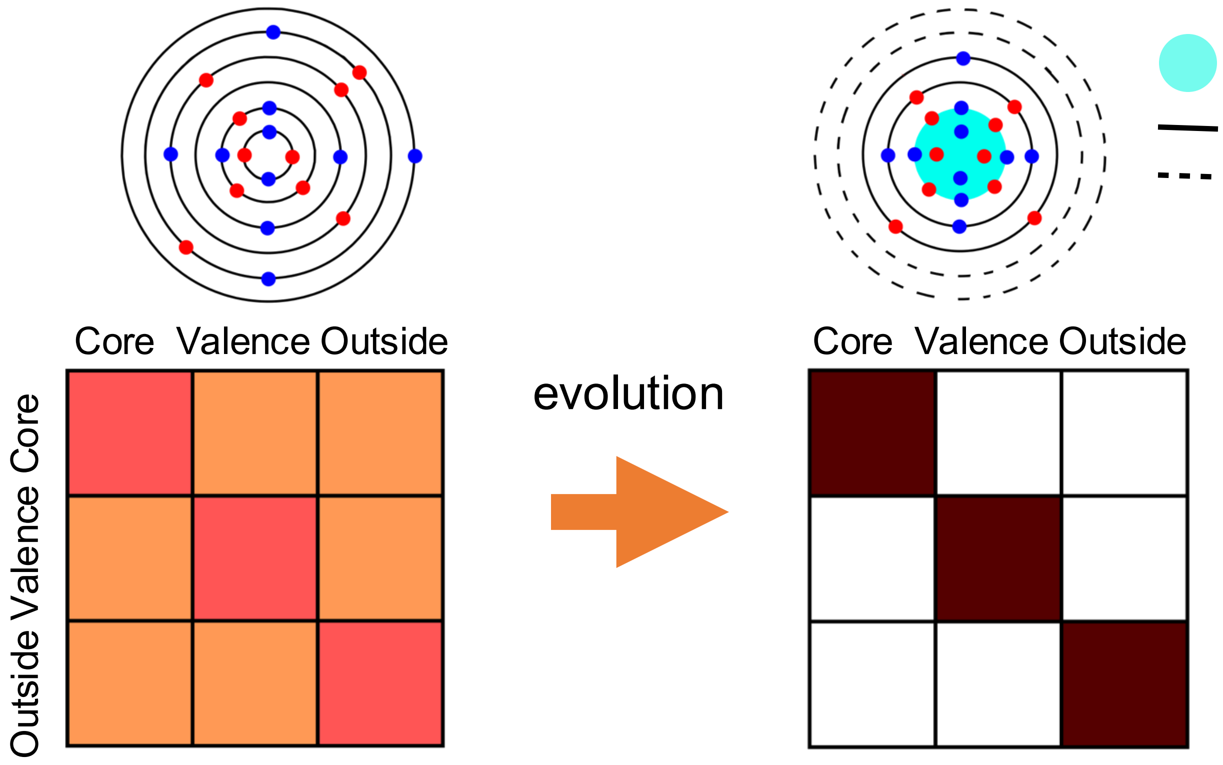
$$r_{ch}^2 = -\frac{6}{Z}\frac{1}{(4\pi)^{3/2}}\lim_{Q\to 0}\frac{d}{dQ^2}\int d\hat{\boldsymbol{Q}}\,\tilde{\rho}(\boldsymbol{Q})$$

$$Q_{2\mu} = -\frac{15}{8\pi}\lim_{Q\to 0}\frac{d^2}{dQ^2}\int d\hat{\boldsymbol{Q}}\,Y_{2\mu}(\hat{\boldsymbol{Q}})\tilde{\rho}(\boldsymbol{Q})$$

$$M_{1\mu} = -i\frac{3}{8\pi}\lim_{Q\to 0}\frac{d}{dQ}\int d\hat{\boldsymbol{Q}}\{[\boldsymbol{Q}\times\nabla_{\boldsymbol{Q}}]Y_{1\mu}(\hat{\boldsymbol{Q}})\}\cdot\tilde{\boldsymbol{j}}(\boldsymbol{Q})$$

E. Epelbaum, arXiv:1908.09349.

Valence-Space In-Medium Similarity Renormalization Group



: frozen core
: valence
: outside

Similarity transformation

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

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

s: flow parameter

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

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

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

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

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

f_{12}, Γ_{1234} : matrix elements to be suppressed

$$\mathcal{O}(s) = e^{\Omega(s)}\mathcal{O}e^{-\Omega(s)} \approx \mathcal{O}^{[0]}(s) + \sum_{12} \mathcal{O}^{[1]}_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234} \mathcal{O}^{[2]}_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, Annu. Rev. Nucl. Part. Sci. **69**, 307 (2019).

Valence-Space In-Medium Similarity Renormalization Group

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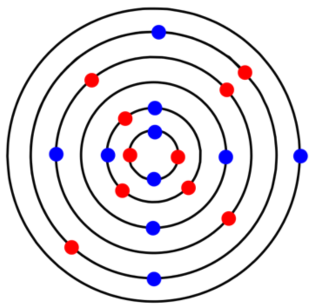
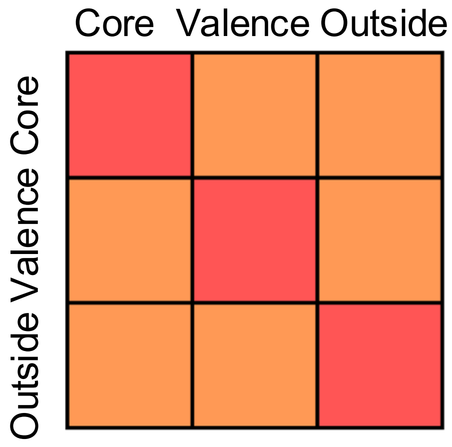
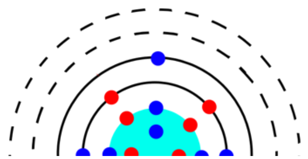




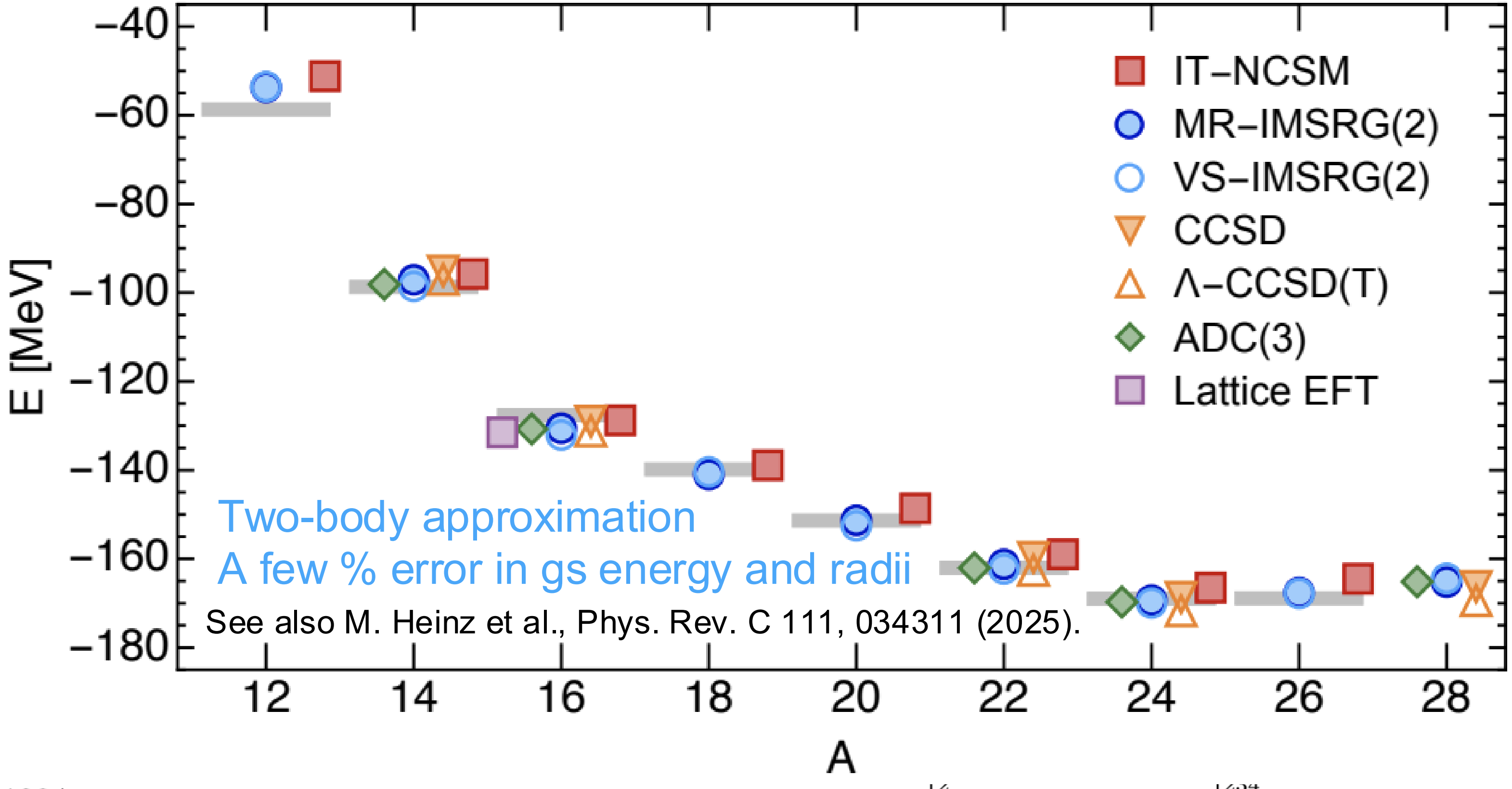
evolution



: frozen core

: valence

H. Hergert, Front. Phys. 8, 1 (2020).



Two-body approximation

A few % error in gs energy and radii

See also M. Heinz et al., Phys. Rev. C 111, 034311 (2025).

Similarity transforma

H

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

s: flow parameter

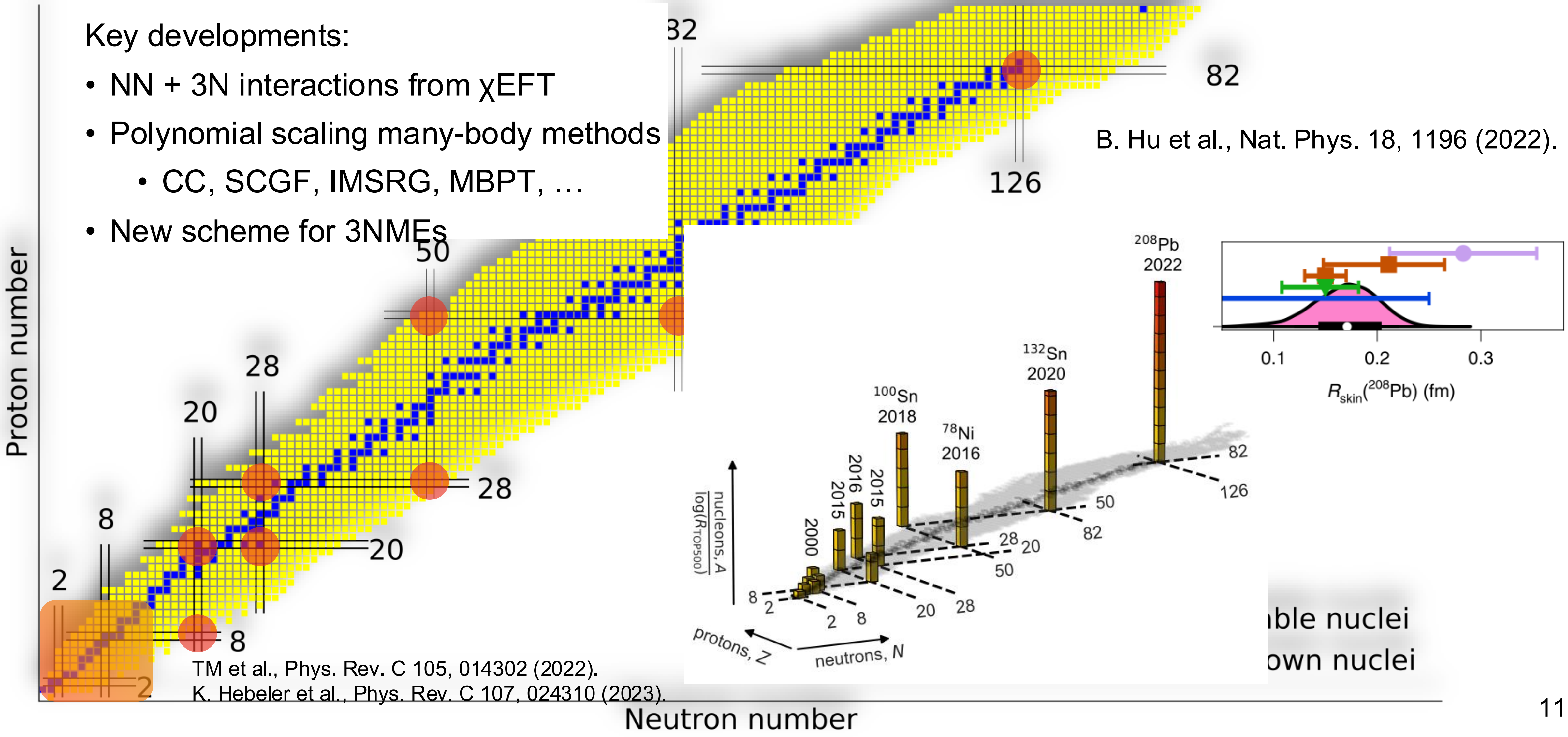
H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).

S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, Annu. Rev. Nucl. Part. Sci. **69**, 307 (2019).

Range of applicability

Key developments:

- NN + 3N interactions from χEFT
- Polynomial scaling many-body methods
  - CC, SCGF, IMSRG, MBPT, …
- New scheme for 3NMEs



B. Hu et al., Nat. Phys. 18, 1196 (2022).

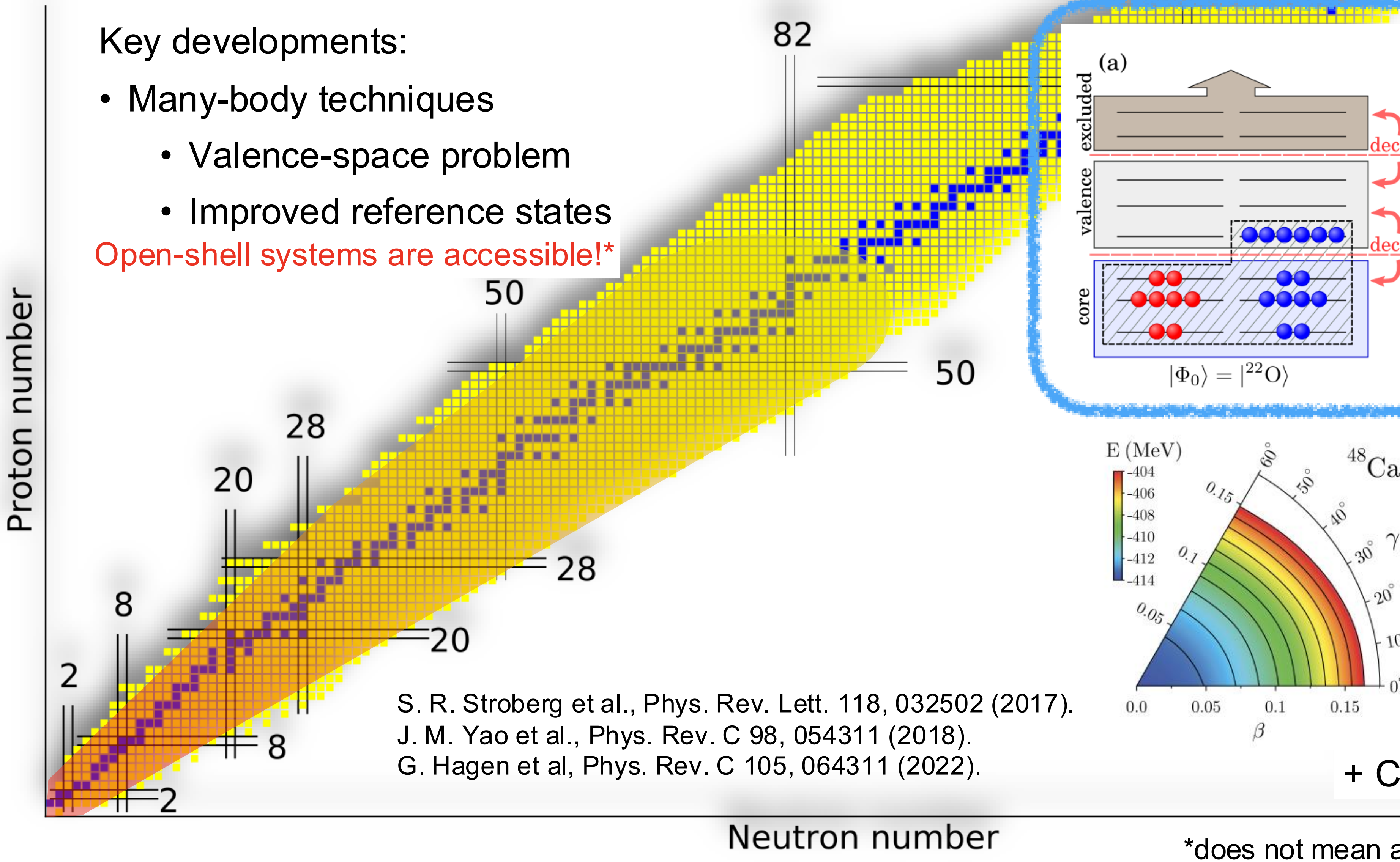
TM et al., Phys. Rev. C 105, 014302 (2022).
K. Hebeler et al., Phys. Rev. C 107, 024310 (2023).

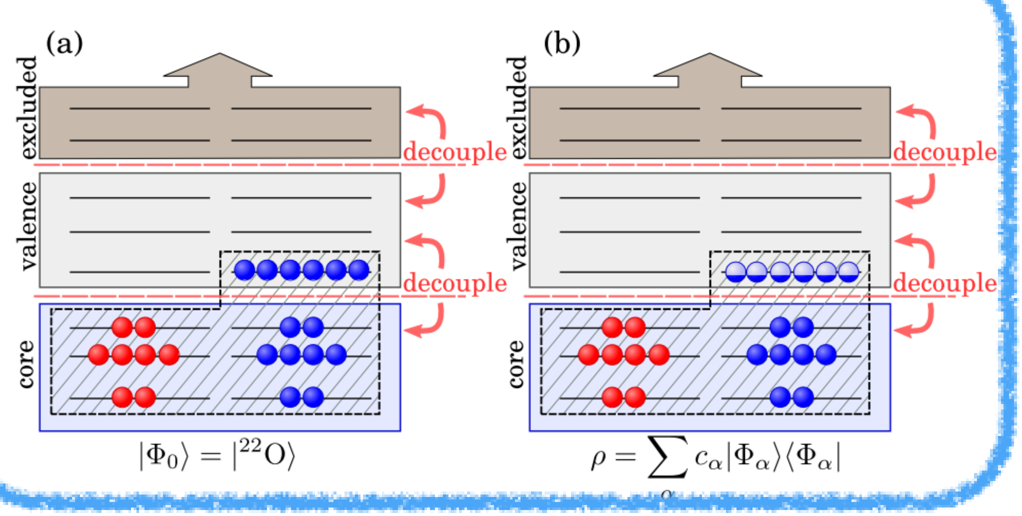
Range of applicability

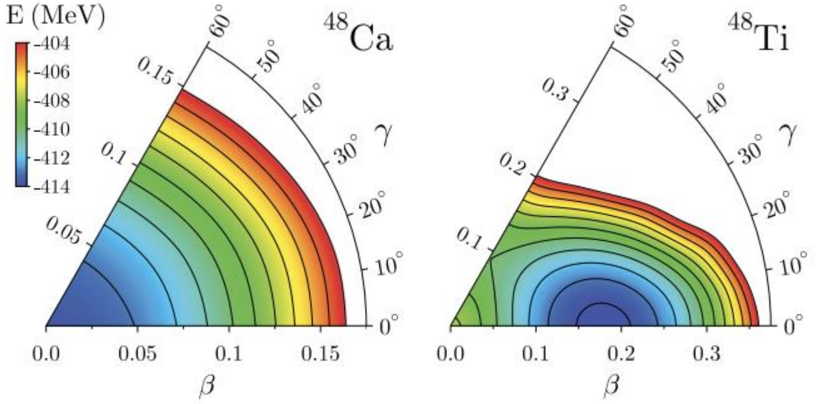
Key developments:

- Many-body techniques
    - Valence-space problem
    - Improved reference states

Open-shell systems are accessible!*







S. R. Stroberg et al., Phys. Rev. Lett. 118, 032502 (2017).
J. M. Yao et al., Phys. Rev. C 98, 054311 (2018).
G. Hagen et al, Phys. Rev. C 105, 064311 (2022).

+ CC, IMSRG, …

*does not mean all nuclei are accessible

Ground-state energies

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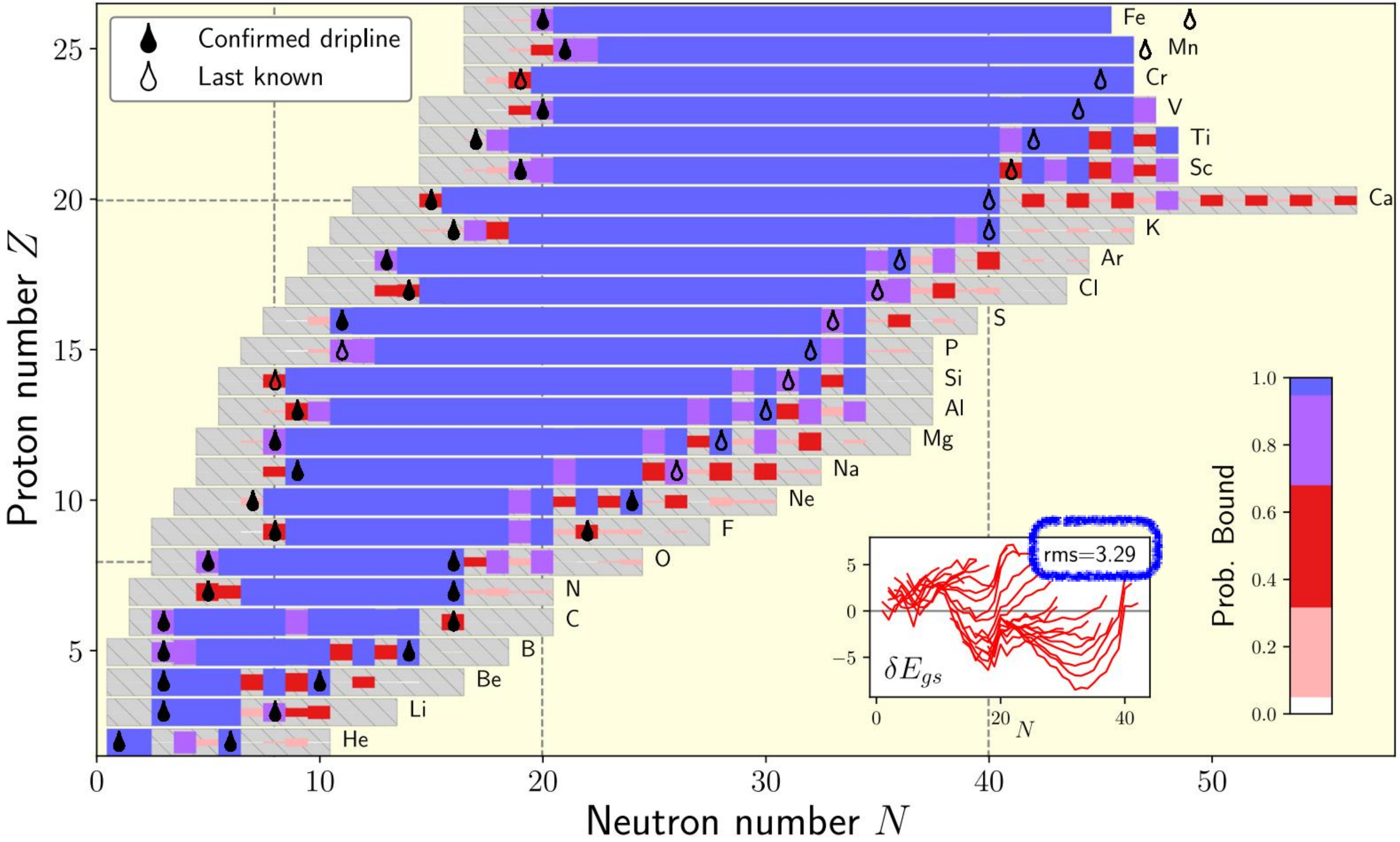
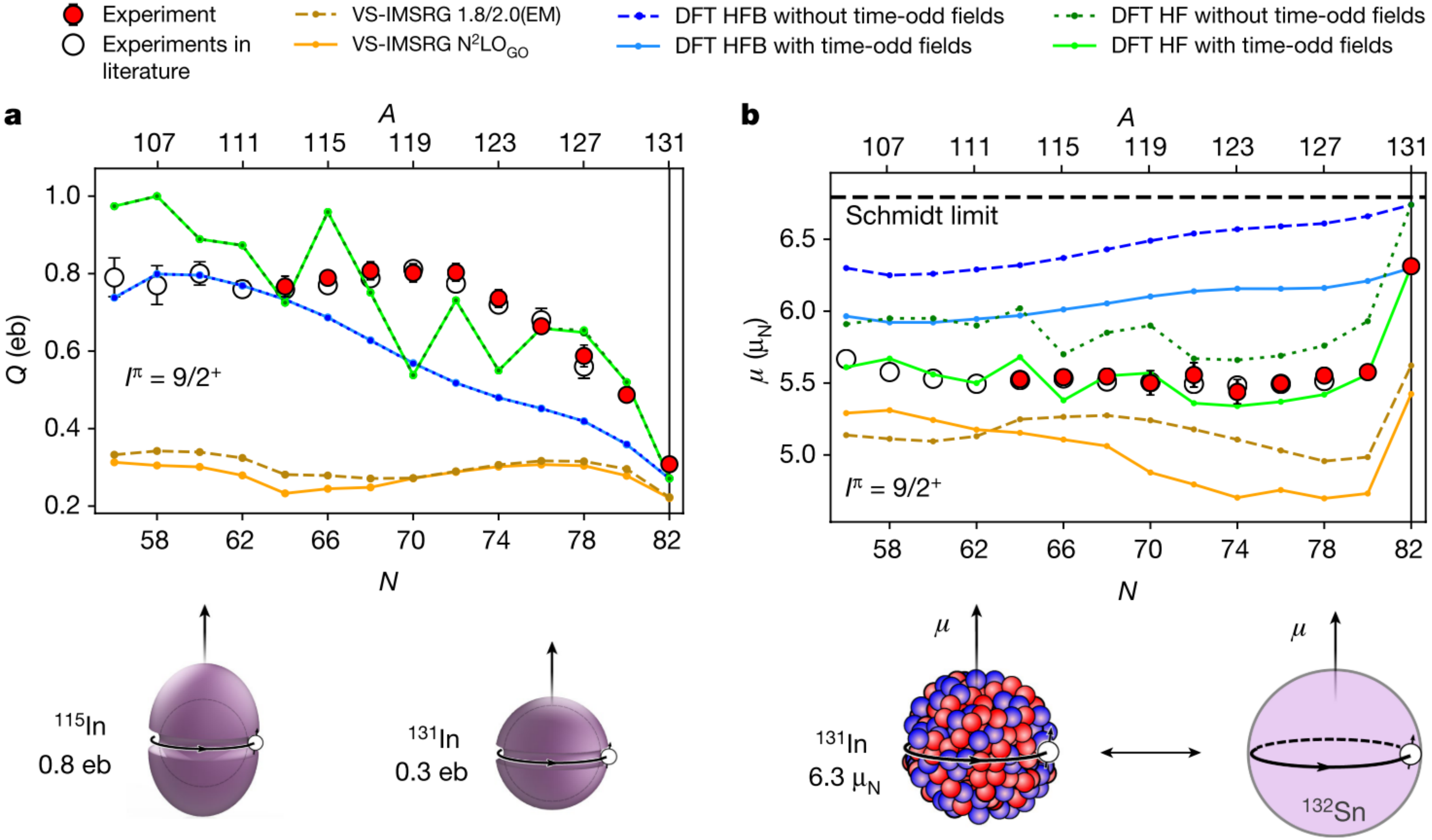
S. R. Stroberg et al., Phys. Rev. Lett. 126, 022501 (2021).



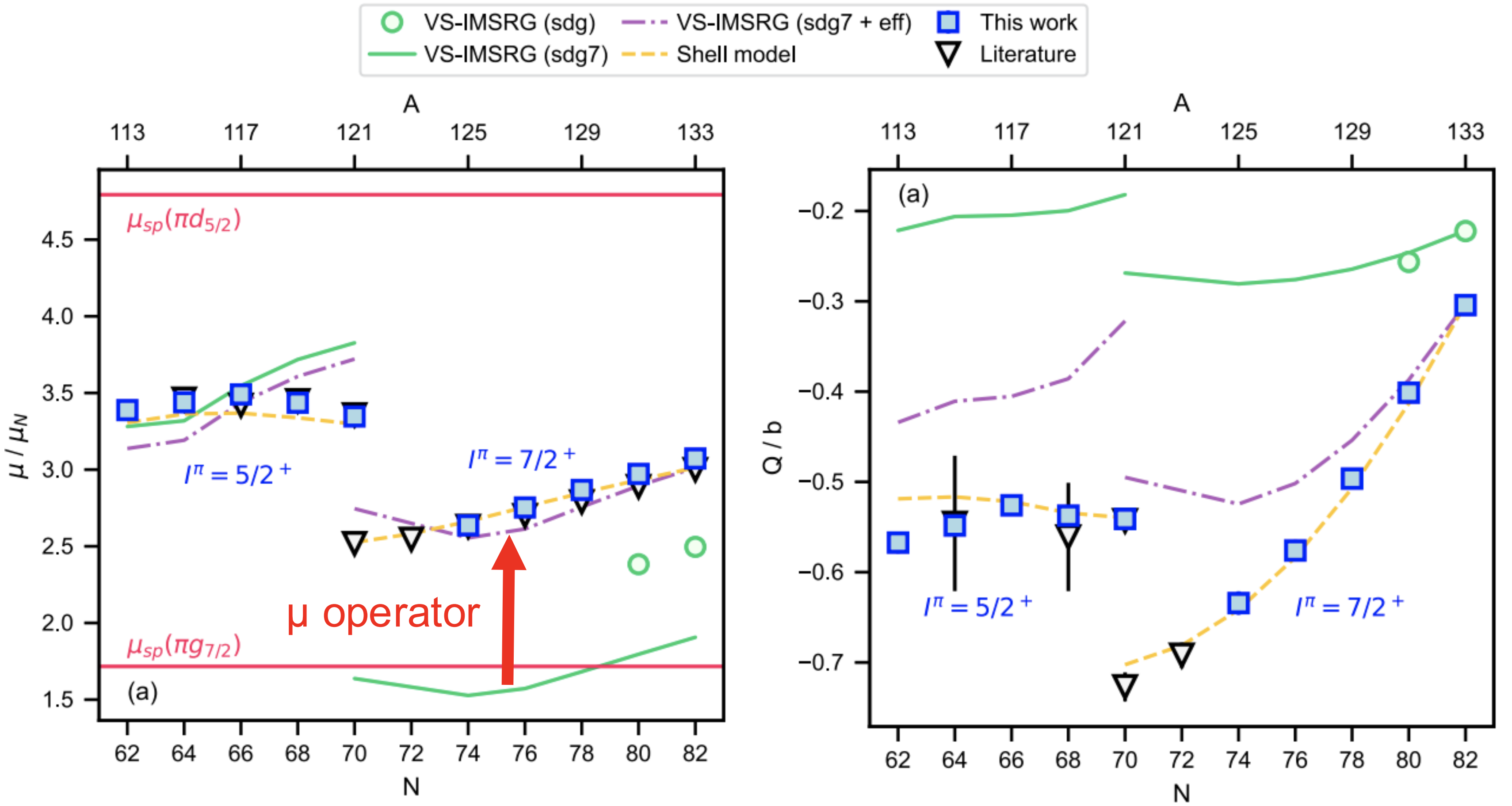
Nuclear moments in In isotopes



A. R. Vernon et al., Nature 607, 260 (2022).

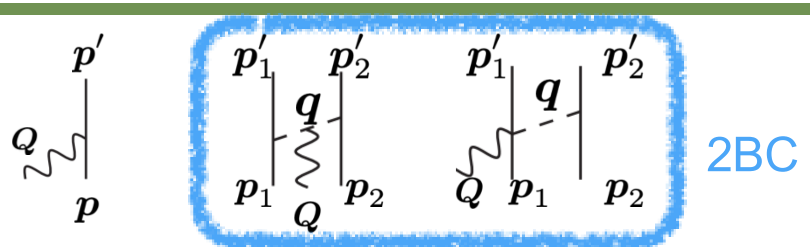
Nuclear moments in Sb isotopes

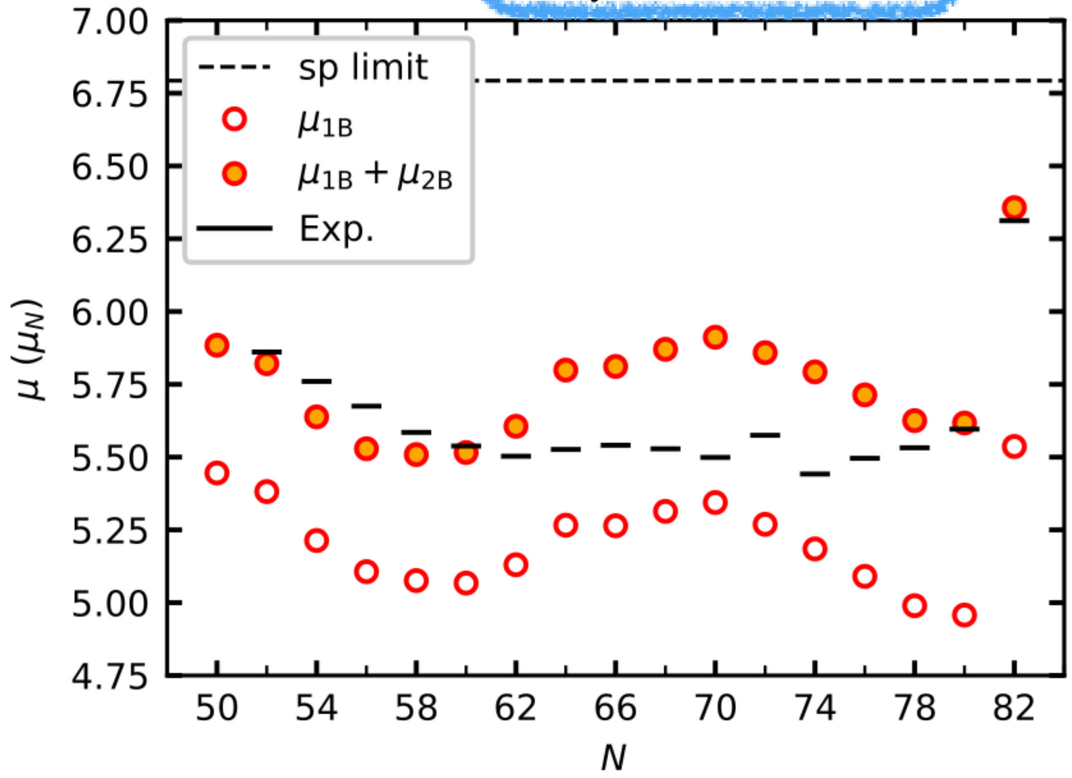
- Comparison with phenomenological CI results
- Magnetic moments
  - ✦ Operator (eff params.)
- Quadrupole moments
  - ✦ Operator (eff. params.)
  - ✦ Wave function



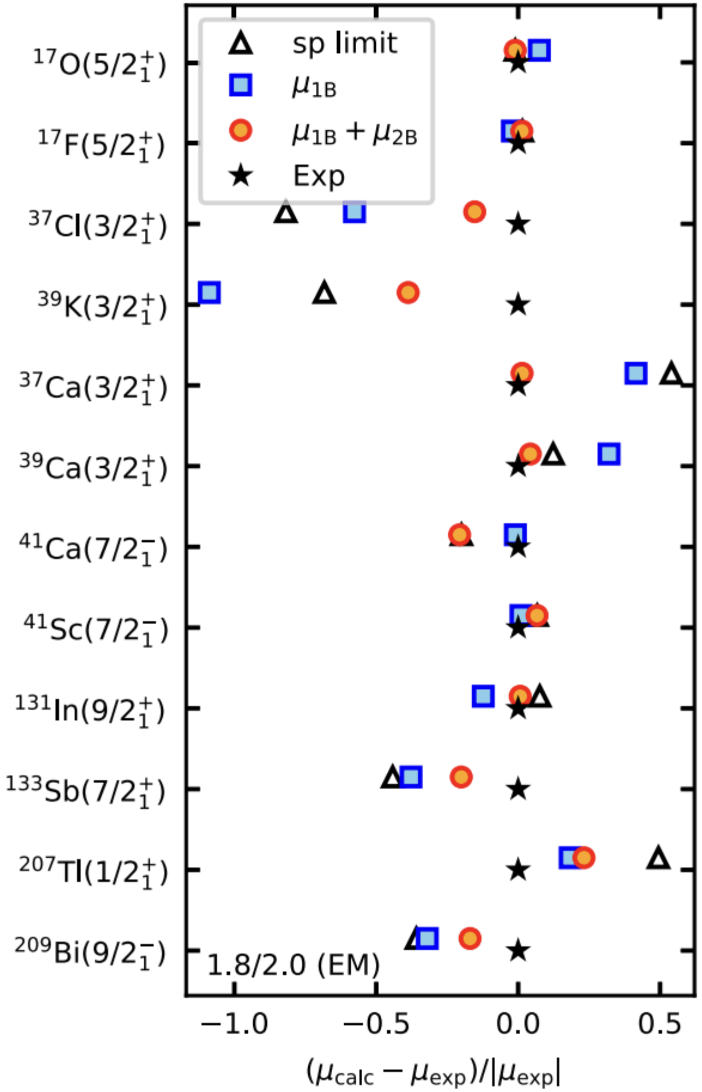
S. Lechner et al., Phys. Lett. B 847, 138278 (2023).

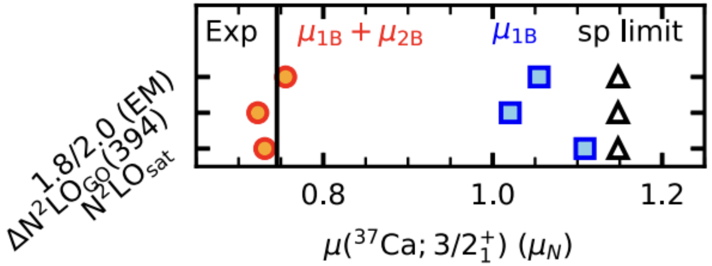
Role of 2BCs: magnetic moments





EM 2BC significantly improves magnetic moments.

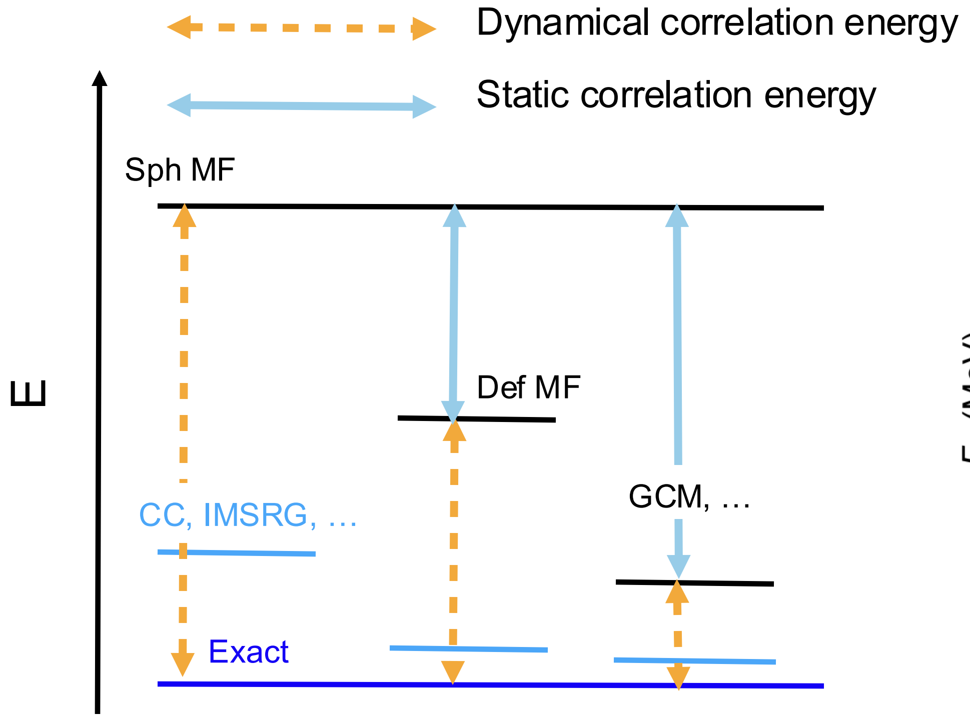




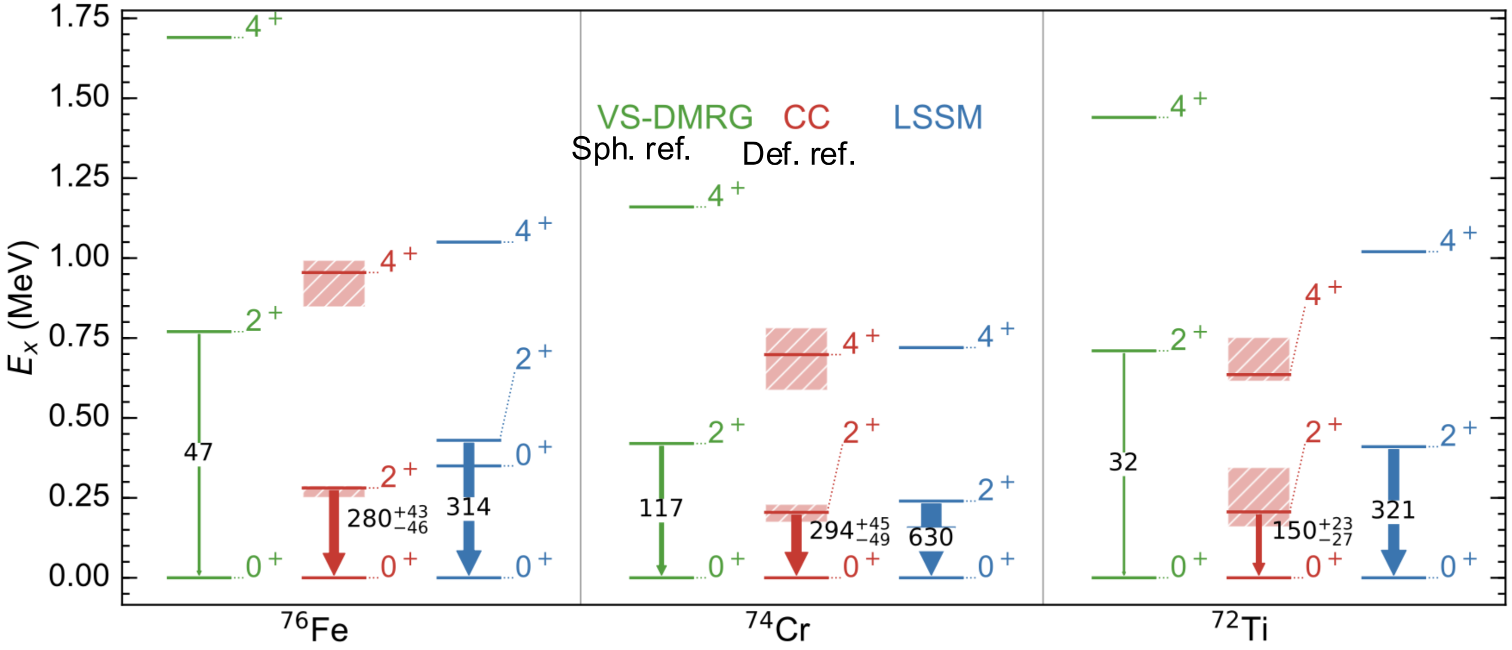
TM et al., Phys. Rev. Lett. 132, 232503 (2024).

Deformation

- Collective deformation cannot be captured by 1p1h and 2p2h excitations from the spherical reference.
- One can begin with a deformed reference.



B. S. Hu et al., Phys. Lett. B 858, 139010 (2024).

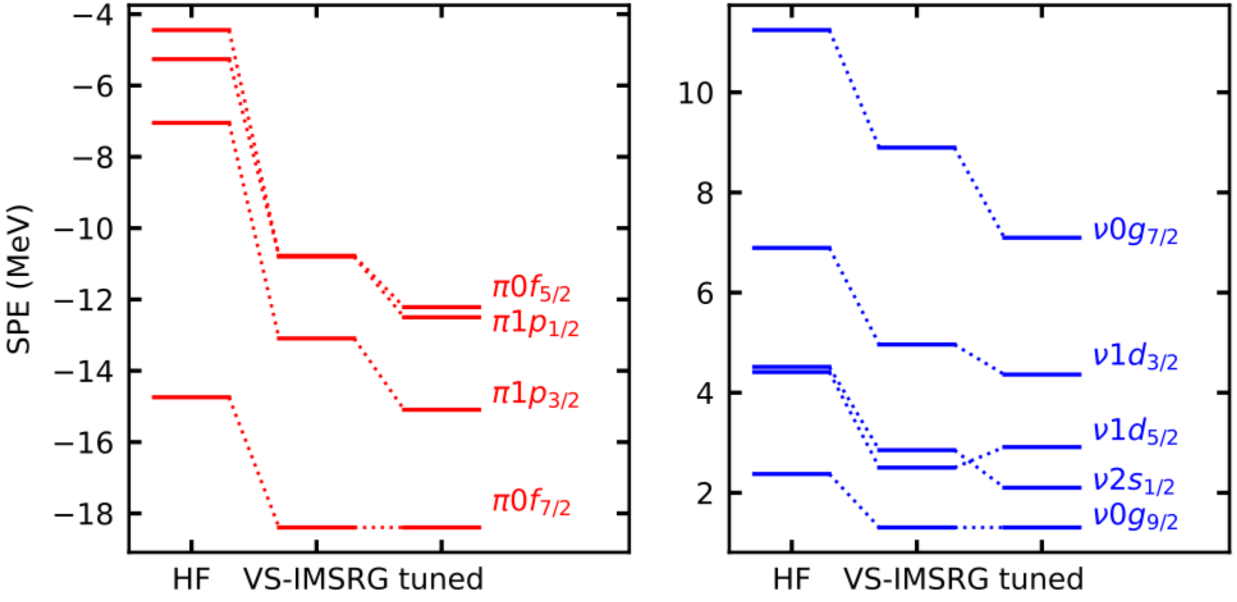


Deformation

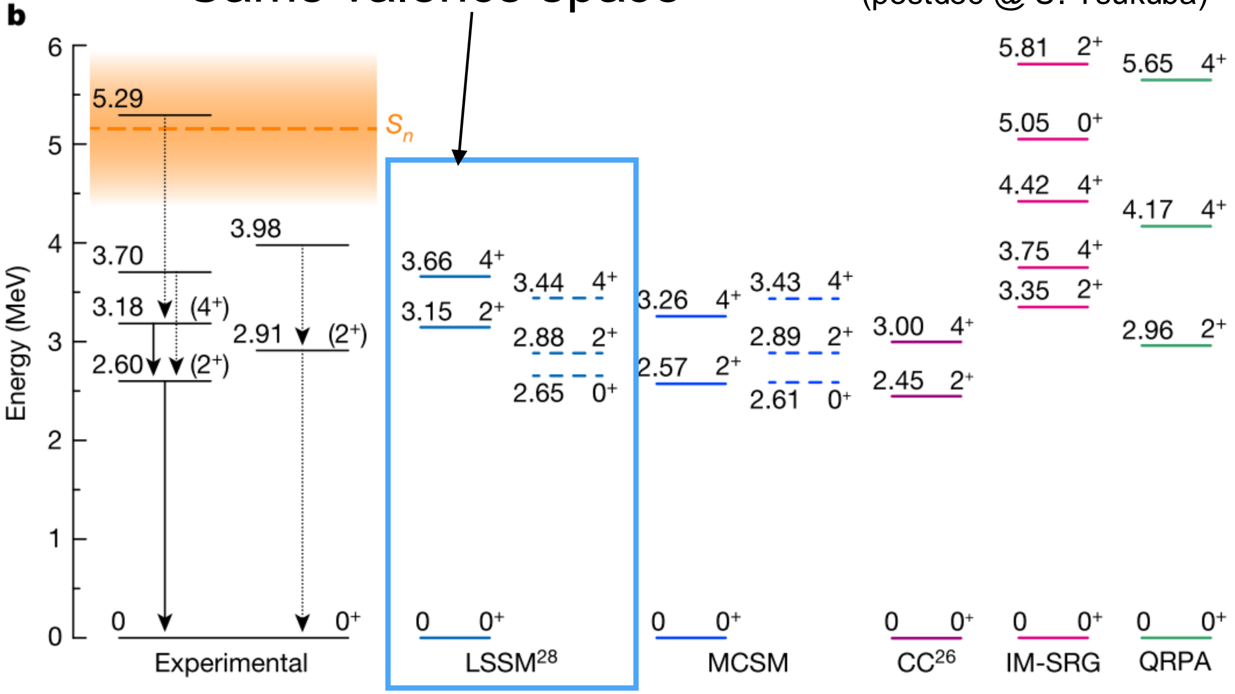
- A possible way to improve

  See also J. A. Purcell et al., Phys. Rev. C 111, 044313 (2025).

  - As a first step, try to tune single-particle energies.
  - 79Cu and 79Zn low-lying spectra

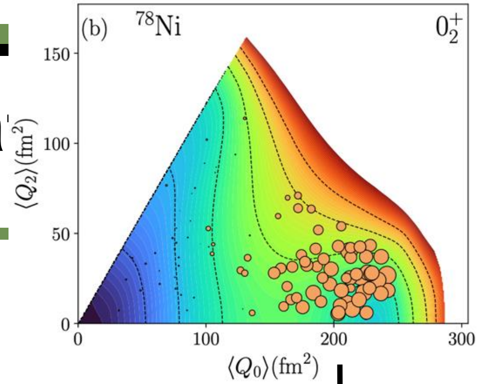


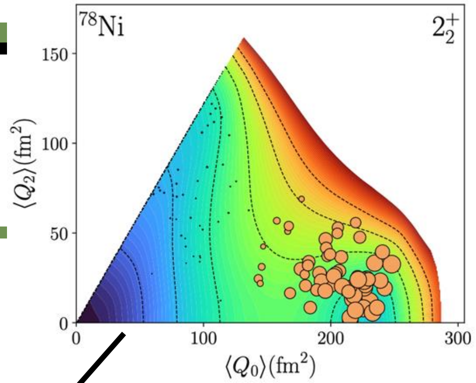
Same valence space

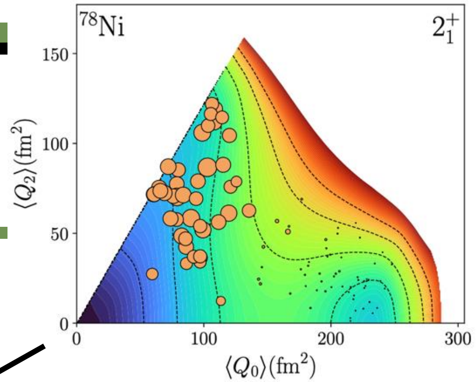


R. Taniuchi et al., Nature 569, 53 (2019).

Deforma

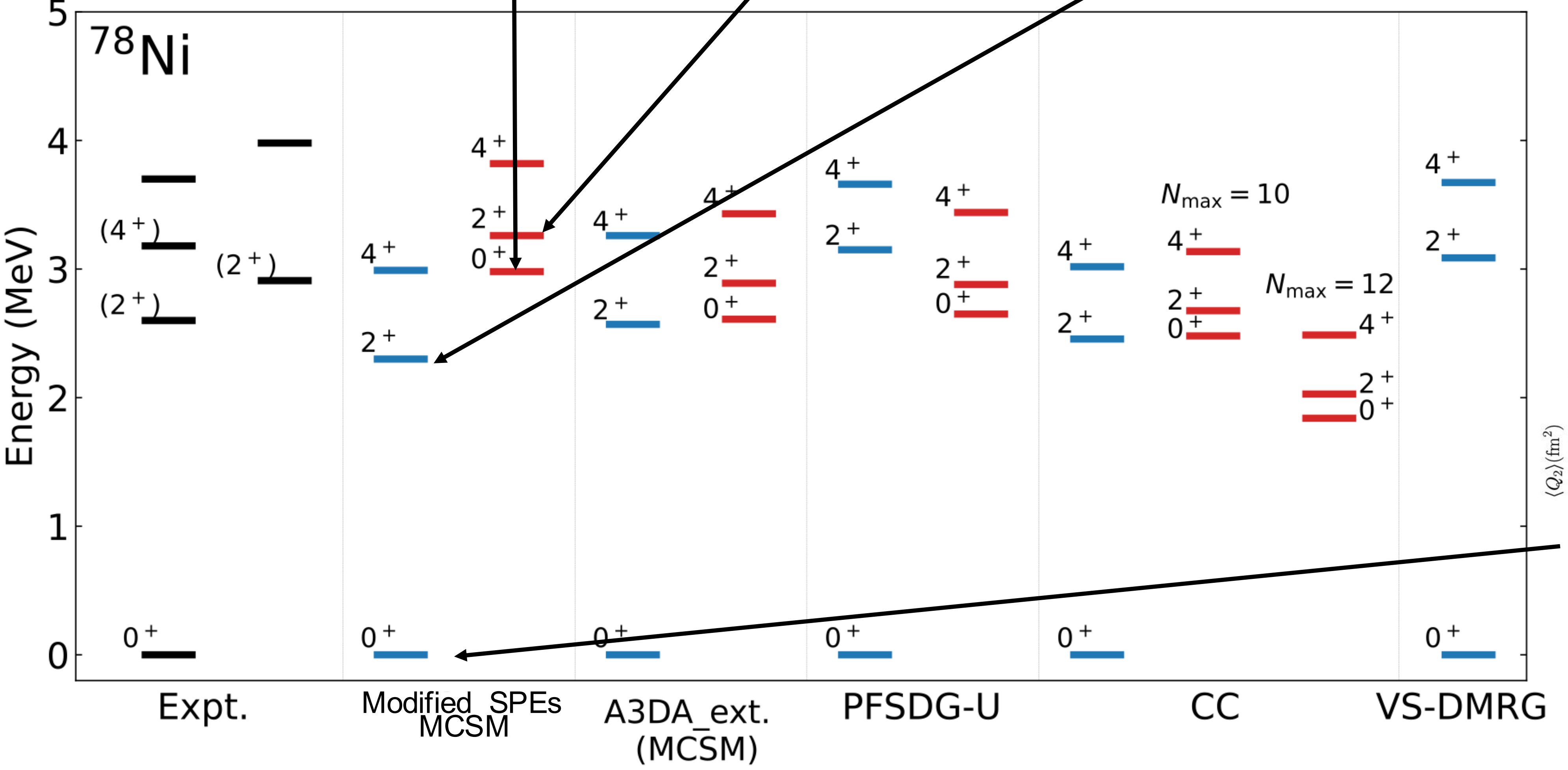


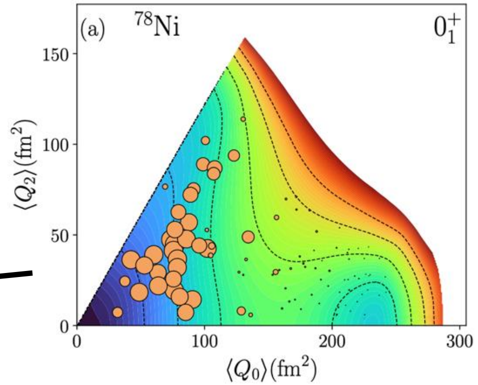




A. Kumar

(postdoc @ U. Tsukuba)





Summary

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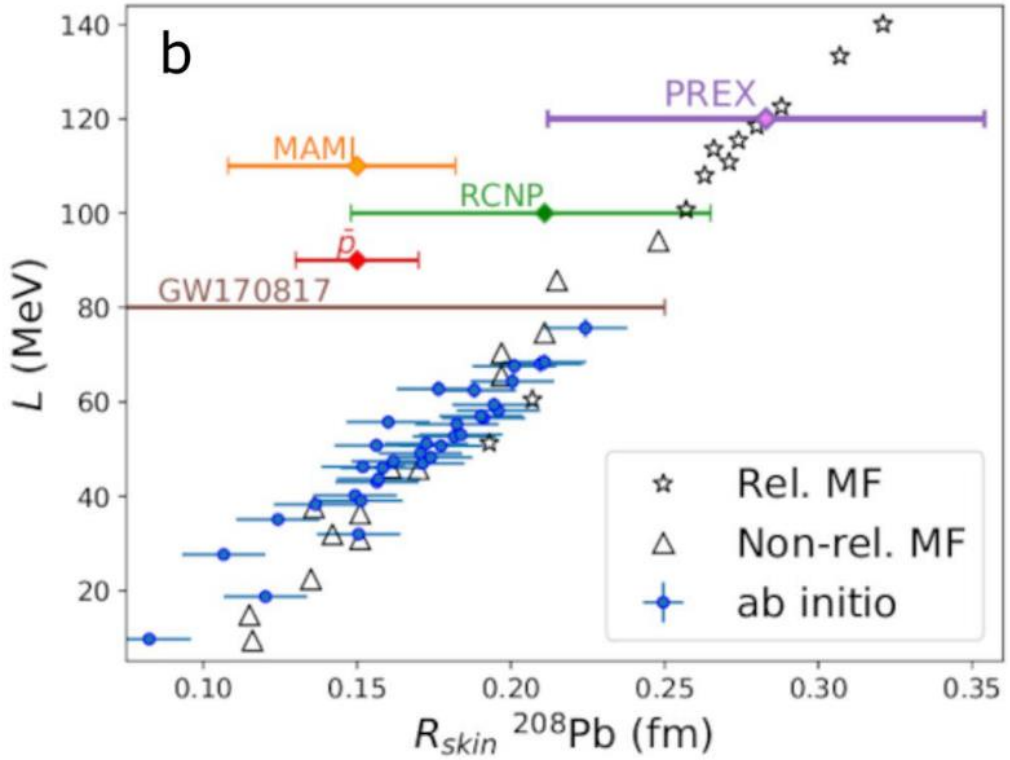
- Developments in ChEFT and many-body techniques enable us to perform nuclear ab initio calculations.
  - Heavier systems
  - Open-shell systems

- EM 2BCs are needed for the magnetic moment reproductions.
- E2 observables are significantly underestimated
  - Improvements in many-body methods are required.

- It seems a posteriori SPE tuning captures the deformation.
  - Perturbative correction of SPEs may solve the issue?

Neutron skin of ^{208}Pb



Observable	median	68% CR	90% CR
$R_{\mathrm{skin}}(^{48}\mathrm{Ca})$	0.164	[0.141, 0.187]	[0.123, 0.199]
$R_{\mathrm{skin}}(^{208}\mathrm{Pb})$	0.171	[0.139, 0.200]	[0.120, 0.221]

Neutron skins

B. Hu, W. Jiang, T. Miyagi, et al., Nat. Phys. 18, 1196 (2022).

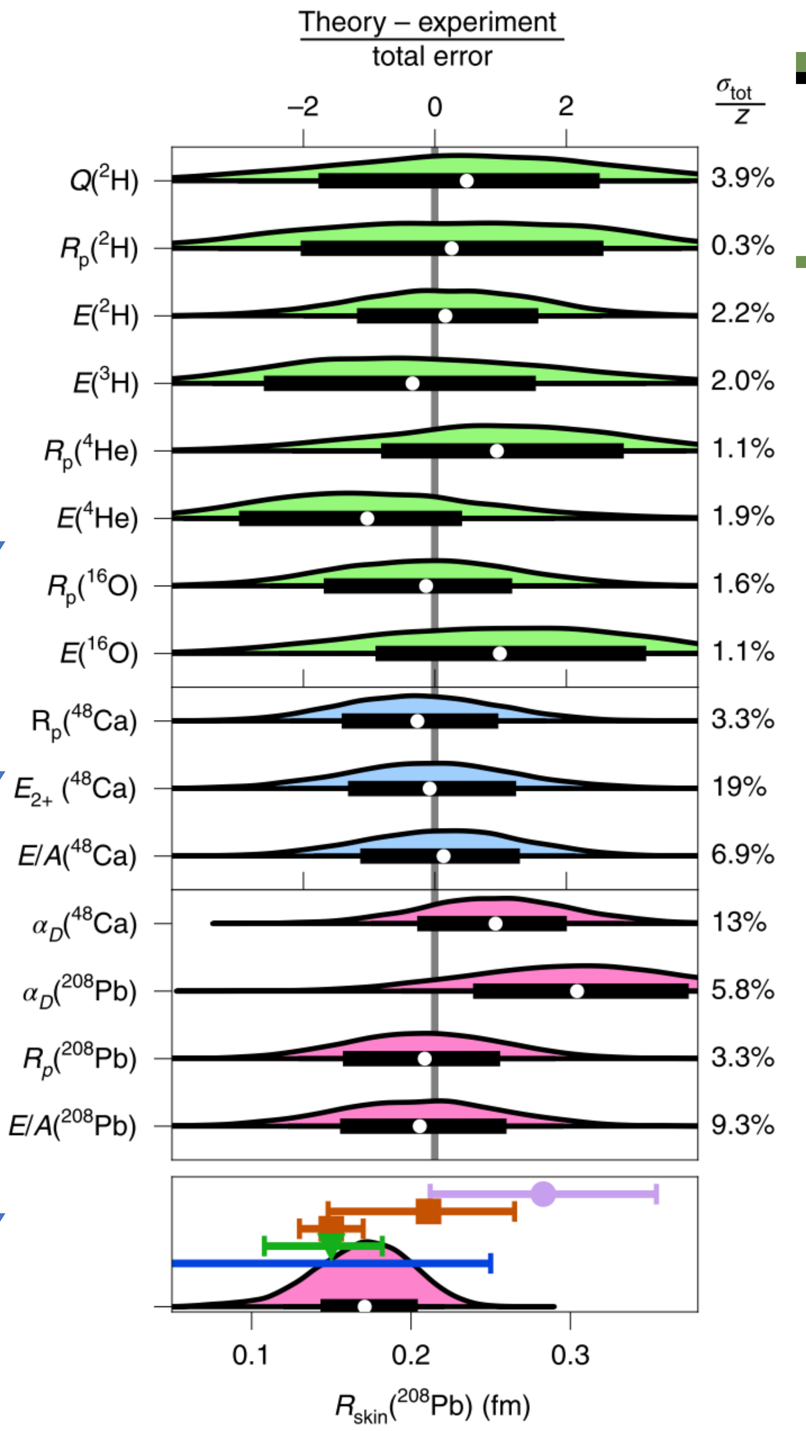
History matching

17 parameters
NN scattering
few-body + ^{16}O
$10^9 \rightarrow 34$

Calibration

Sampling/Importance resampling

Validation
Prediction



Is ^{40}Ca magic?

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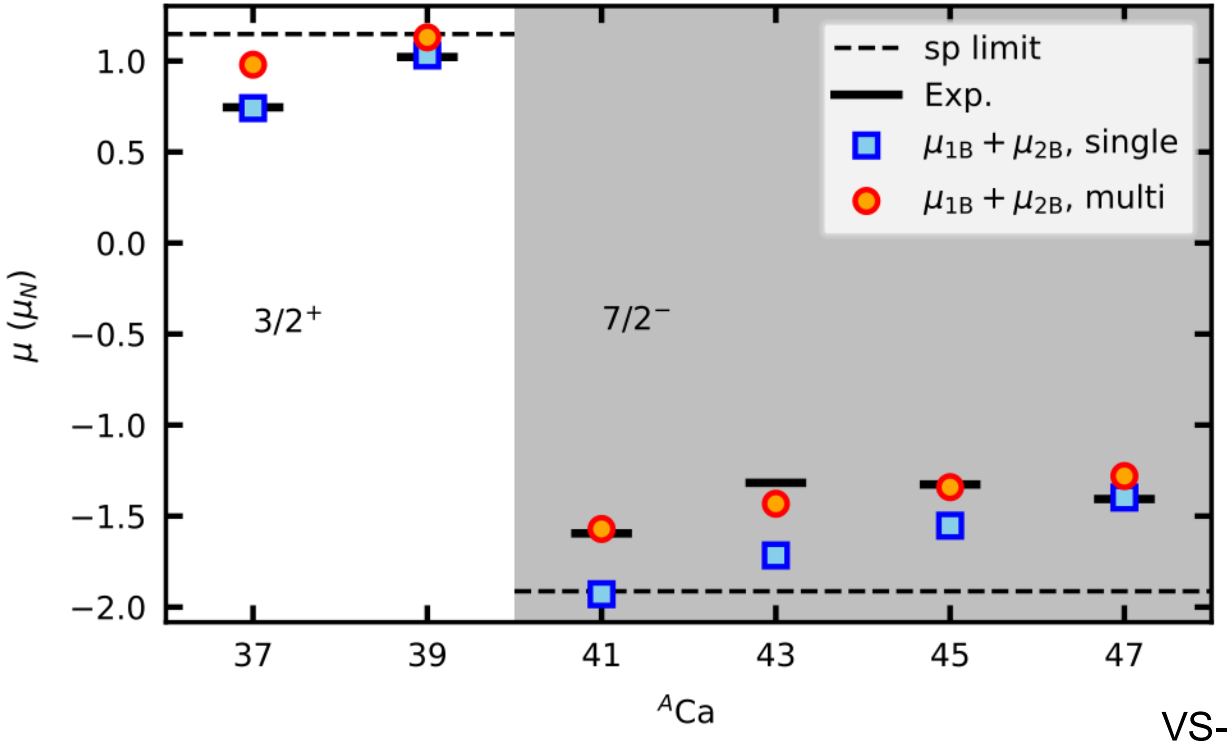
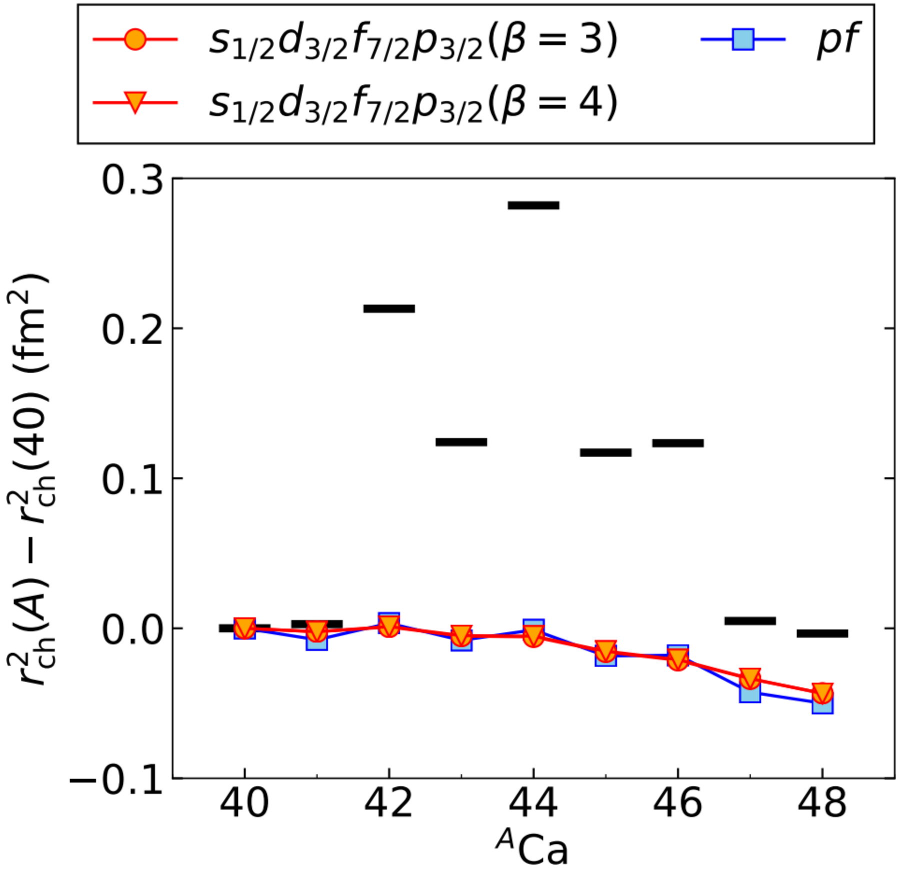
- 2BC makes agreement worse.
- Activating the ^{40}Ca core explains the magnetic moments better.
- The radii are not explained. Further investigations are needed!





VS-IMSRG(2), 1.8/2.0 (EM)

TM et al., Phys. Rev. Lett. 132, 232503 (2024).

Mass dependence of 2B contribution

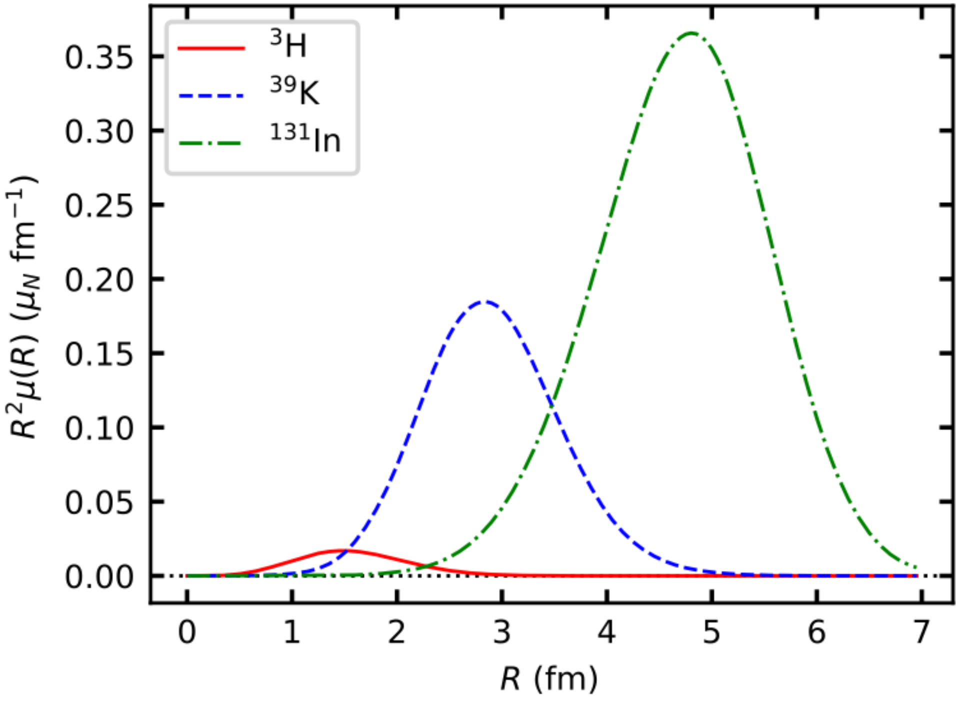
$$\mu^{2B} = \mu^{2B}_{\rm intr} + \boxed{\mu^{2B}_{\rm Sachs}} \qquad \mu^{2B}_{\rm Sachs} \propto \sum_{i<j} (\boldsymbol{R}_{ij} \times \boldsymbol{r}_{ij}) V^{\rm OPE}(r_{ij})$$

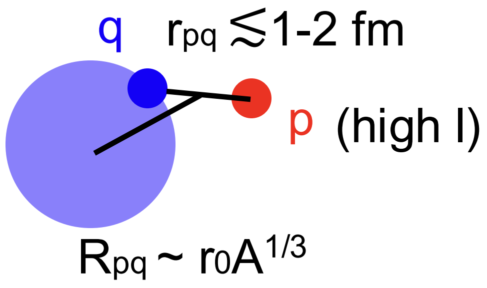
Dominant in heavy systems

- The size of 2BC contribution is larger in heavier systems.
- The simplest configuration limit is 0^+ core + 1 particle (or hole)

$$\langle J || \mu || J \rangle \sim \sum_{q \in \rm core} \sum_{I} f(j_p, j_q, I) \langle pq : I || \mu || pq : I \rangle$$

- $|r_p - r_q| \lesssim$ 1-2 fm because of pion-exchange potential





$$\boldsymbol{\mu}^{\rm Sachs}_{pq} \propto (\boldsymbol{R}_{pq} \times \boldsymbol{r}_{pq}) V^{\pi}(r_{pq})$$

The peak position moves to larger R for heavier systems.

TM et al., Phys. Rev. Lett. 132, 232503 (2024).