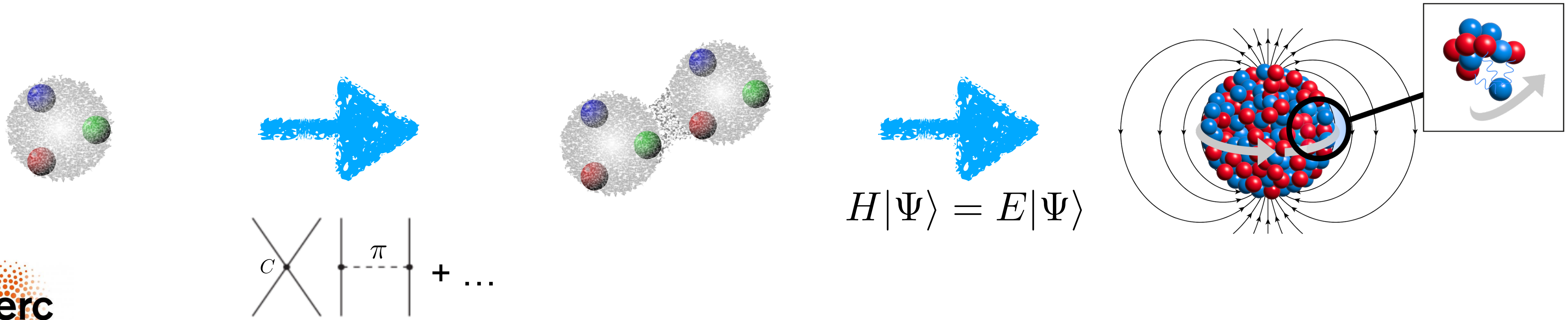
筑波大学
計算科学研究センター
Center for Computational Sciences

Nuclear magnetic dipole moments from ab initio calculation



SFB 1245
European Research Council
Established by the European Commission
ERATO
TOMOE

Takayuki Miyagi

10th International Conference on Quarks and Nuclear Physics (July 8, 2024)

Collaborators

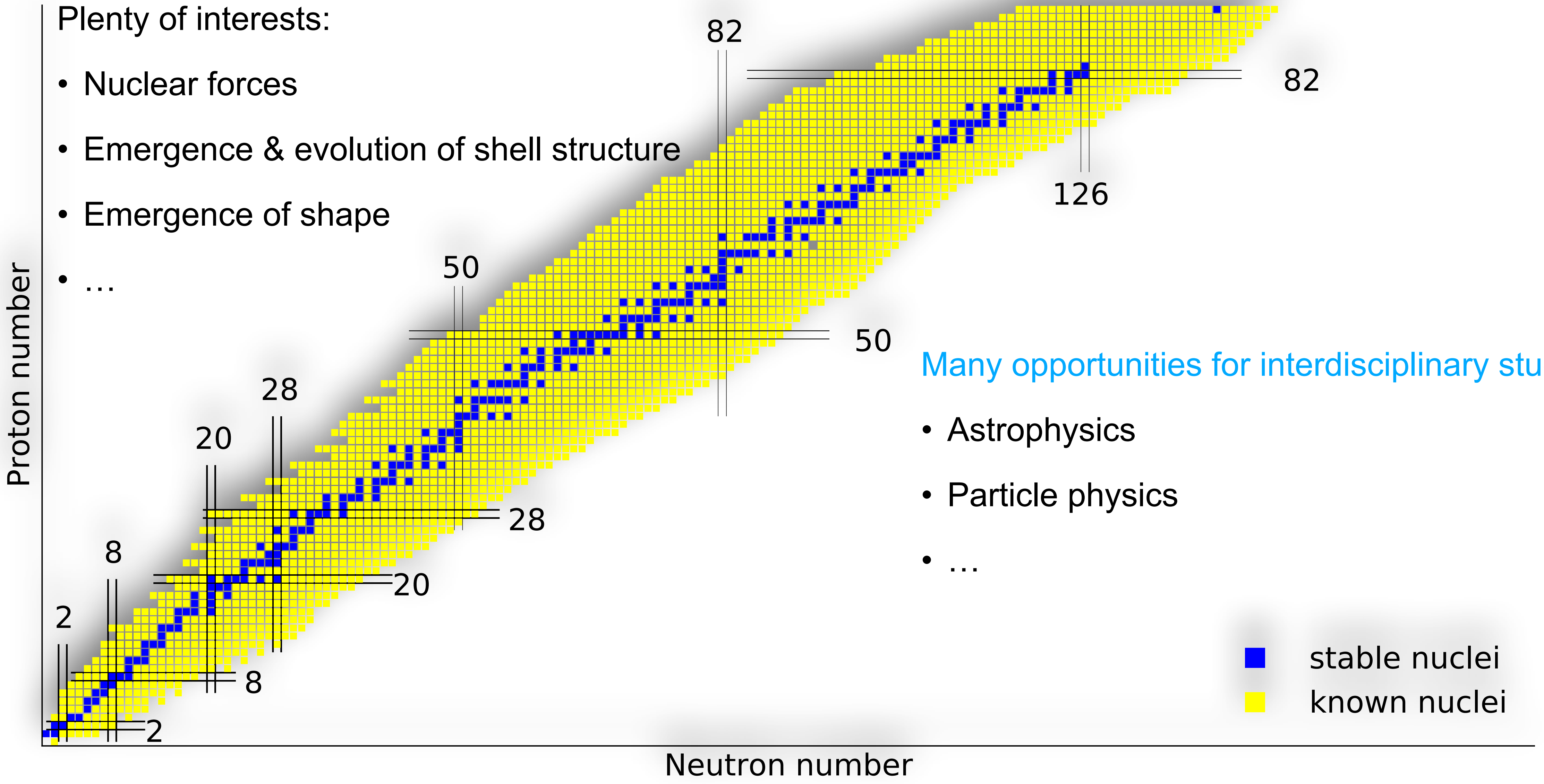
- TU Darmstadt: C. Brase, K. Hebeler, A. Schwenk, R. Seutin
- TRIUMF: J. D. Holt
- University of Illinois: X. Cao
- Massachusetts Institute of Technology: R. G. Ruiz
- University of Barcelona: J. Menendez
- Johannes Gutenberg University of Mainz: S. Bacca

Motivations

筑波大学 計算科学研究センター Center for Computational Sciences

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

Plen

- Nu
- En
- En
- …

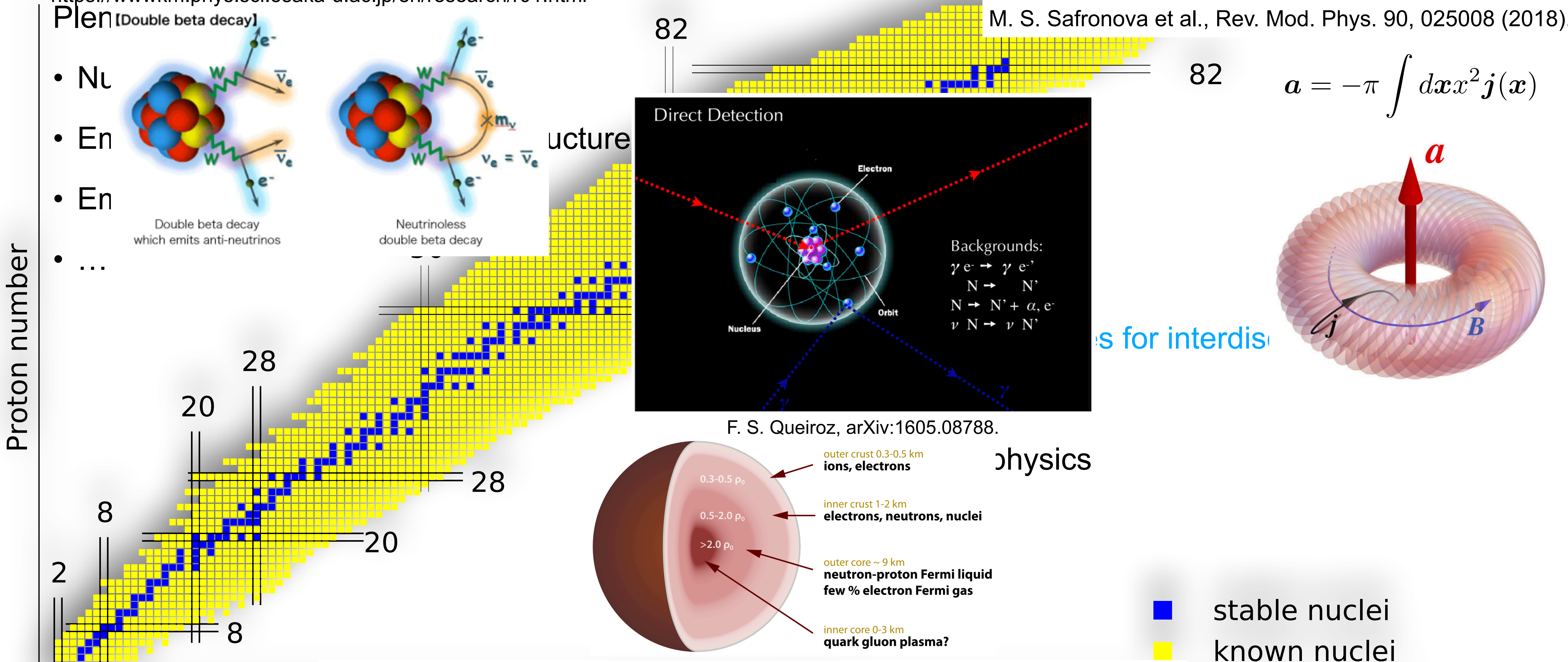
ucture

s for interdis

physics

M. S. Safronova et al., Rev. Mod. Phys. 90, 025008 (2018).

$$a = -\pi \int dx\, x^2 j(x)$$



F. S. Queiroz, arXiv:1605.08788.

Tests of current knowledge are needed!

Motivations

- 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 (focus of this talk)

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

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

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

Motivations

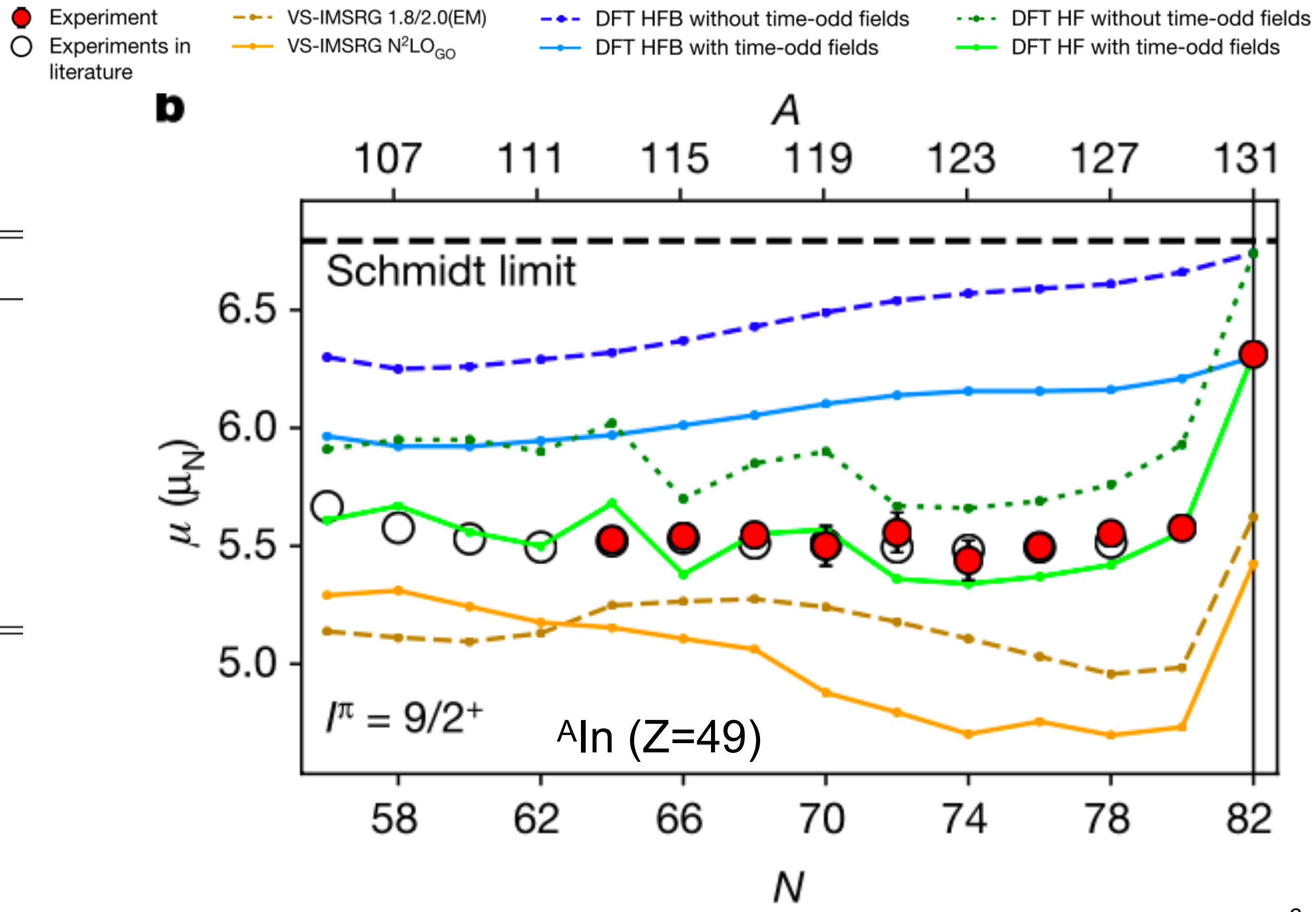
- Ab initio IMSRG calculations

A. Klose et al., Phys. Rev. C 99, 061301 (2019).

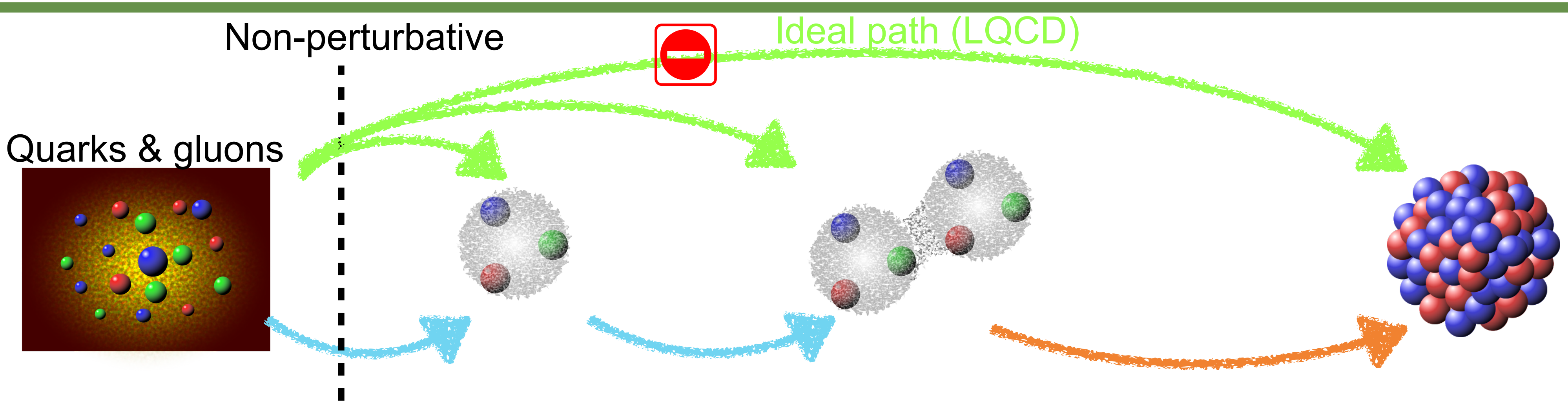
A		$Z = 20$	$N = 20$
	sp g^{free}	+1.148	+0.124
39	Expt.	+1.0217(1) [23]	+0.3915073(1) [24]
	sp g^{eff}	+0.930	+0.469
	VS-IMSRG	+1.349	−0.035
37	Expt.	+0.7453(72)	+0.6841236(4) [25]
	USDA-EM1	+0.770	+0.677
	USDB-EM1	+0.754	+0.675
	VS-IMSRG	+1.055	+0.290

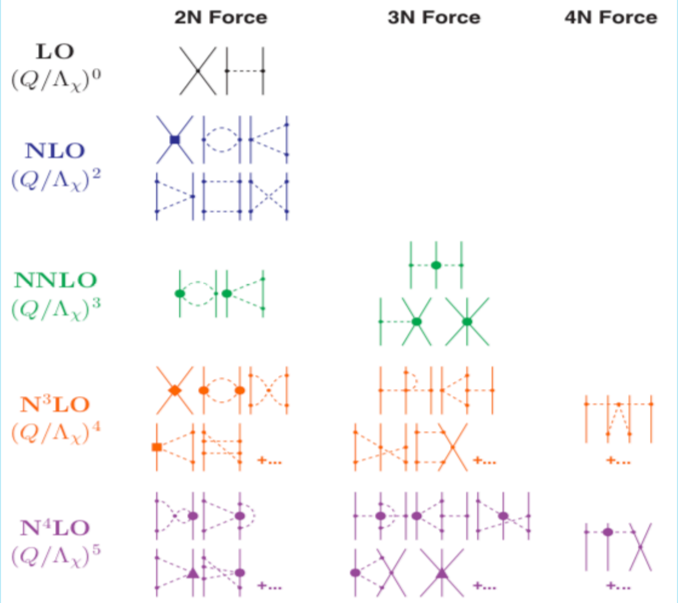
of ^{36}Ca. Compared to the USDA/B-EM1 calculations, the VS-IMSRG agrees with the dominance of the (620) partition for ^{36}Ca. However, the amount of the (522) partition that gives the core-polarization correction is a factor of 2 larger. The deviation is likely due to meson-exchange currents [39], which are not included in the present VS-IMSRG calculations, but are included indirectly through the effective g factors in the USDA/B-EM1 calculations.

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



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
- …

Nuclear interaction from chiral EFT

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

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

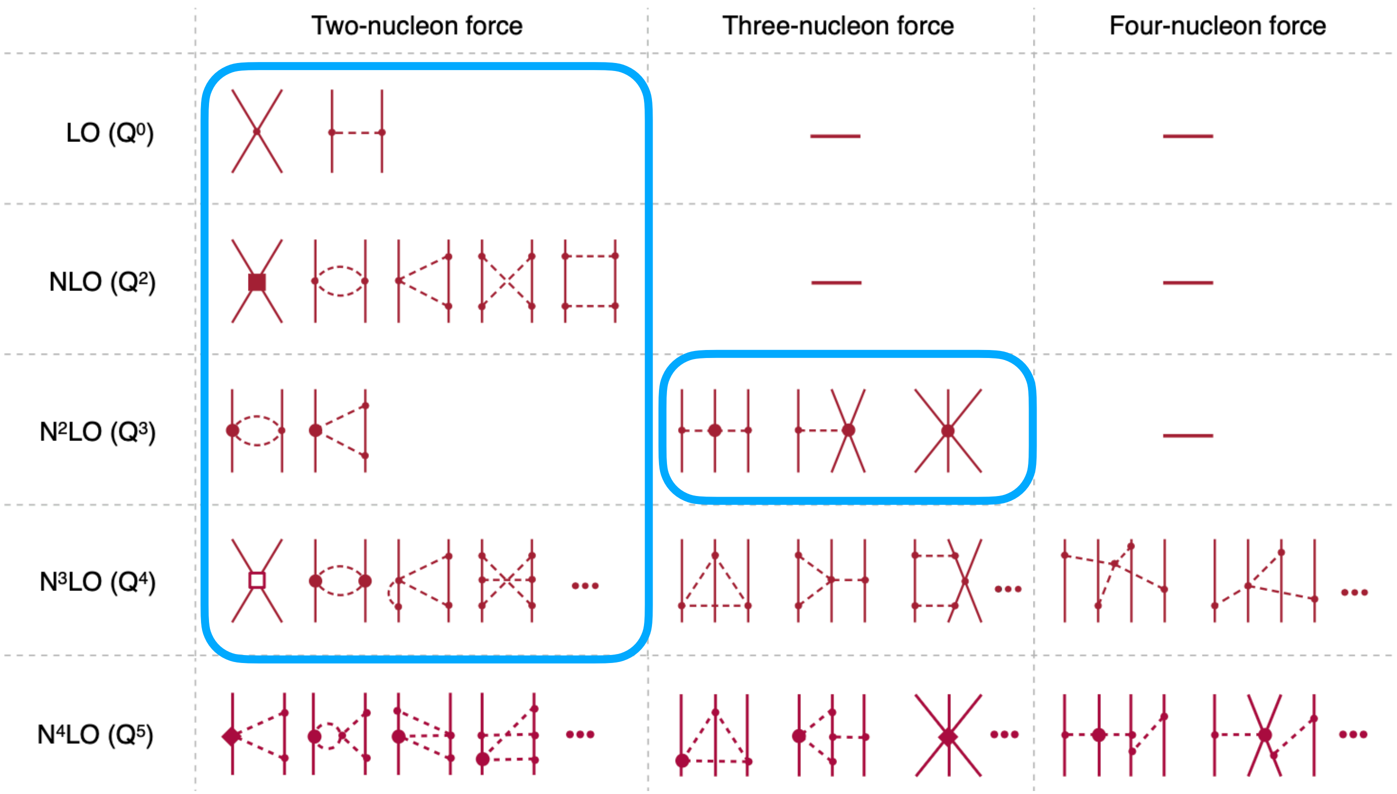
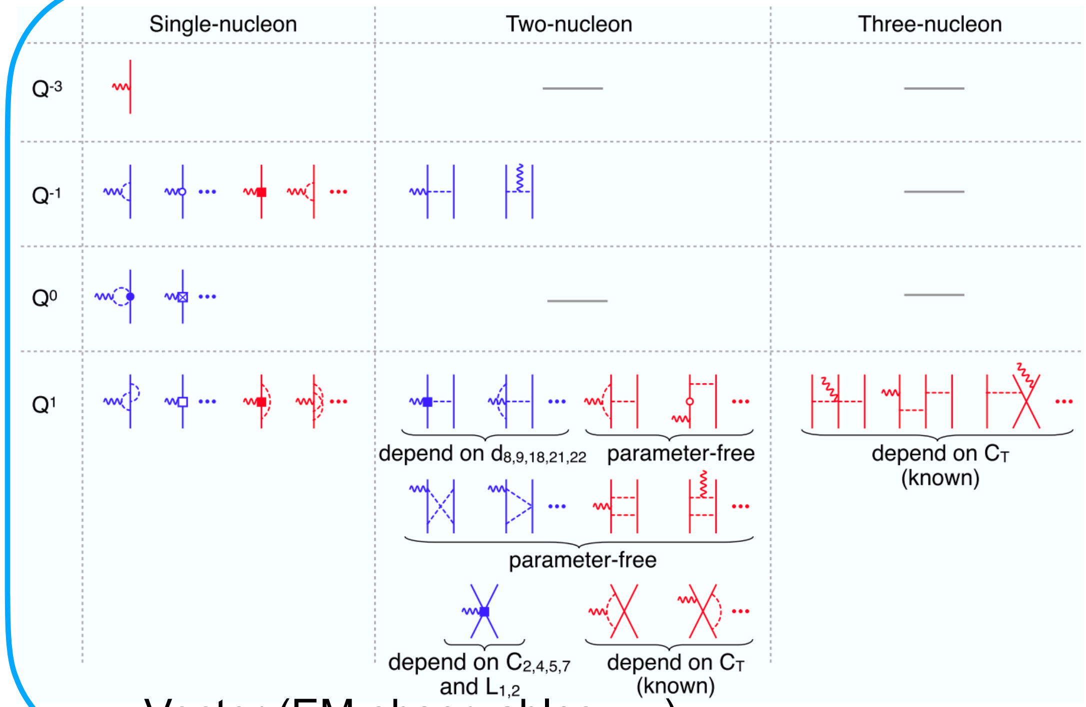


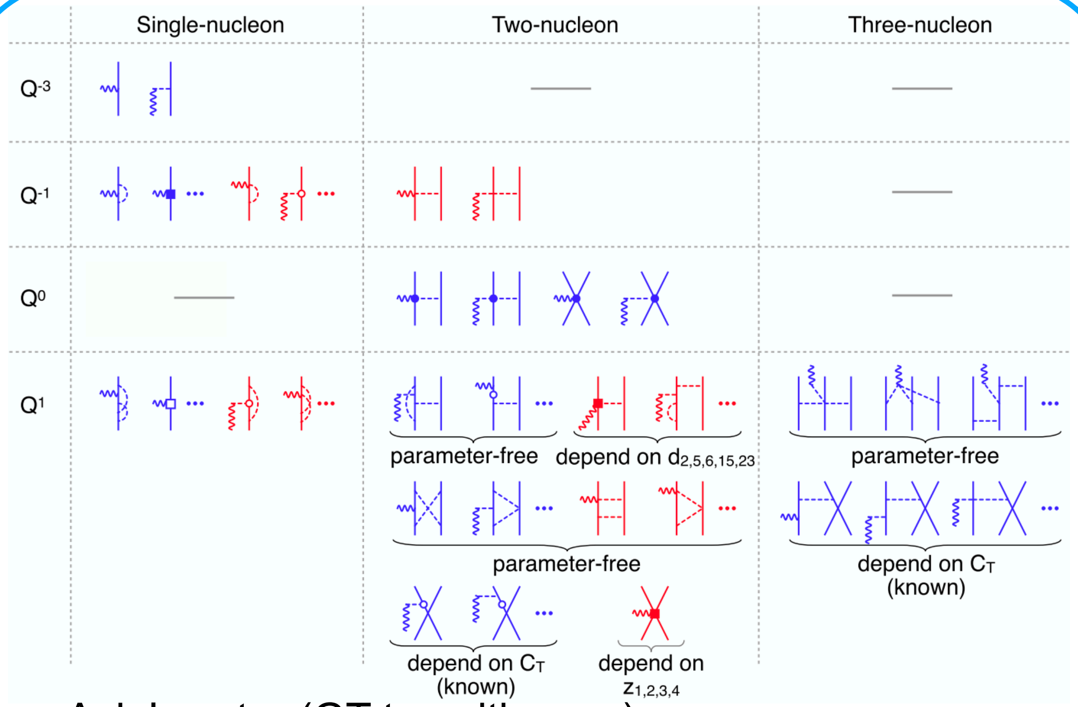
Figure is from E. Epelbaum, H. Krebs, and P. Reinert, Front. Phys. 8, 1 (2020).

Nuclear currents from chiral EFT

- Nuclear observables (EM properties, beta decay, …) are measured through the interaction between a nucleus and external field.
- Chiral EFT allows us a systematic expansion for charge and current operators.



Vector (EM observables, …)

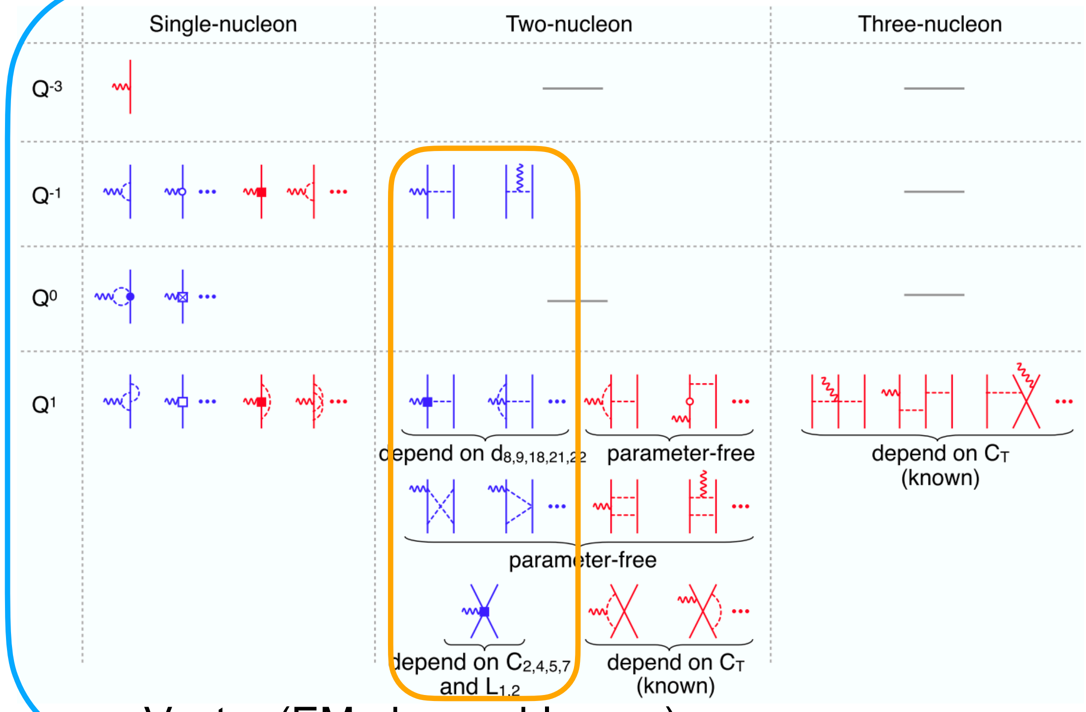


Axial vector (GT transition, …)

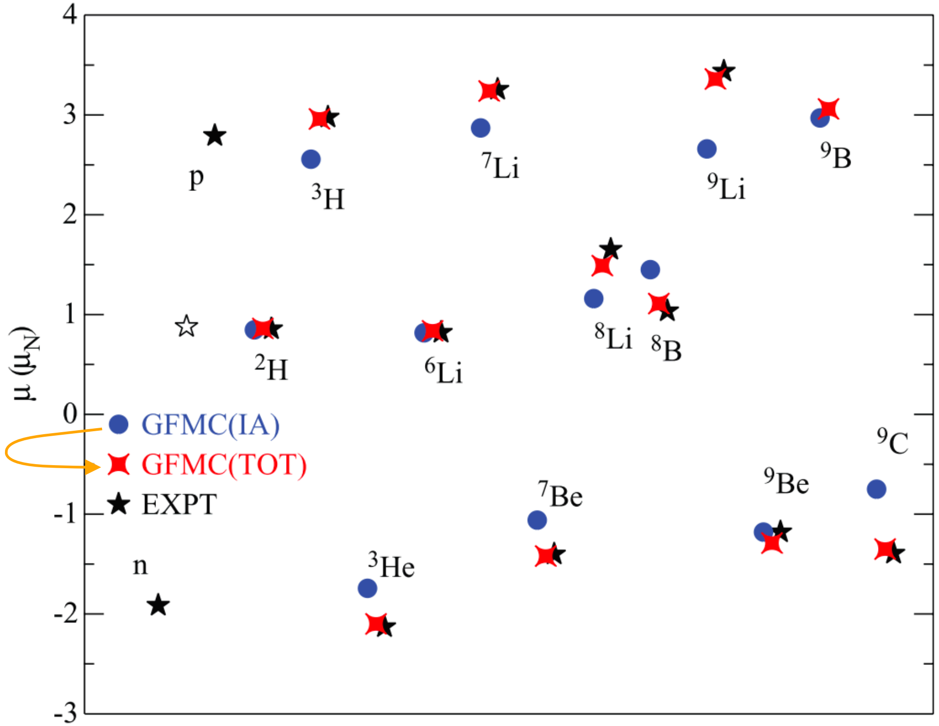
E. Epelbaum, arXiv:1908.09349.

Nuclear currents from chiral EFT

- Nuclear observables (EM properties, beta decay, …) are measured through the interaction between a nucleus and external field.
- Chiral EFT allows us a systematic expansion for charge and current operators.

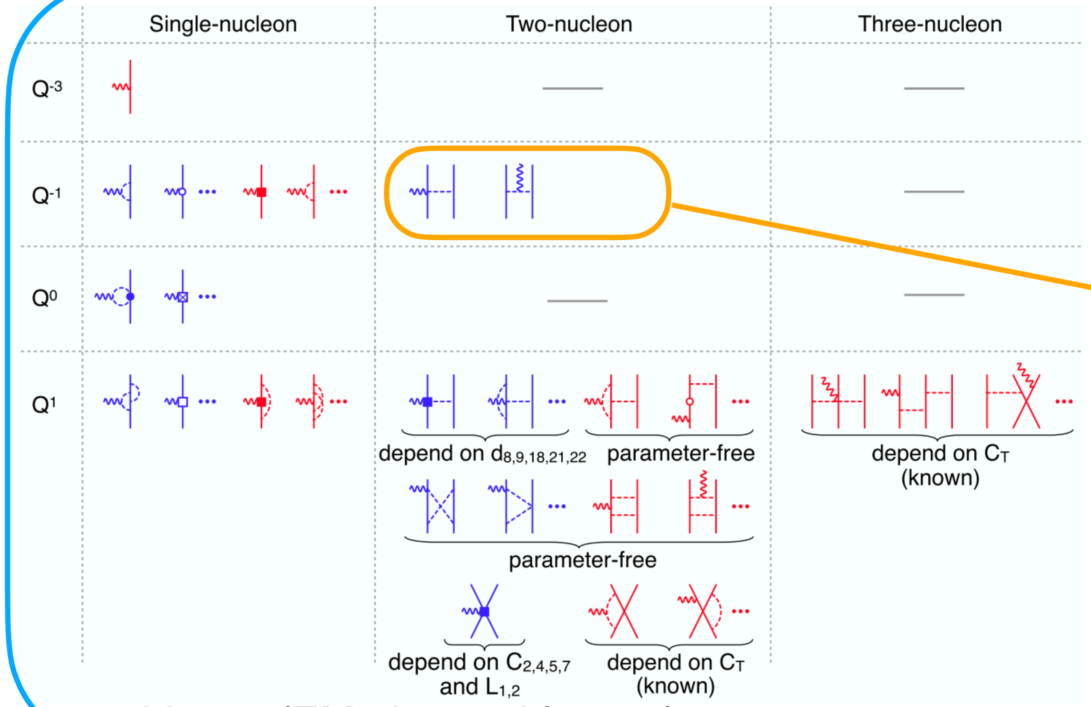


S. Pastore et al., Phys. Rev. C 87, 035503 (2013).



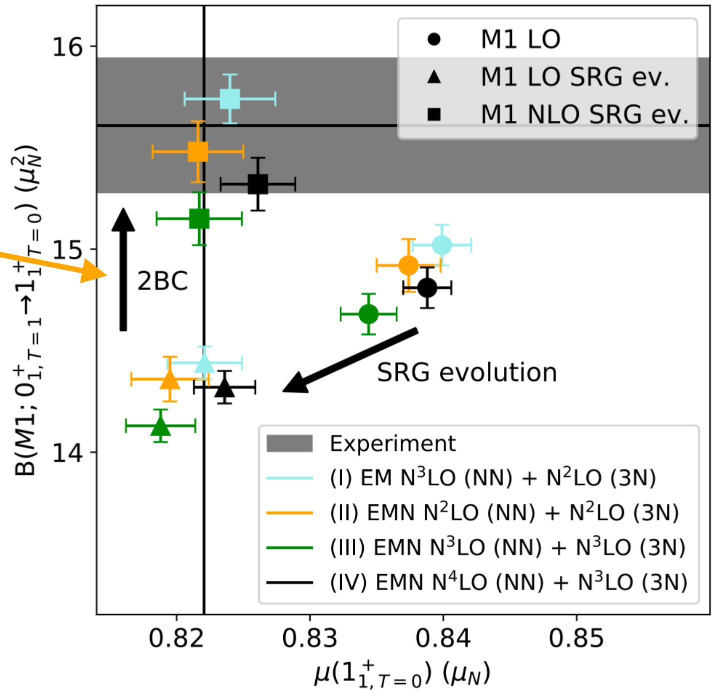
Nuclear currents from chiral EFT

- Nuclear observables (EM properties, beta decay, …) are measured through the interaction between a nucleus and external field.
- Chiral EFT allows us a systematic expansion for charge and current operators.



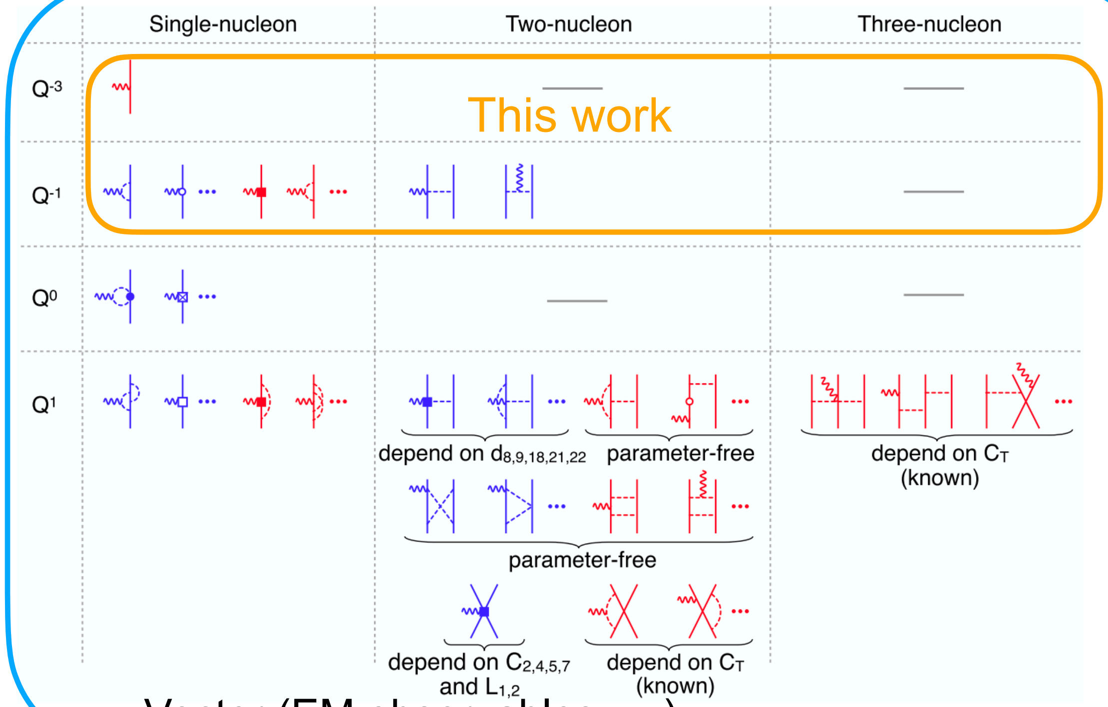
Vector (EM observables, …)

U. Friman-Gayer et al., Phys. Rev. Lett. 126, 102501 (2021).



Nuclear currents from chiral EFT

- Nuclear observables (EM properties, beta decay, …) are measured through the interaction between a nucleus and external field.
- Chiral EFT allows us a systematic expansion for charge and current operators.



Vector (EM observables, …)

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

LO 2BC appear at Q^1 order (N^3LO)

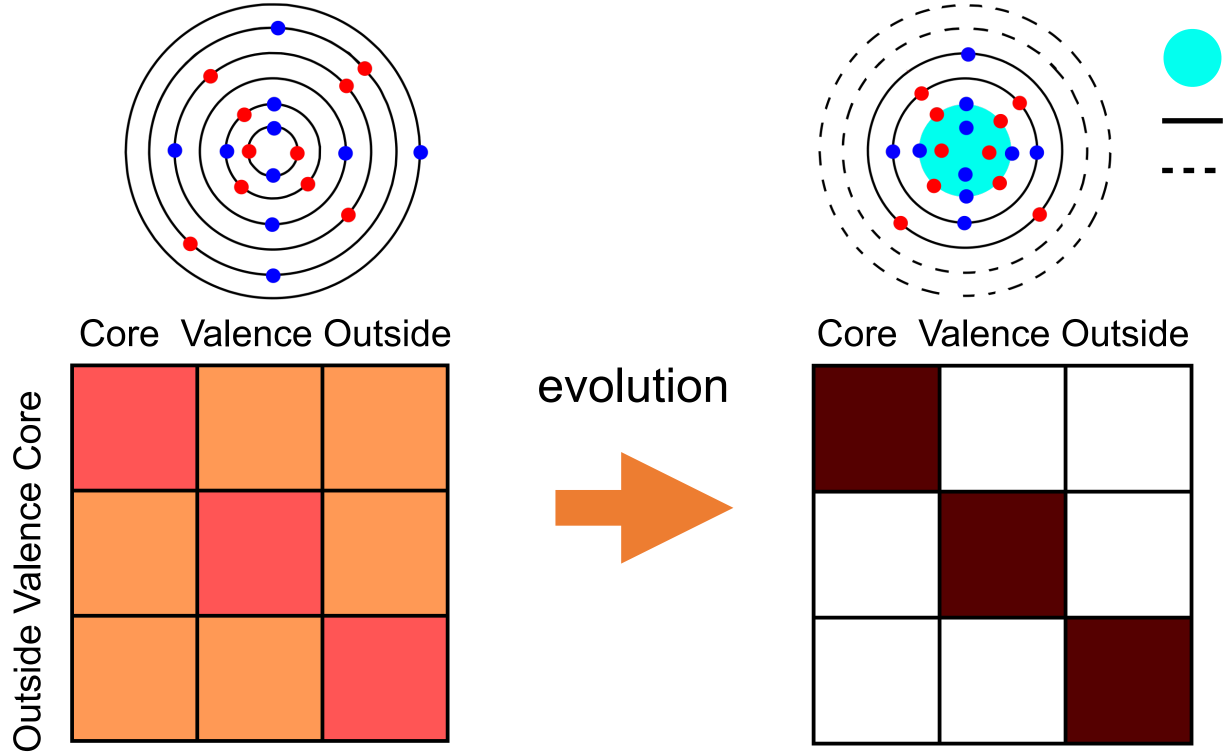
$$Q_{20} = -\frac{15}{8\pi}\lim_{Q\to 0}\frac{d^2}{dQ^2}\int d\hat{\boldsymbol{Q}}\,Y_{20}(\hat{\boldsymbol{Q}})\tilde{\rho}(\boldsymbol{Q})$$

$$M_{10} = -i\frac{3}{8\pi}\lim_{Q\to 0}\frac{d}{dQ}\int d\hat{\boldsymbol{Q}}\left\{[\boldsymbol{Q}\times\nabla_{\boldsymbol{Q}}]Y_{10}(\hat{\boldsymbol{Q}})\right\}\cdot\tilde{j}(\boldsymbol{Q})$$

or $\boldsymbol{M} = -\frac{i}{2}\sqrt{\frac{3}{4\pi}}\lim_{Q\to 0}\nabla_{\boldsymbol{Q}}\times\tilde{\boldsymbol{j}}(\boldsymbol{Q})$

LO 2BC appear at Q^{-1} order (NLO)

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

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

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

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

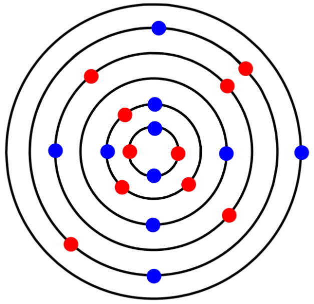
$$\eta_{1234} = \frac{1}{2}\arctan\left(\frac{2\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta}\right)$$

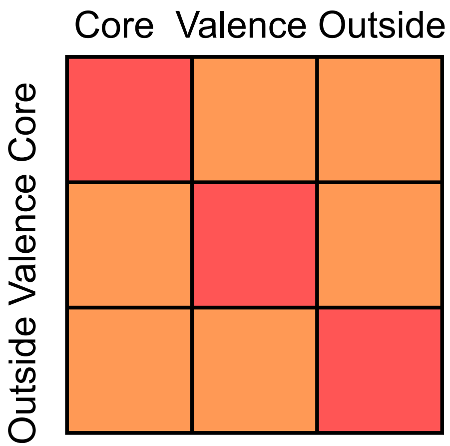
$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

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

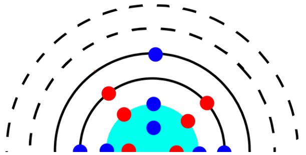
$$\mathcal{O}(s) = e^{\Omega(s)} \mathcal{O} e^{-\Omega(s)} \approx \mathcal{O}^{[0]}(s) + \sum_{12} \mathcal{O}^{[1]}_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234} \mathcal{O}^{[2]}_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

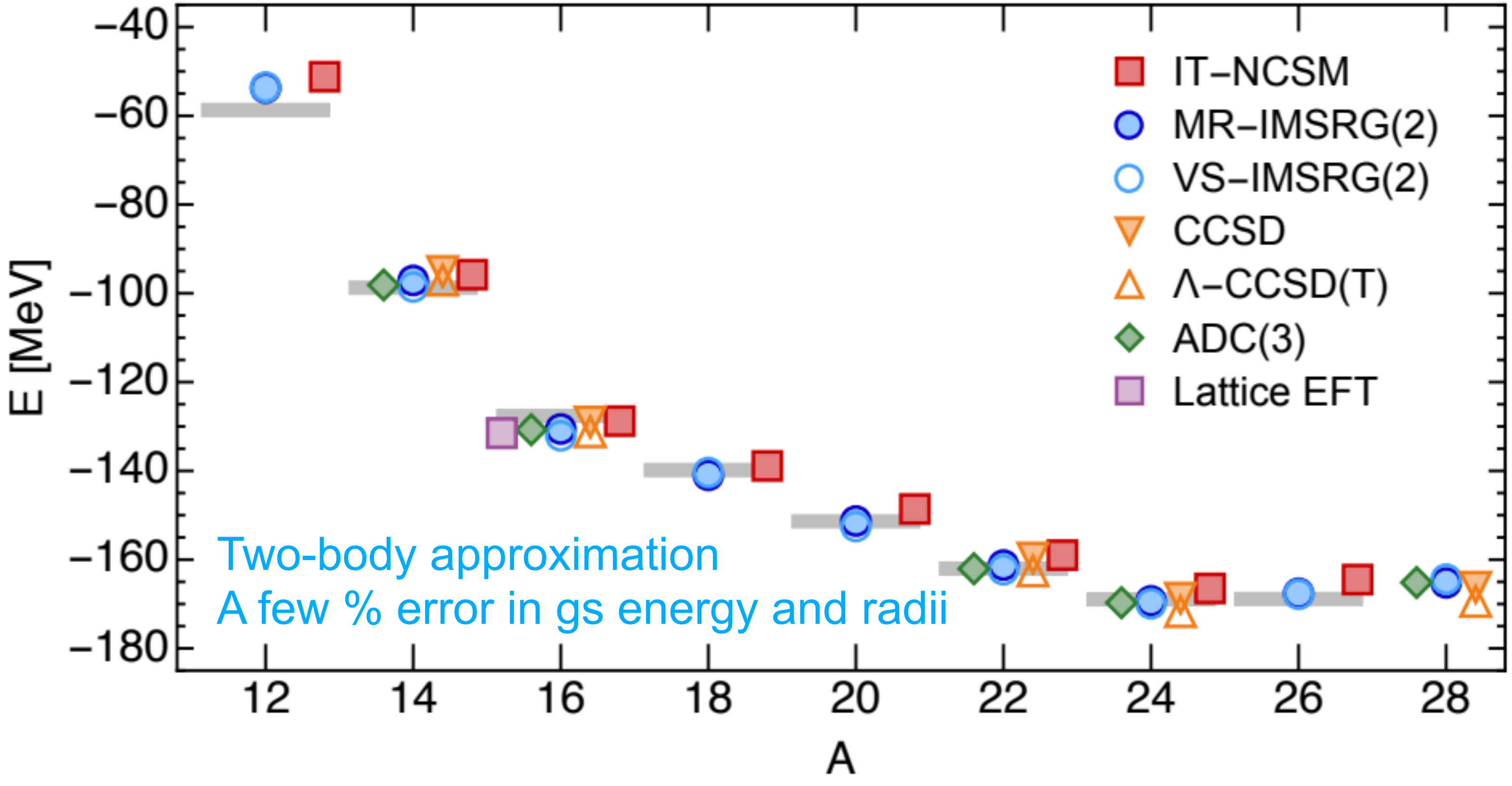
Valence-space in-medium similarity renormalization group





evolution





Similarity transformat

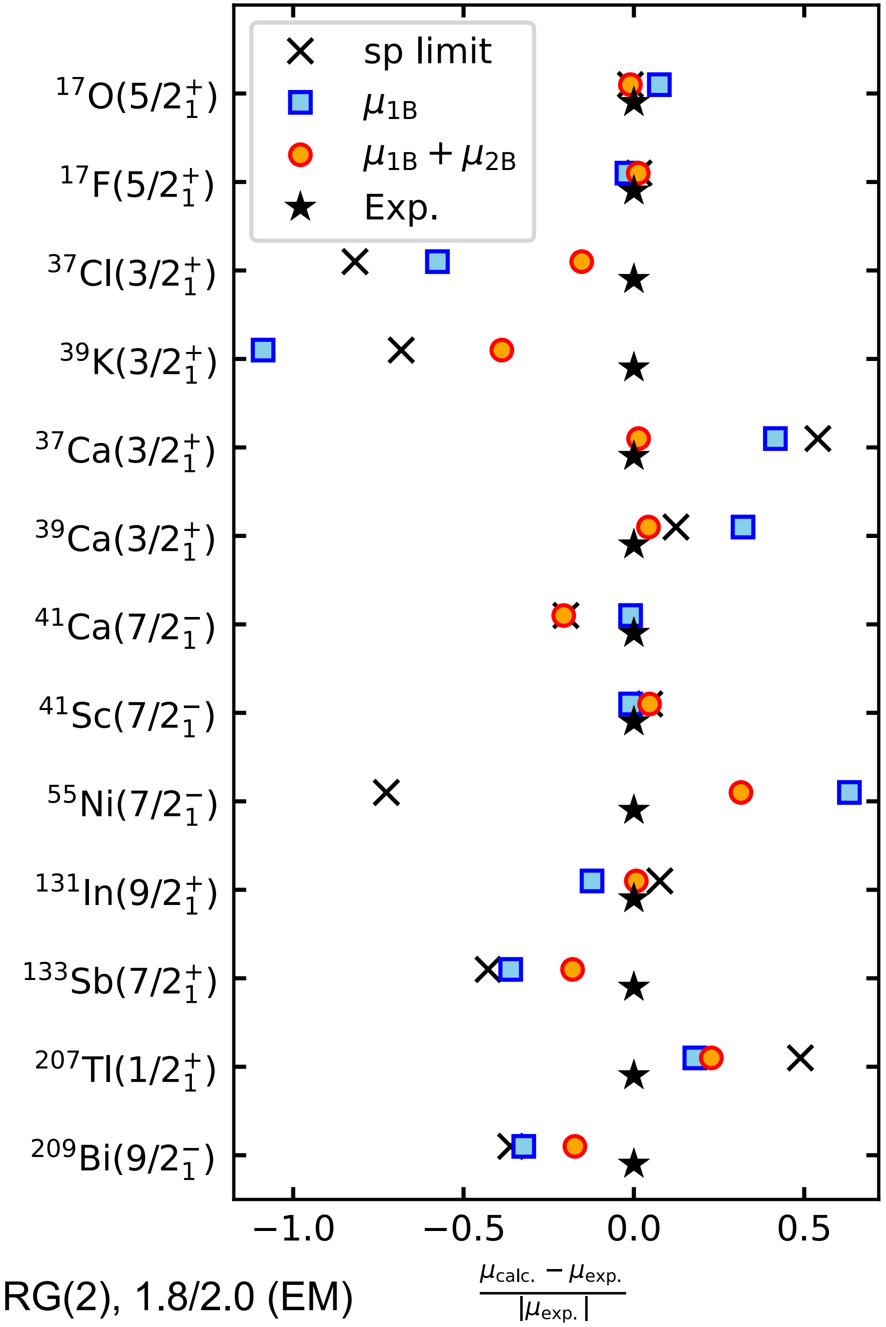
H

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

s: flow parameter

Magnetic dipole moments

- Magnetic moment from IMSRG.
- Single-particle analytical limits do not always explain the experimental data.
- A better agreements with IMSRG, but not perfect.
- 2BC globally improves the magnetic moments.
  - ✦ Enhancement from 2BC

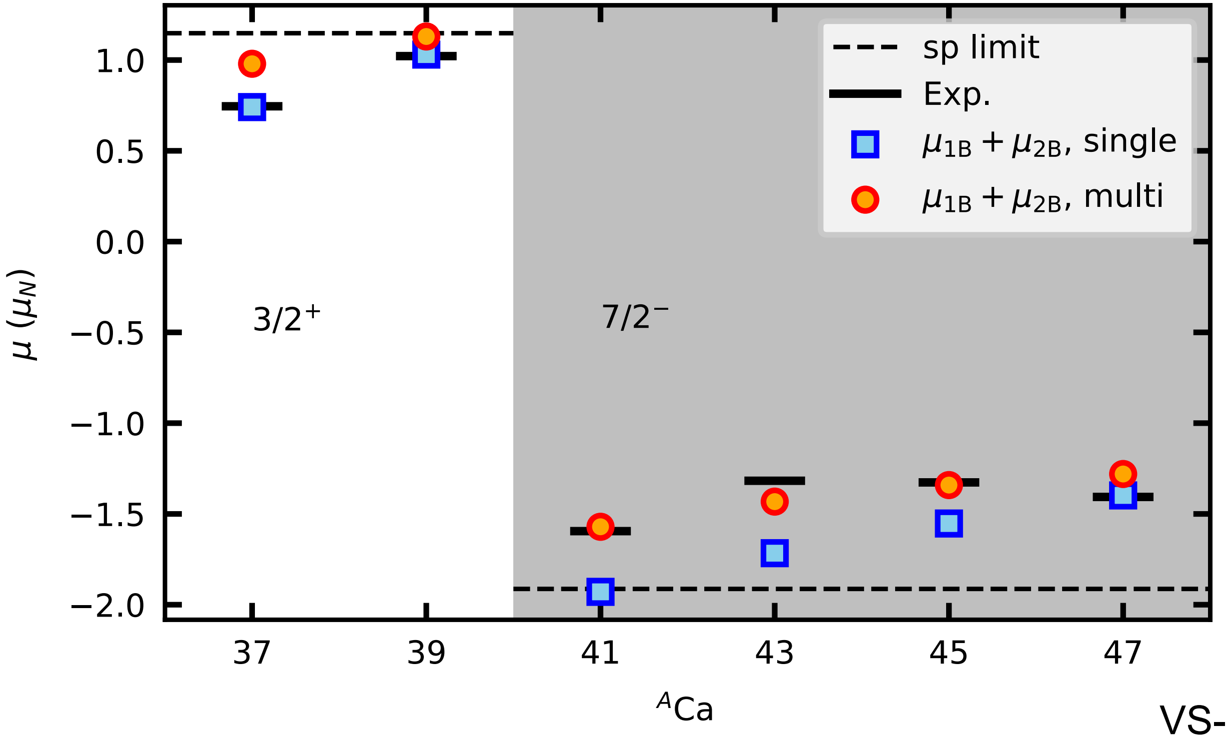


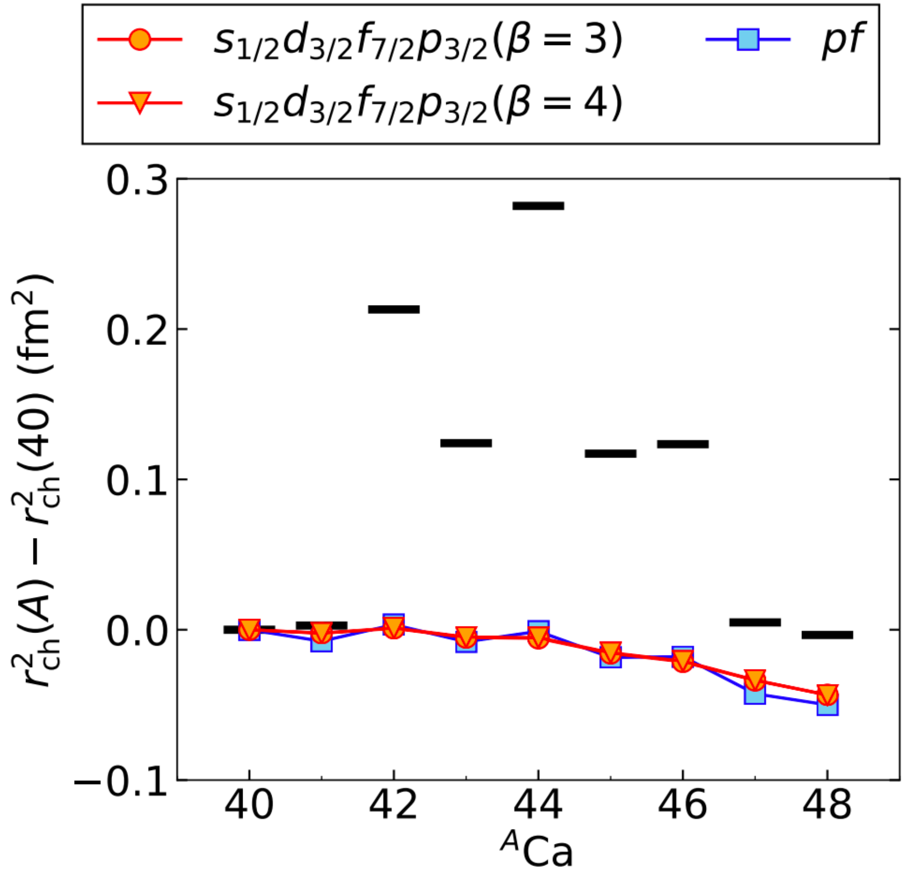
VS-IMSRG(2), 1.8/2.0 (EM)

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

Is ^{40}Ca magic?

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



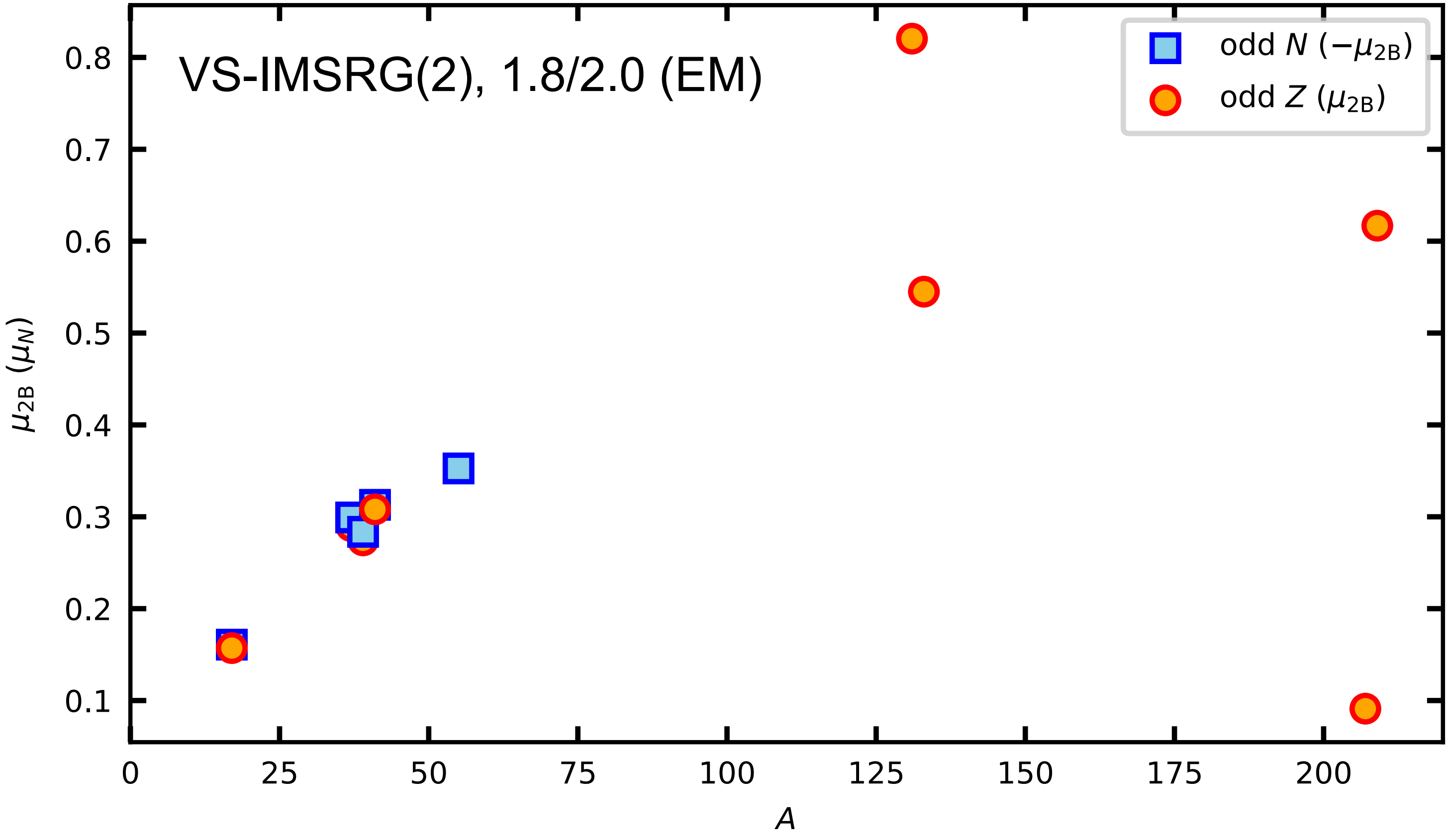


VS-IMSRG(2), 1.8/2.0 (EM) TM et al., Phys. Rev. Lett. 132, 232503 (2024).

Mass dependence of 2B contribution

筑波大学
計算科学研究センター
Center for Computational Sciences

- The size of 2BC contribution is larger in heavier systems.



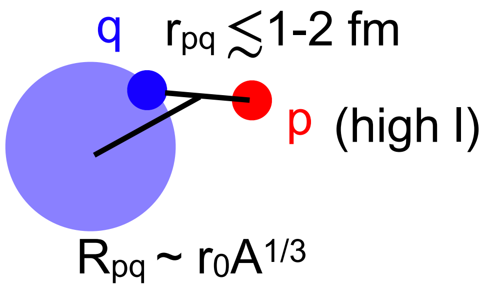
Mass dependence of 2B contribution

筑波大学 計算科学研究センター Center for Computational Sciences

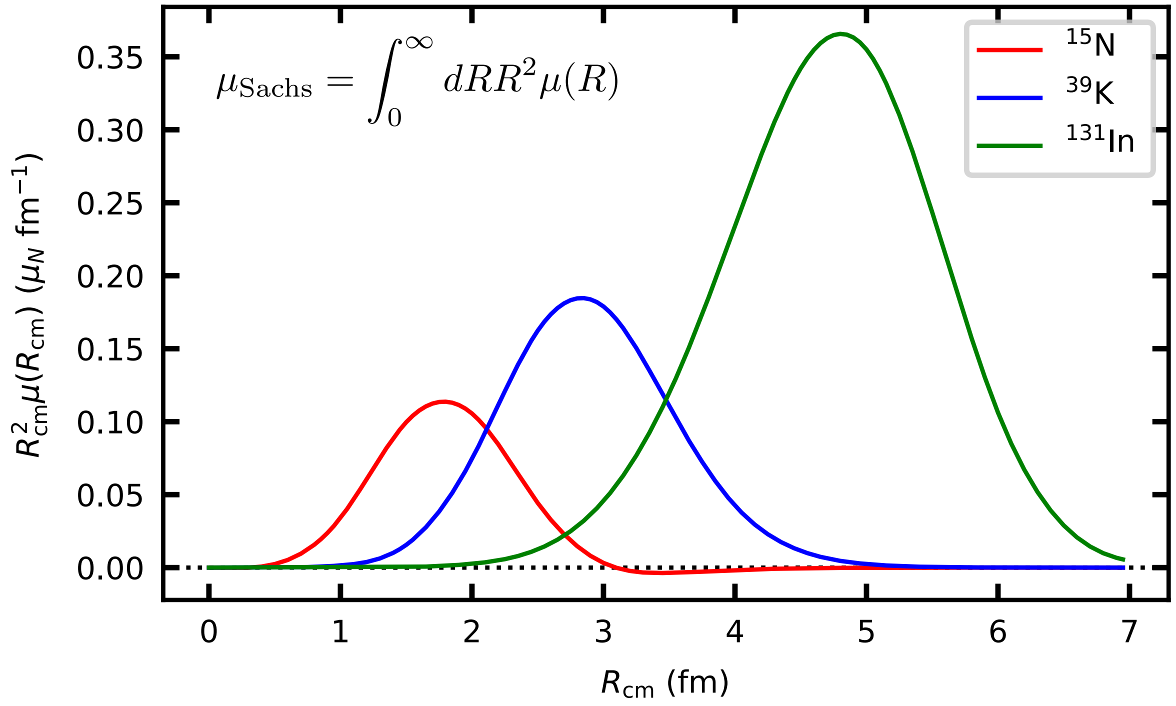
- The size of 2BC contribution is larger in heavier systems.
- The simplest configuration limit is 0^+ core + 1 particle (or hole)

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

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



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



The peak position moves to larger R for heavier systems.

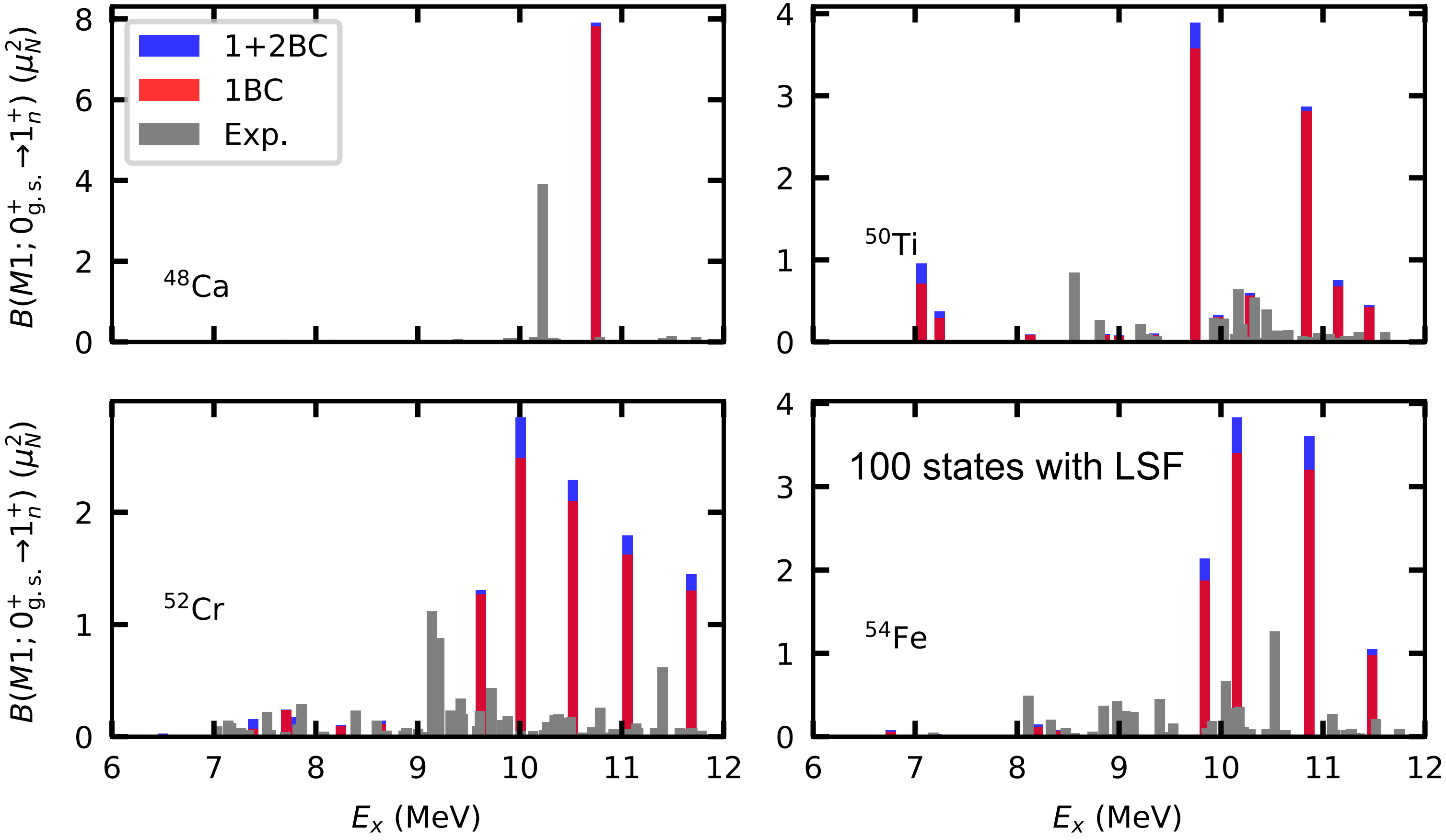
TM et al., Phys. Rev. Lett. 132, 232503 (2024).

2BC effect on M1 transition

筑波大学 計算科学研究センター Center for Computational Sciences

- M1 transition in pf-shell nuclei
- 2BC slightly enhances the major B(M1)'s.

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



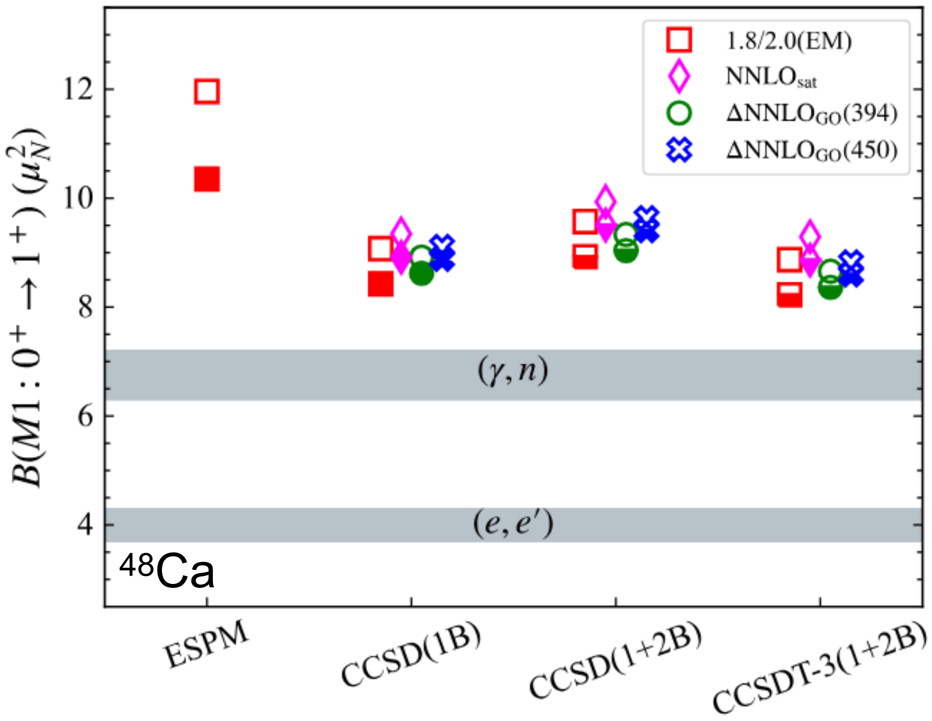
Exp. W. Steffen et al., Nucl. Phys. A 404, 413 (1983); D. I. Sober et al., Phys. Rev. C 31, 2054 (1985).

2BC effect on M1 transition

筑波大学 計算科学 Center for Co

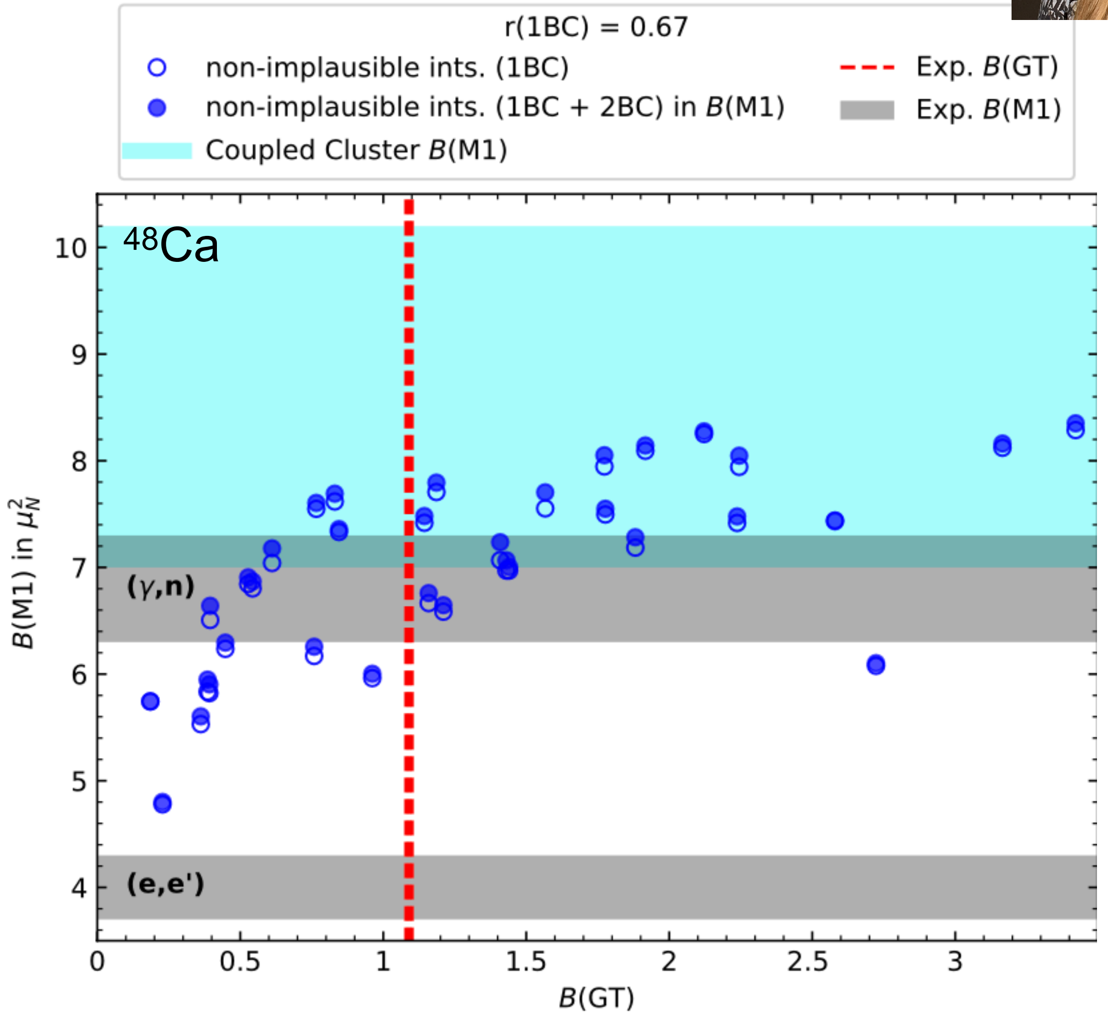
C. Brase
TU Darmstadt

Coupled-cluster calculations



Recent CC study found a similar disagreement

B. Acharya et al., Phys. Rev. Lett. 132, 232504 (2024).



Summary

- Magnetic dipole moments
  - For most of doubly-closed shell nuclei +/- 1 systems, the 2BC improves the agreements.
  - 2BC effect becomes large for heavier systems due to the 2B CM dependence of the operator.

- M1 transition
  - The 2BC effect is small for N=28 isotones. CC calculation also found a similar 2BC effect.
  - (e, e’) or (p, p’) result? Further investigation is needed

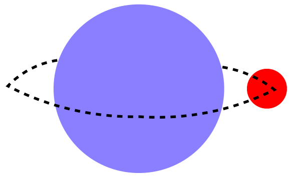
Backup slides

Motivations

- Magnetic dipole moment: $\langle\mu\rangle = \sqrt{\frac{J}{(J+1)(2J+1)}}\langle J||\mu||J\rangle$

- Magnetic dipole operator: $\boldsymbol{\mu} = \frac{e\hbar}{2m_p}\sum_i \left(g_i^l \boldsymbol{l}_i + g_i^s \boldsymbol{\sigma}_i\right)$ Point-nucleon approximation

- Neighbors of doubly magic: $|J\rangle \approx |\mathrm{Core}:0^+\rangle \otimes |j_p\rangle,\ j_p = J$



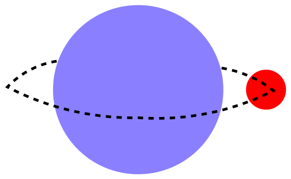
Schmidt limit

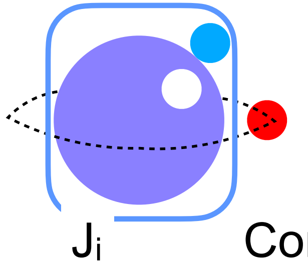
$$\langle\mu\rangle = \frac{e\hbar}{2m_p}\langle l_p j_p||g_i^l \boldsymbol{l}_i + g_i^s \boldsymbol{\sigma}_i||l_p j_p\rangle = j_p\left[g_l \mp (g_l - 2g_s)\frac{1}{2l_p+1}\right],\ \left(j_p = l_p \pm \frac{1}{2}\right)$$

T. Schmidt 1937

Motivations

- Configuration mixing effect: $|J\rangle \approx c_0[|\mathrm{Core}:0^+\rangle \otimes |j_p\rangle] + \sum_i c_i[[|j_h^{-1}\rangle \otimes |j_q\rangle]_{J_i} \otimes |j_p\rangle]_J$





Core polarization

- Arima and Horie computed c_i perturbatively: $c \sim \frac{V}{\varepsilon}$

NN interaction

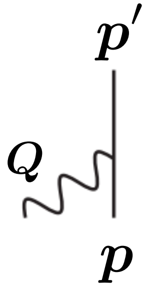
SPE energy gap

A. Arima & H. Horie 1954

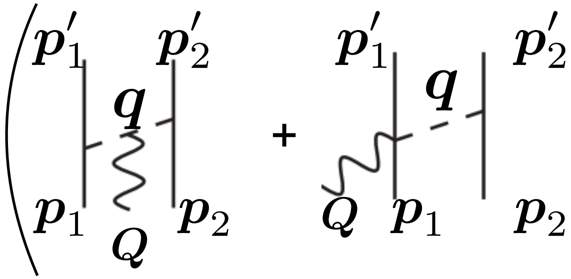
- Good agreement with data.
  - ✦ The deviation from the Schmidt value indicates how much the 0+ core is broken.

Magnetic dipole operator

$$\boldsymbol{\mu} = -\frac{i}{2}\nabla_{\boldsymbol{Q}}\times\left(\quad \right) \to \mu_N \sum_i \left(g_i^s \boldsymbol{\sigma}_i + g_i^l \boldsymbol{l}_i\right) \qquad (Q \to 0)$$



$$\boldsymbol{\mu} = -\frac{i}{2}\nabla_{\boldsymbol{Q}}\times\left(\quad + \quad \right) \to \sum_{i<j} \boldsymbol{\mu}_{ij}^{\text{intr}} + \boldsymbol{\mu}_{ij}^{\text{Sachs}} \qquad (Q \to 0)$$



$$\boldsymbol{\mu}_{ij}^{\text{intr}} = -\mu_N \frac{g_A^2 m_\pi m_p}{16\pi f_\pi^2}(\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j)_z \left\{ \left(1 + \frac{1}{x_{ij}}\right) \frac{[(\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j)\cdot \boldsymbol{x}_{ij}]\boldsymbol{x}_{ij}}{x_{ij}^2} - (\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j) \right\} e^{-x_{ij}}$$

$$\boldsymbol{\mu}_{ij}^{\text{Sachs}} = -\mu_N \frac{g_A^2 m_\pi^2 m_p}{48\pi f_\pi^2}(\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j)_z (\boldsymbol{R}_{ij} \times \boldsymbol{x}_{ij}) V_{ij}(x_{ij})$$

$$V_{ij}(x_{ij}) = \left[S_{ij}\left(1 + \frac{3}{x_{ij}} + \frac{3}{x_{ij}^2}\right) + (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \right] \frac{e^{-x_{ij}}}{x_{ij}} - \frac{1}{x_{ij}^2}(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\delta(x_{ij})$$

$$\boldsymbol{x}_{ij} = m_\pi \boldsymbol{r}_{ij}$$

Normal ordering wrt a single Slater determinant

筑波大学 計算科学研究センター Center for Computational Sciences

- Initial Hamiltonian is expressed with respect to nucleon vacuum

$$H = \sum_{pq} t_{pq} a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} V_{pqrs} a_p^\dagger a_q^\dagger a_s a_r + \frac{1}{36} V_{pqrstu} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

✦ Hamiltonian normal ordered with respect to a single Slater determinant

$$H = E_0 + \sum_{pq} f_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} \{a_p^\dagger a_q^\dagger a_s a_r\} + \frac{1}{36} W_{pqrstu} \{a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s\}$$

$$E_0 = \sum_{pq} t_{pq} \rho_{pq} + \frac{1}{2} \sum_{pqrs} V_{pqrs} \rho_{pr} \rho_{qs} + \frac{1}{6} \sum_{pqrstu} V_{pqrstu} \rho_{ps} \rho_{qt} \rho_{ru}, \qquad \Gamma_{pqrs} = V_{pqrs} + \sum_{tu} V_{pqtrsu} \rho_{tu}$$

$$f_{pq} = t_{pq} + \sum_{rs} V_{prqs} \rho_{rs} + \frac{1}{2} \sum_{rstu} V_{prsqtu} \rho_{rt} \rho_{su}, \qquad W_{pqrstu} = V_{pqrstu}$$

✦ Normal ordered two-body (NO2B) approximation:

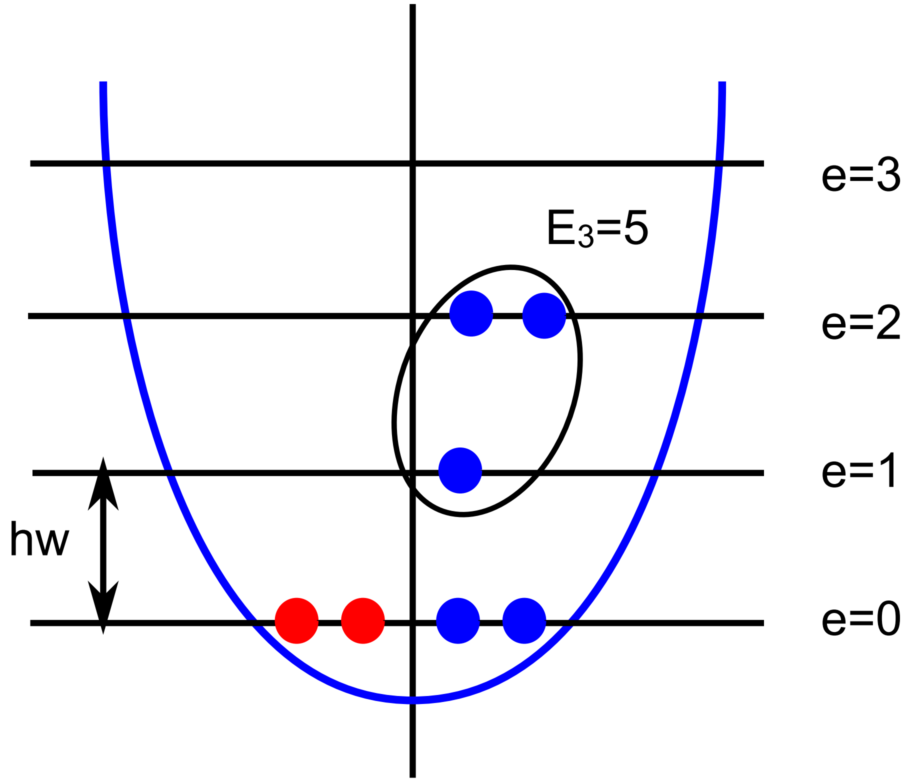
$$H \approx E_0 + \sum_{pq} f_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} \{a_p^\dagger a_q^\dagger a_s a_r\}$$

Model-space convergence

- NN+3N Hamiltonian (harmonic oscillator basis)

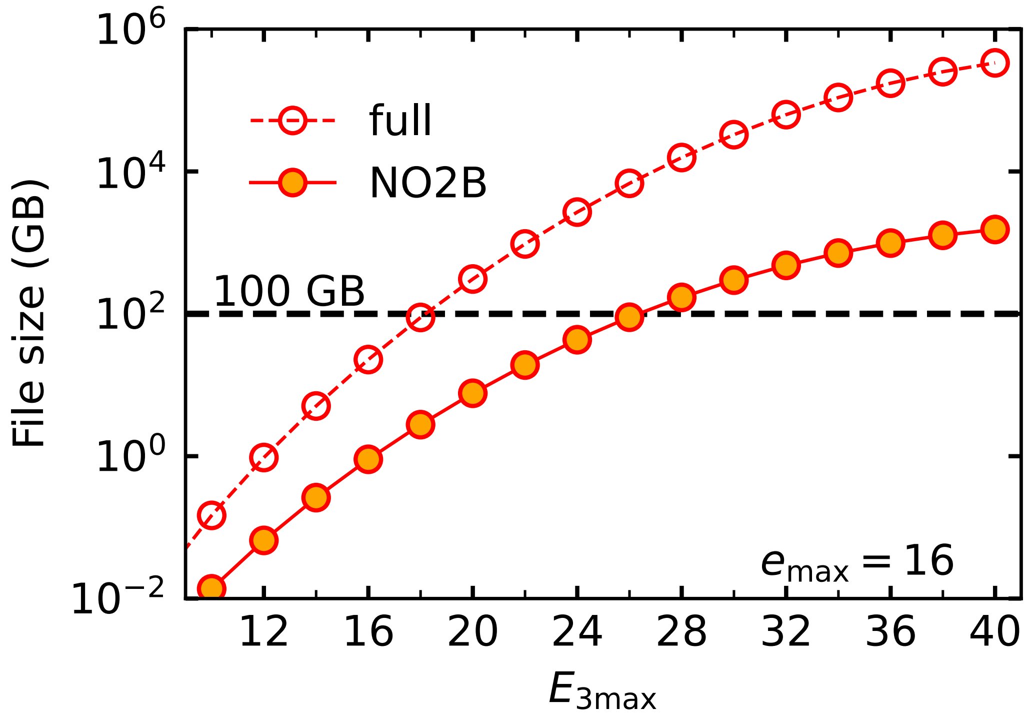
- Parameters:
  - hw
  - e_{max}=max(2n+l)*
  - E_{3max}=max(e_1+e_2+e_3).

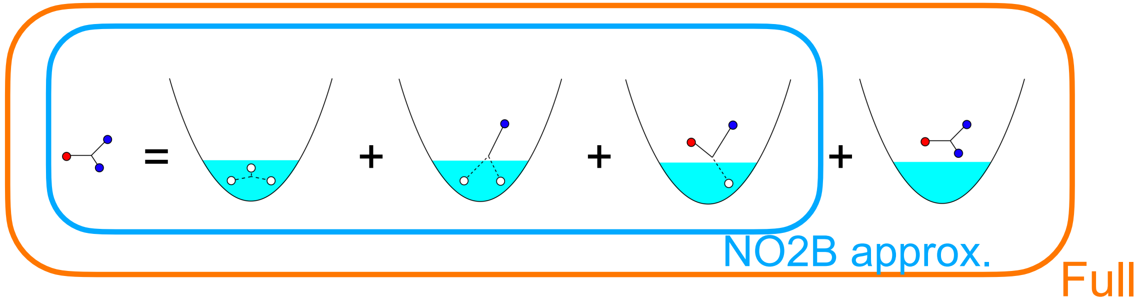
- As e_{max} and E_{3max} increases, the observable should not depend on all the parameters.



*Equivalent to (number of major shells)+1

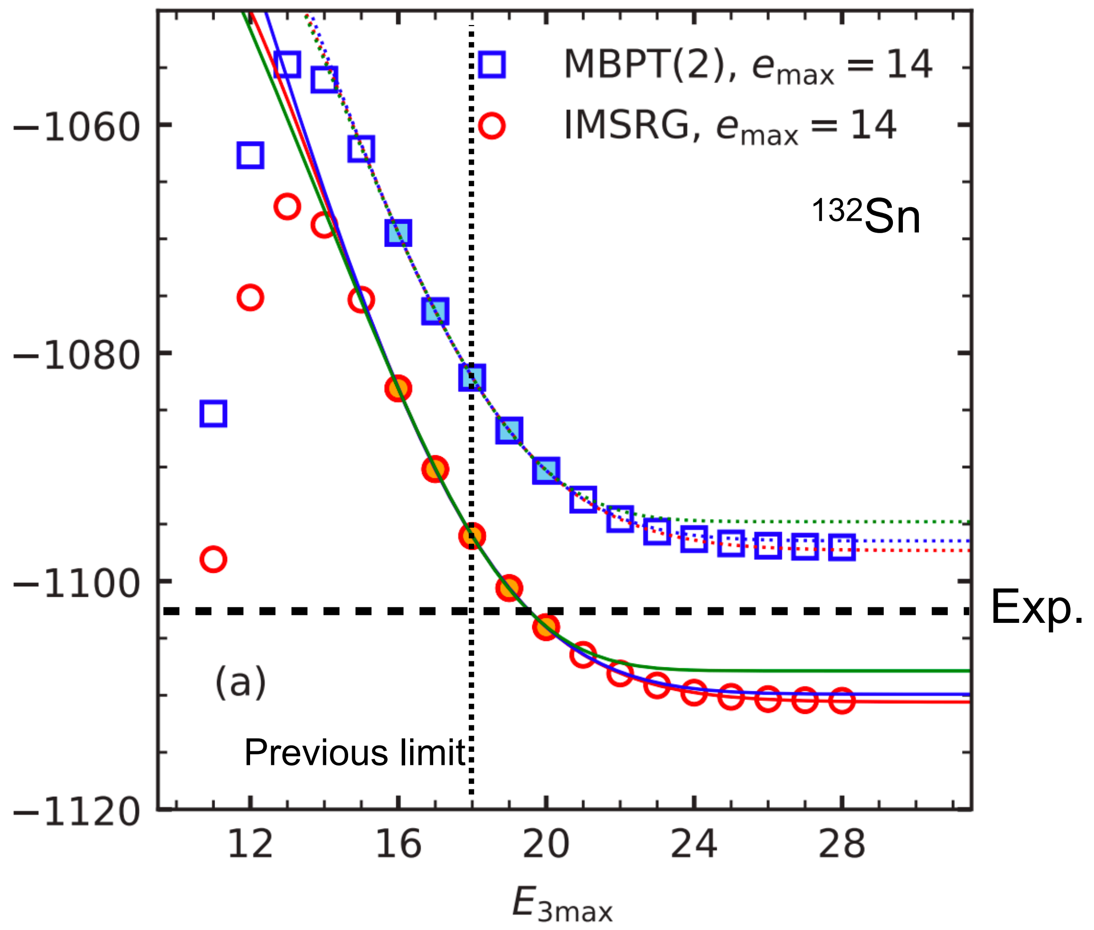
E_{3max} convergence in heavy nuclei





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

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

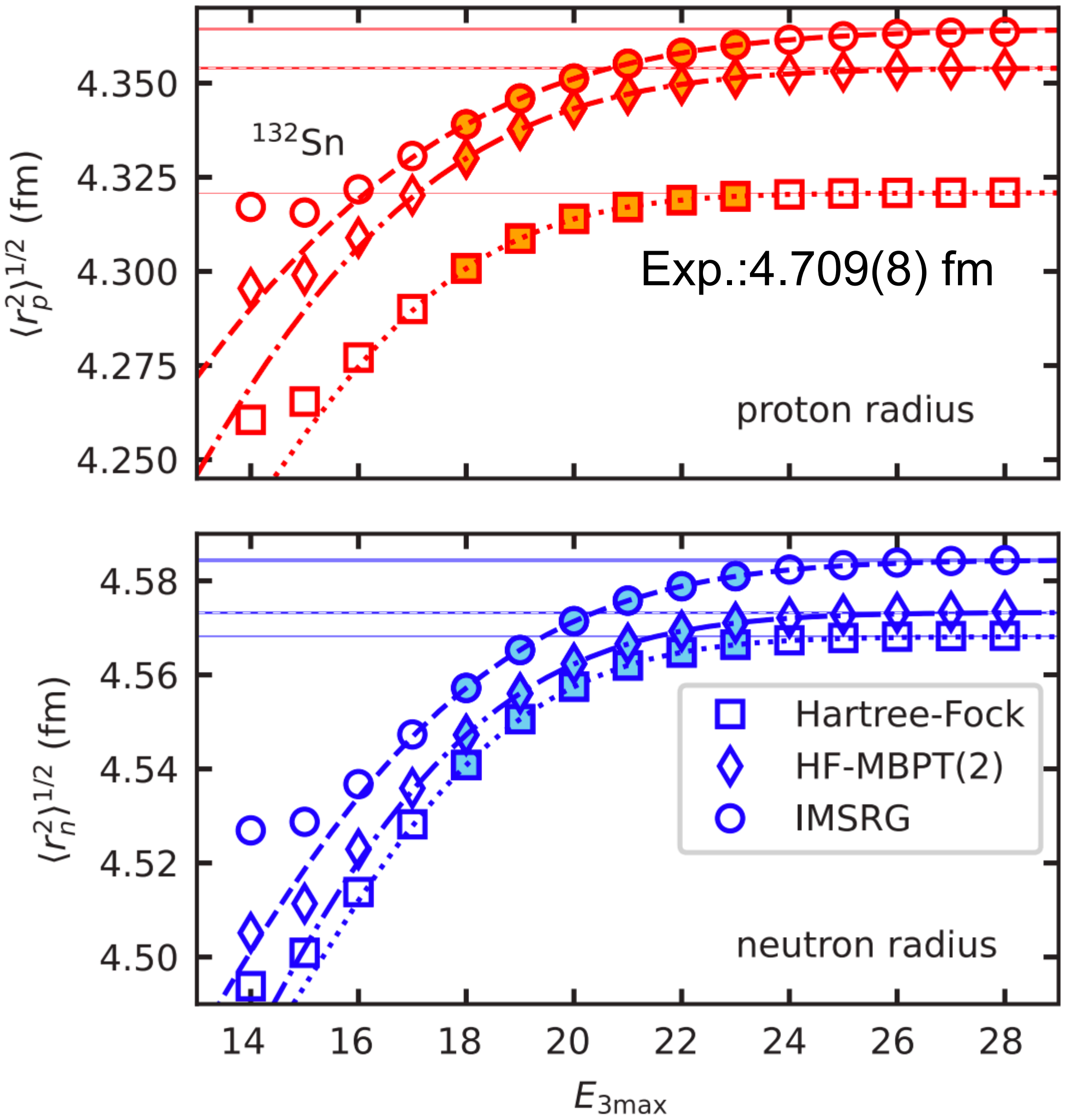


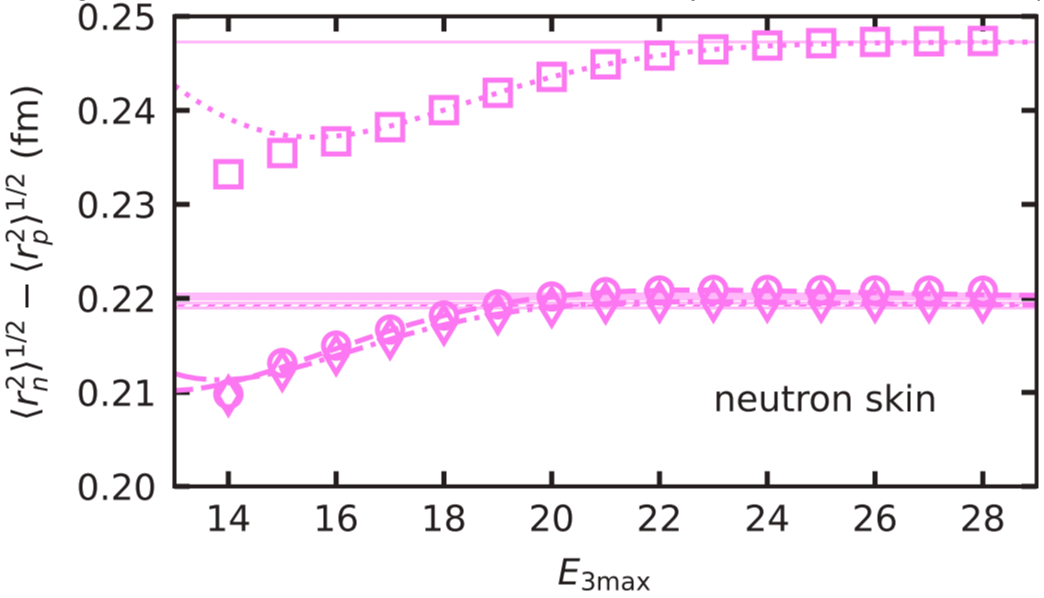
Asymptotic form: $E \approx A\gamma_{\frac{2}{n}}\left[\left(\frac{E_{3max}-\mu}{\sigma}\right)^n\right] + E_\infty$

Radii

筑波大学 計算科学研究センター Center for Computational Sciences

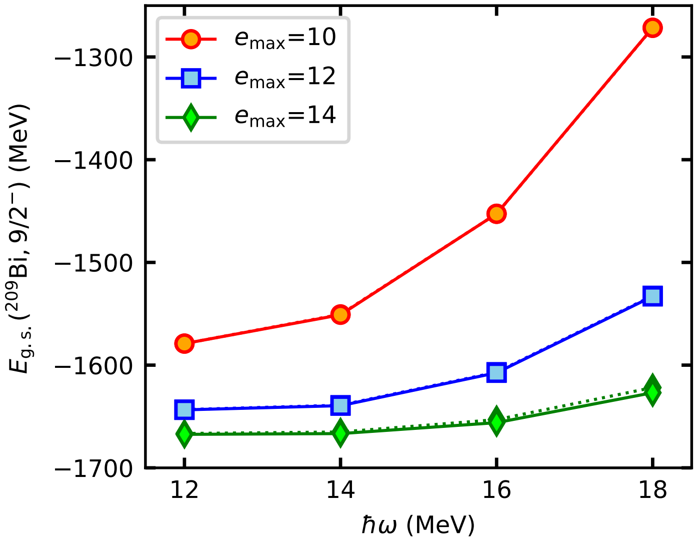
TM, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, Phys. Rev. C 105, 014302 (2022).





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

Convergence of ^{209}Bi



$$E(L_{\rm eff}) = E_\infty + A_\infty \exp(-2k_\infty L_{\rm eff})$$

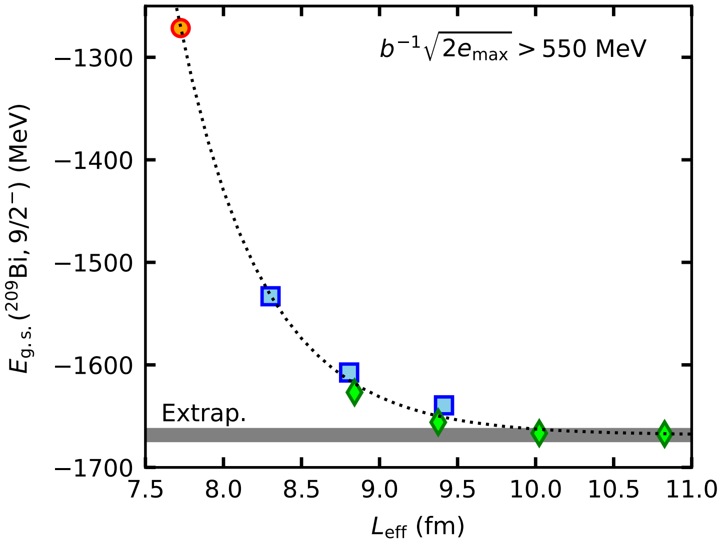
$$L_{\rm eff} = \sqrt{\frac{\sum_{nl} n_{nl}^{\rm occ} a_{nl}^2}{\sum_{nl} n_{nl}^{\rm occ} \kappa_{nl}^2}}, \quad \kappa_{nl}^2 \approx \frac{a_{nl}^2}{2b^2(N_l + 7/2)}$$

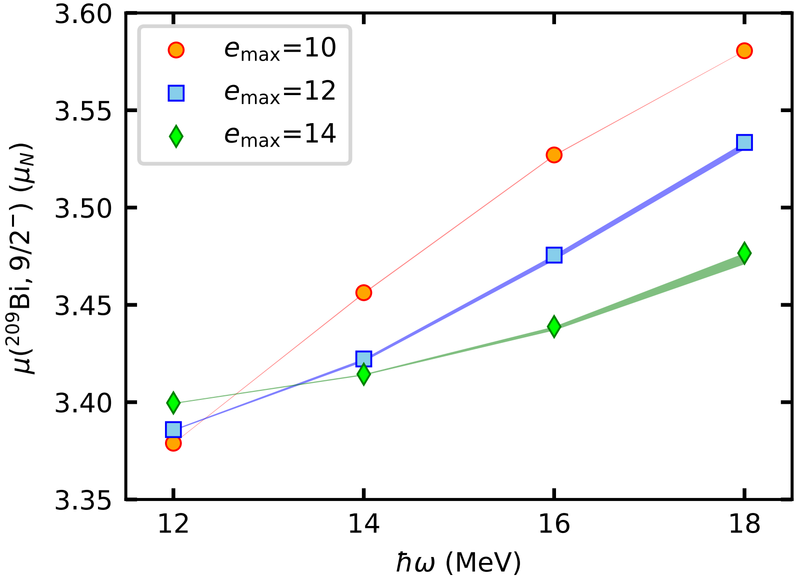
$$b^2 = \frac{\hbar}{m\omega}$$

$$N_l = \begin{cases} e_{\rm max} & e_{\rm max} + l \equiv 0 \pmod 2 \\ e_{\rm max} - 1 & e_{\rm max} + l \equiv 1 \pmod 2 \end{cases}$$

$n_{nl}^{\rm occ}$: occupation number of an orbit specified by n and l

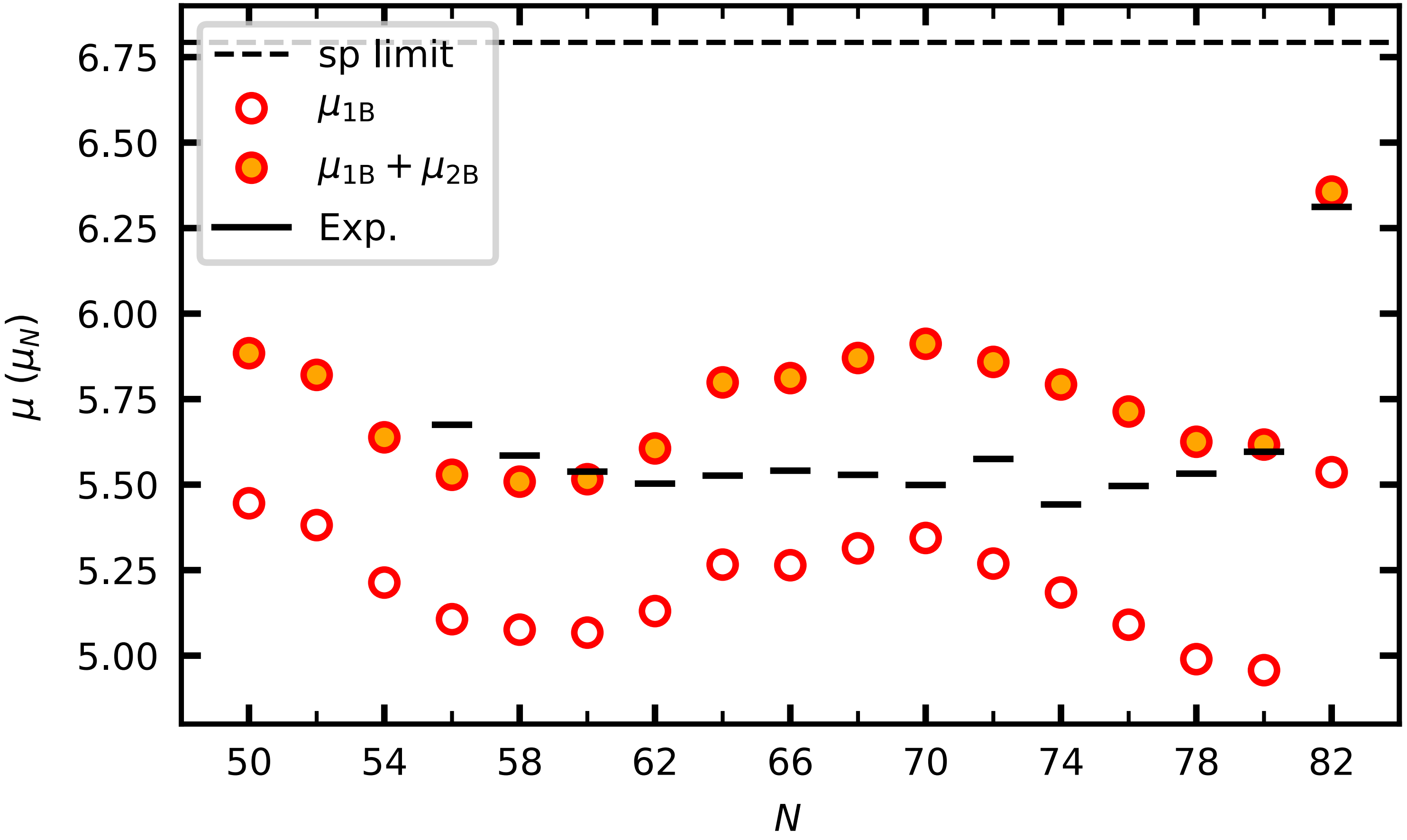
a_{nl} : $(n+1)$-th zero of the spherical Bessel function





Magnetic moments of In isotopes

VS-IMSRG(2), 1.8/2.0 (EM), e_{max}=14, E_{3max}=24, hw = 16 MeV



2B contribution with the simplest limit

筑波大学 計算科学研究センター Center for Computational Sciences

- Expectation value: $\langle J||\mu||J\rangle$
- The simplest limit: $|JM\rangle = [|j_1 \dots j_{A-1} : 0^+\rangle \otimes |j_p m_p\rangle]\delta_{j_p J}\delta_{m_p M}$
- The expectation value depends a particle in the core and last unpaired particle.

$$\begin{aligned}
\langle J||\mu||J\rangle &\approx \delta_{J j_p} \sum_{q\in\mathrm{core}} \langle p0 : j_p||\mu_{pq}||p0 : j_p\rangle \\
&= \delta_{J j_p} \sum_{q\in\mathrm{core}} \sum_{I} \frac{2I+1}{(2j_p+1)(2j_q+1)} \langle((pq)I, q : j_p||\mu_{pq}||(pq)I, q : j_p\rangle \\
&= \delta_{J j_p} \sum_{q\in\mathrm{core}} \sum_{I} \frac{2I+1}{2j_q+1} (-1)^{j_p+j_q+I+1} \begin{Bmatrix} j_p & I & j_q \\ I & j_p & 1 \end{Bmatrix} \langle pq : I||\mu||pq : I\rangle
\end{aligned}$$