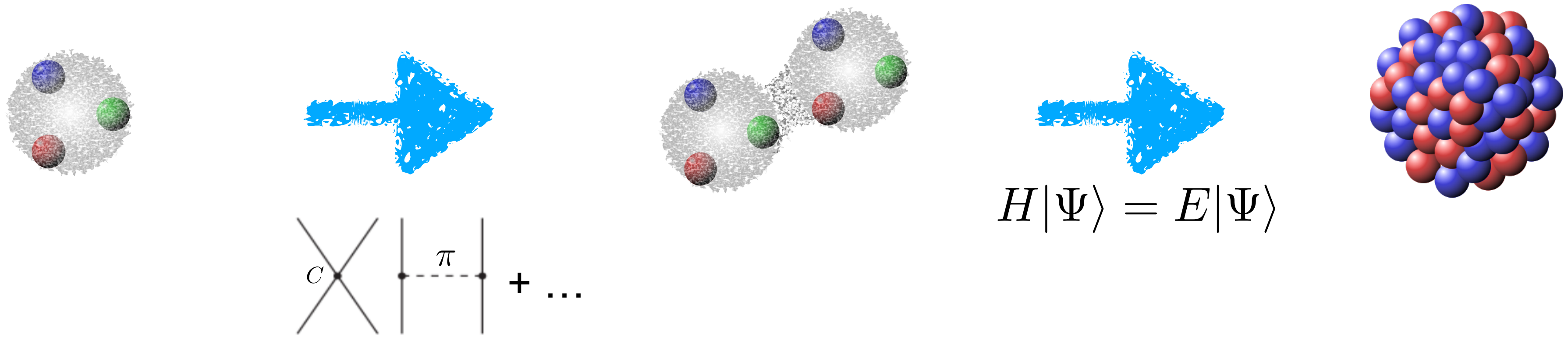
Nuclear ab initio calculations for heavy-mass nuclei



Takayuki Miyagi

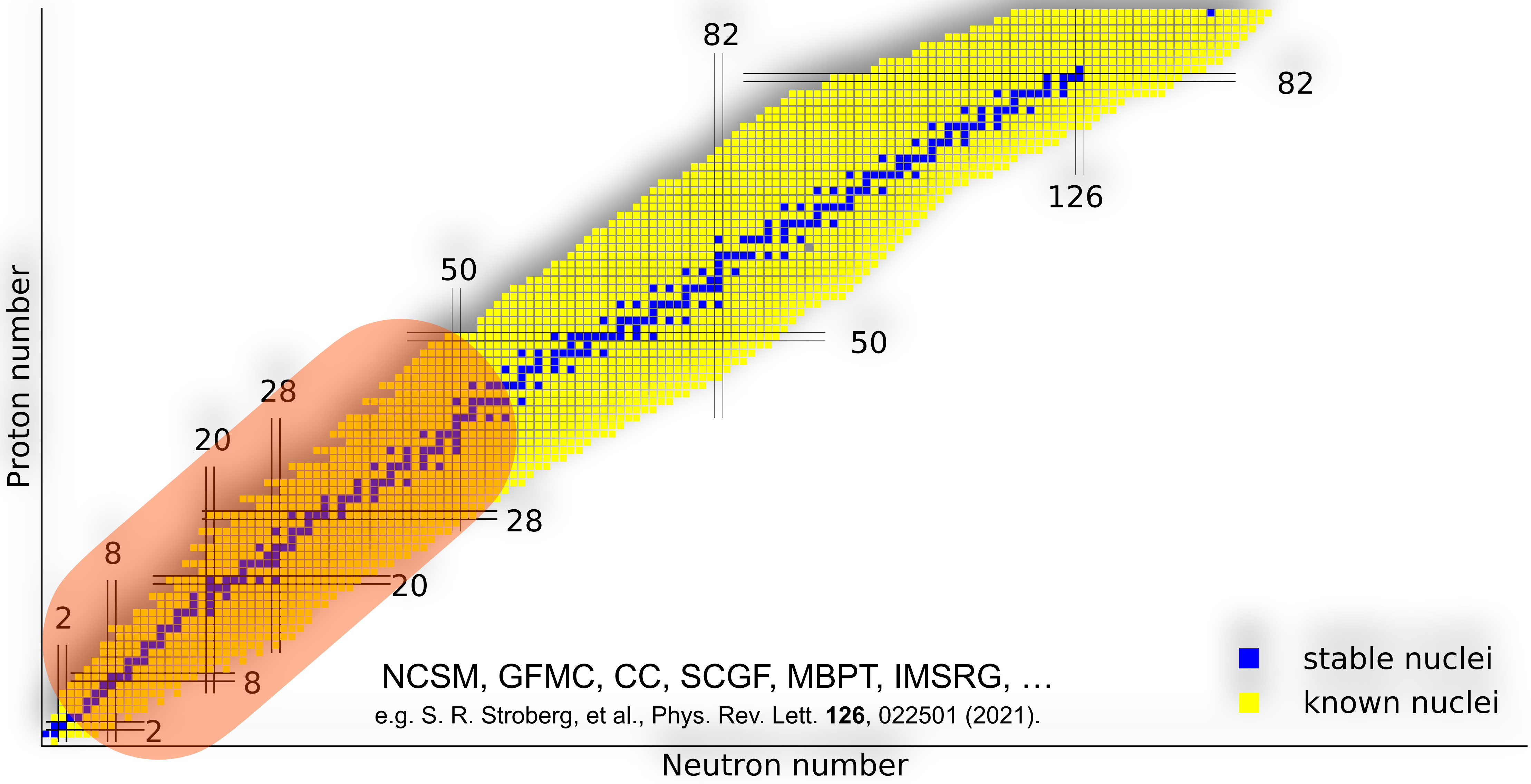
EMMI Workshop and International Workshop XLIX on Gross Properties of Nuclei and Nuclear Excitations (16, Jan. 2023)

Collaborators

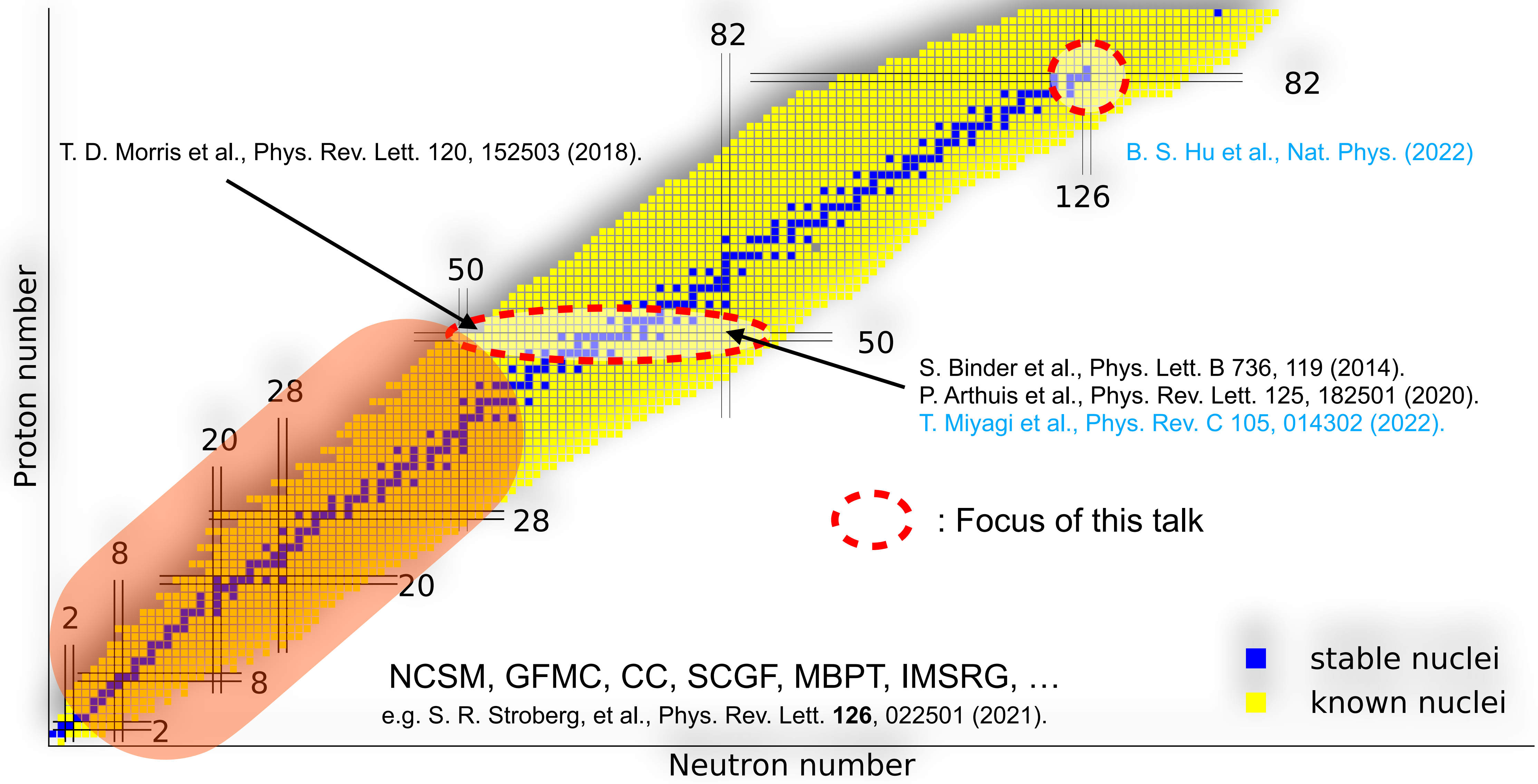
TECHNISCHE UNIVERSITÄT DARMSTADT

- TU Darmstadt: K. Hebeler, A. Schwenk, R. Seutin — Phys. Rev. C 105, 014302 (2022).
- TRIUMF: A. Belley, J. D. Holt, B. S. Hu, P. Navratil
- University of Notre Dame: S. R. Stroberg
- Chalmers University of Technology: A. Ekström, C. Forssen, W. Jiang
- Oak Ridge National Laboratory: G. Hagen
- University of Tennessee: T. Papenbrock, Z. Sun
- University os Tsukuba: N. Shimizu, Y. Tsunoda
- University of Durham: I. Vernon
- Johannes Gutenberg University of Mainz: S. Bacca
- University of Illinois: X. Cao
- Massachusetts Institute of Technology: R. G. Ruiz

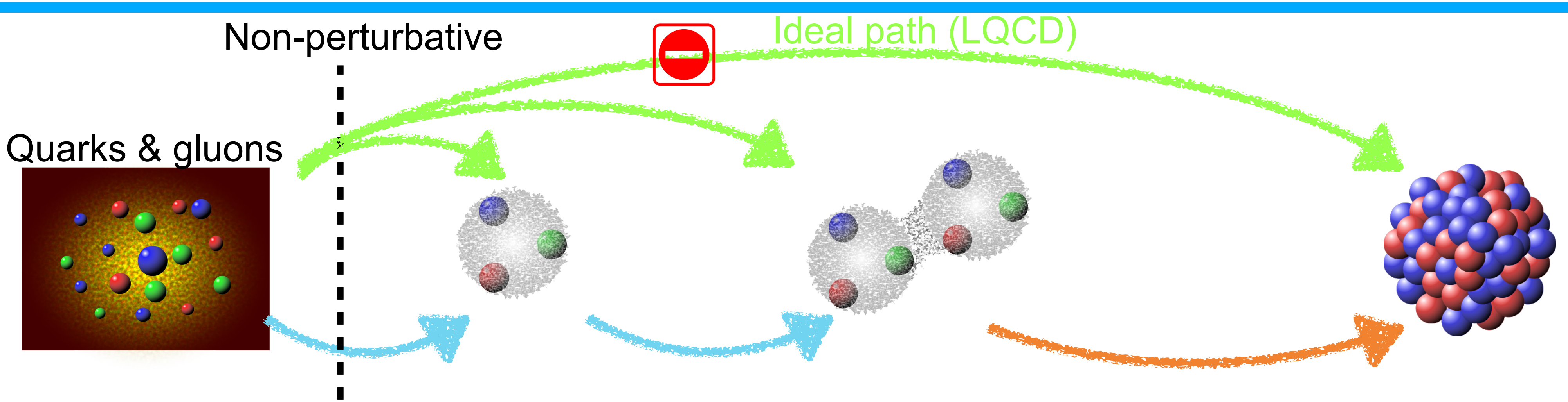
Heavy-mass frontier in ab initio methods

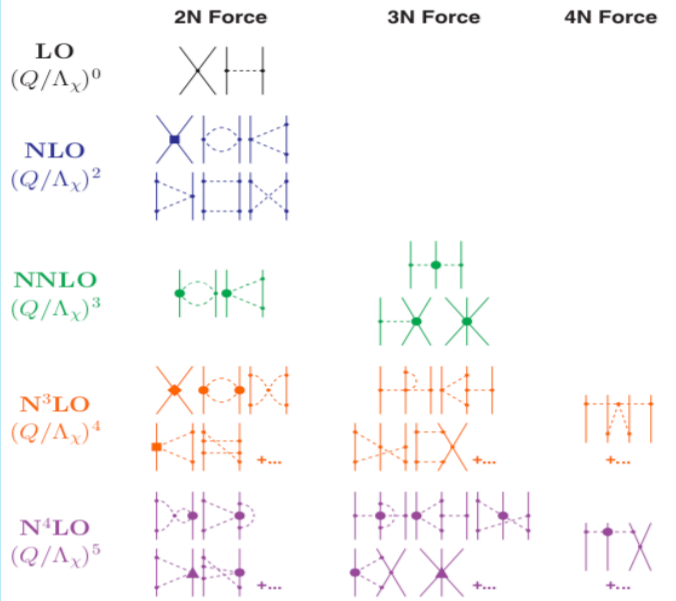


Heavy-mass frontier in ab initio methods



Nuclear ab initio calculation





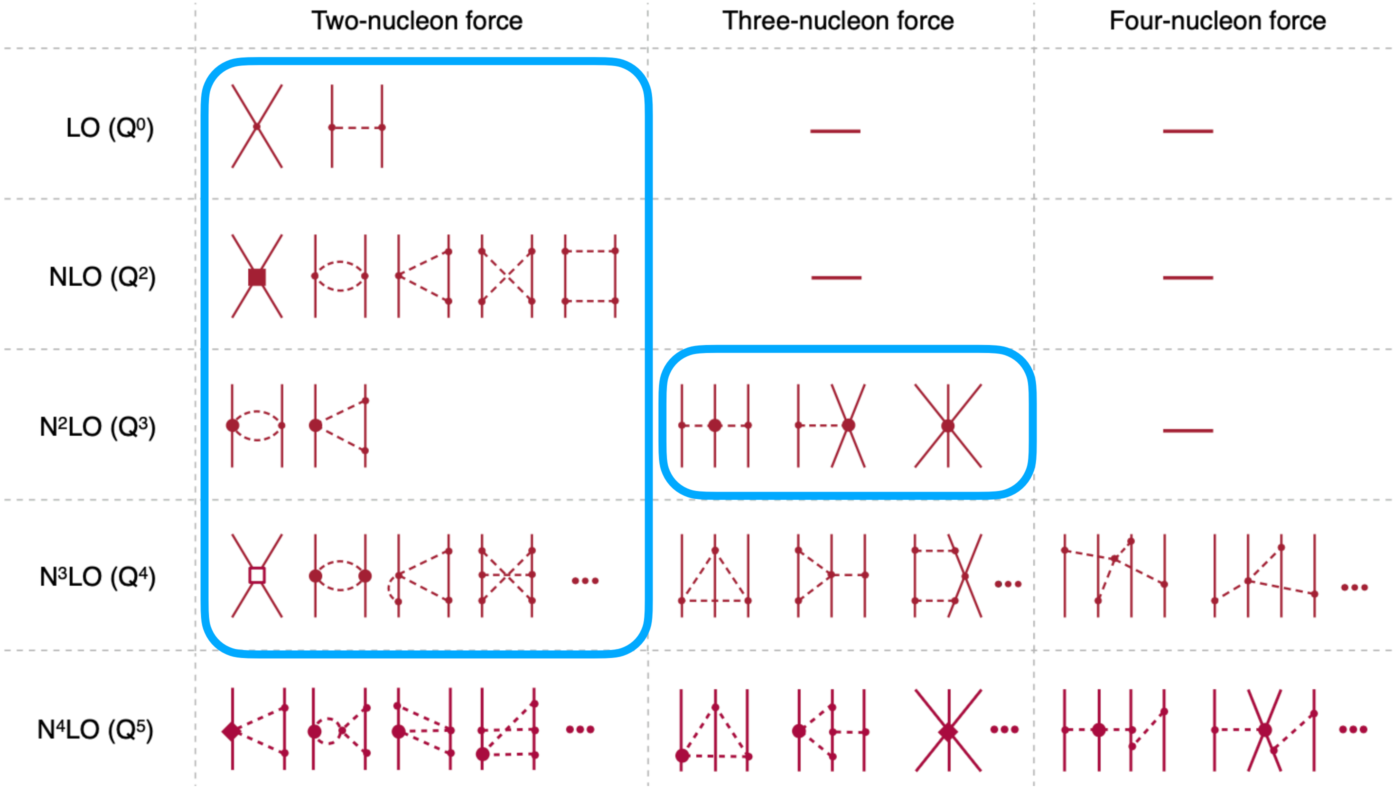
Nuclear many-body problem

- 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
- …

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

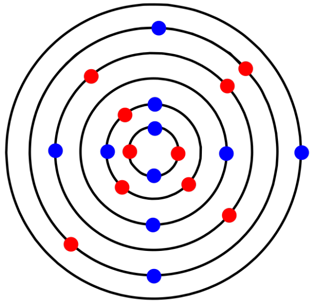


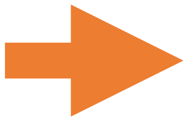
In this talk 1.8/2.0 (EM) is mainly used.

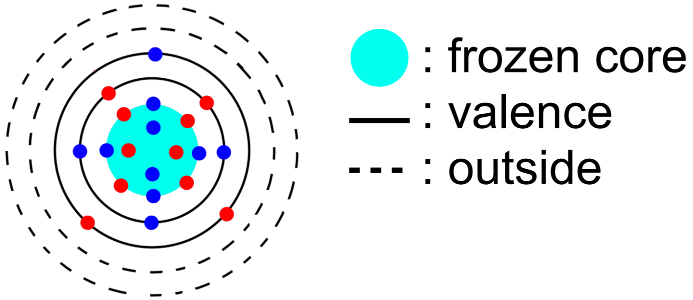
Figure is from E. Epelbaum, arXiv: 1510.07036

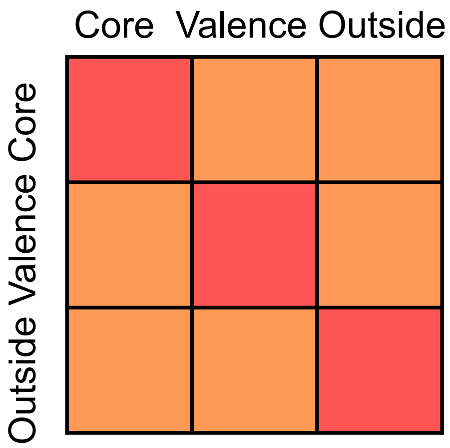
H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, Annu. Rev. Nucl. Part. Sci. **69**, 307 (2019).

Valence-space in-medium similarity renormalization group

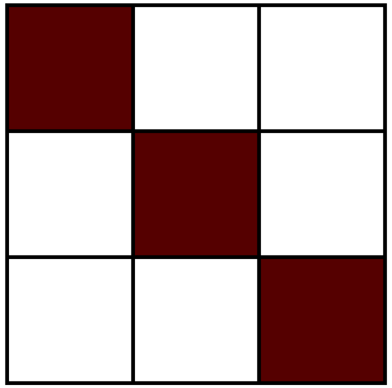








evolution



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

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

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

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

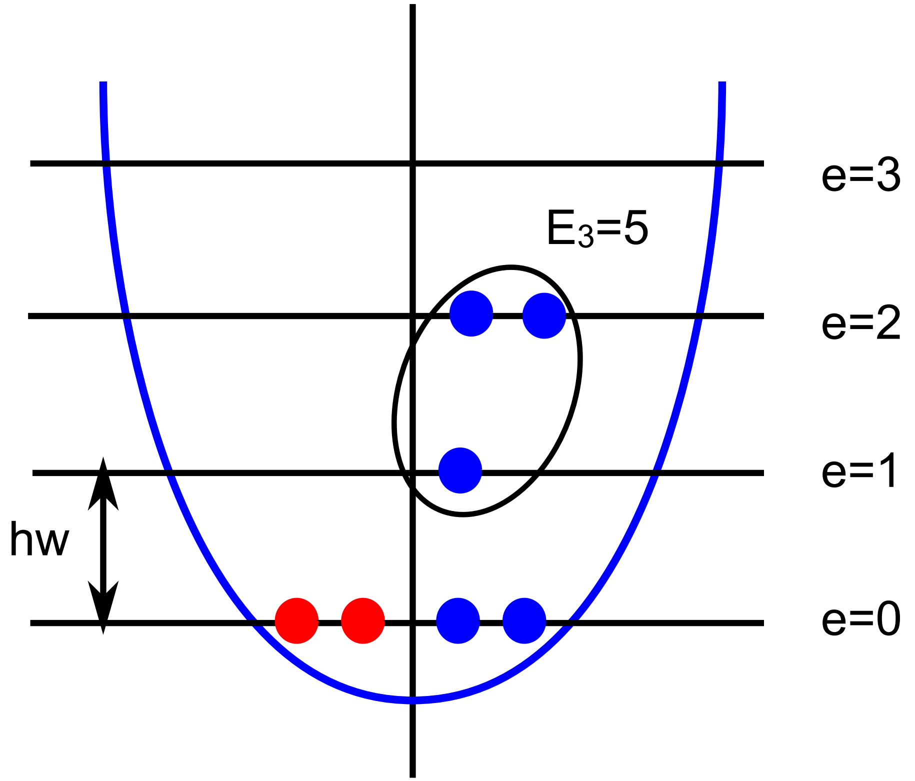
$$\eta_{1234} = \frac{1}{2}\arctan\left(\frac{2\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta}\right)$$

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

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

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.

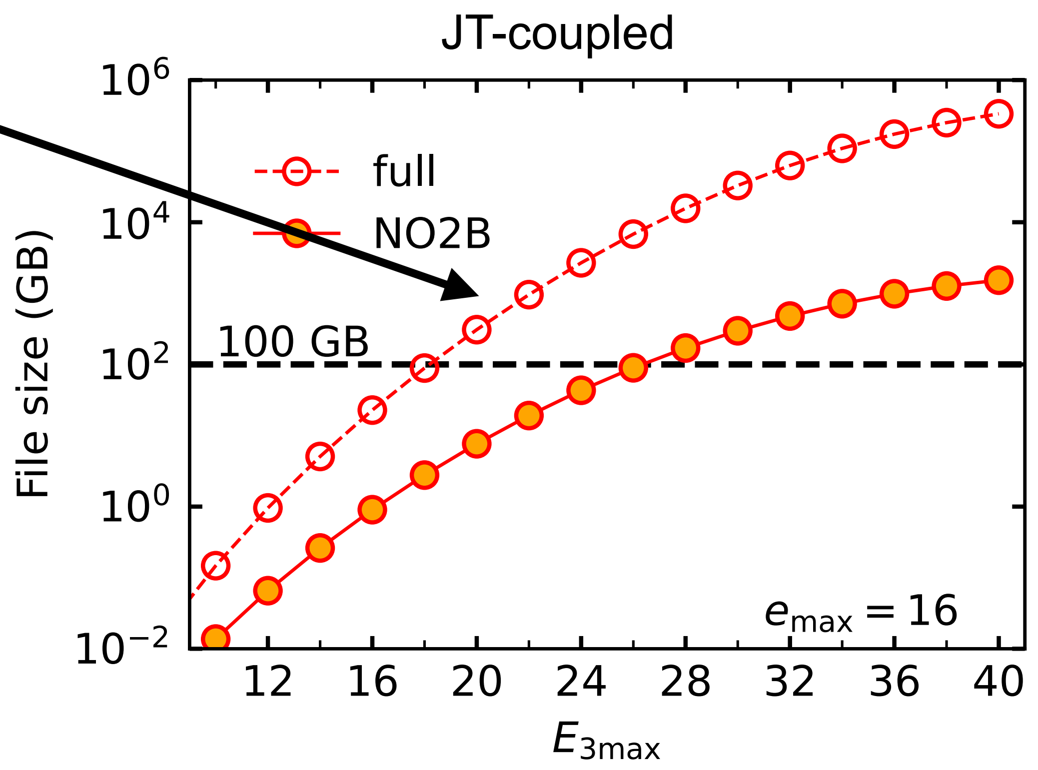


*Equivalent to (number of major shells)+1

Extension of E_{3max} truncation

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

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



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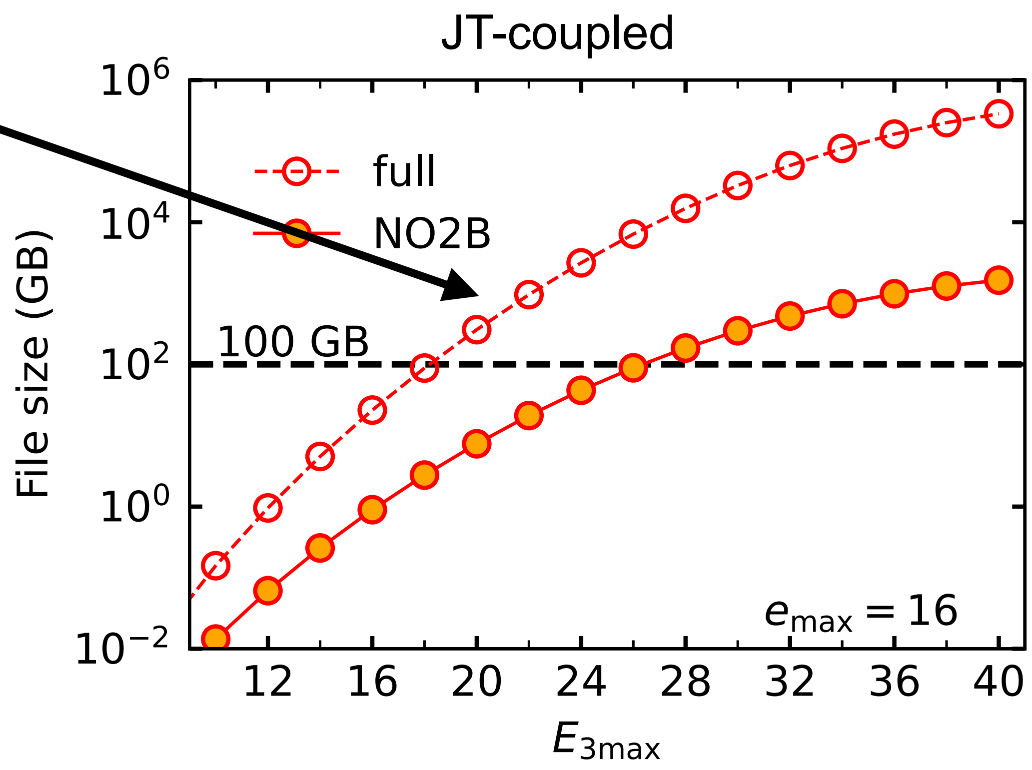
NO wrt reference

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

NO2B approx



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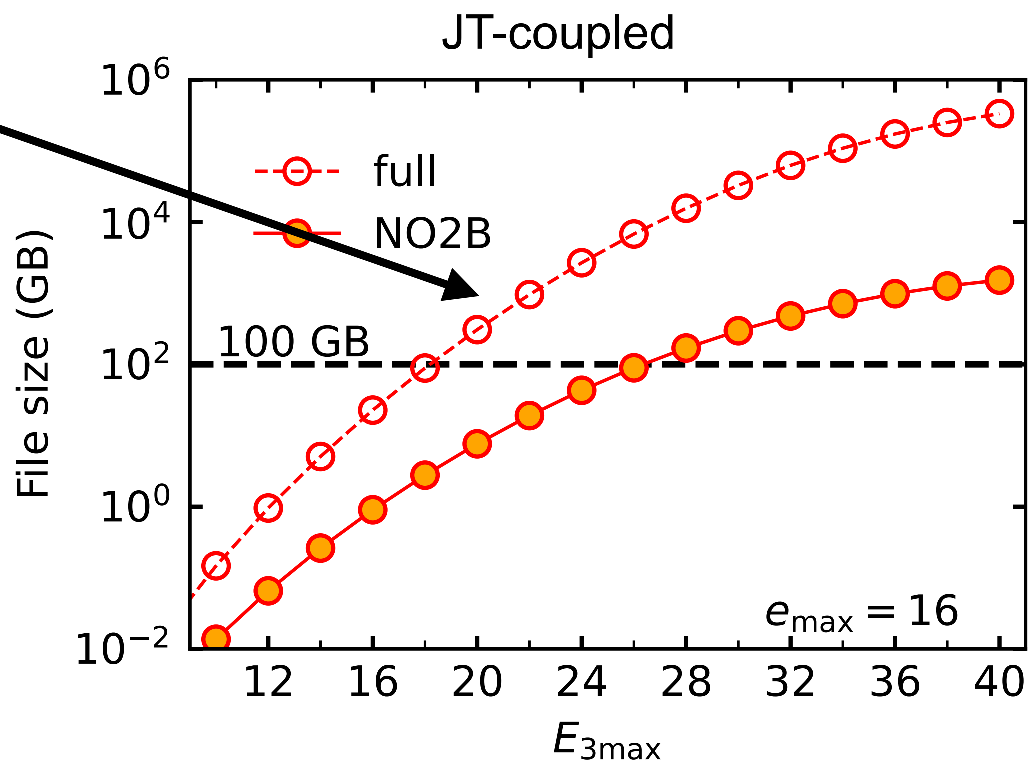
$$E_0 = \sum_{pq} t_{pq}\rho_{pq} + \frac{1}{2}\sum_{pqrs} V_{pqrs}\rho_{pr}\rho_{qs} + \frac{1}{6} V_{pqrstu}\rho_{ps}\rho_{qt}\rho_{ru}$$

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

$$\Gamma_{pqrs} = V_{pqrs} + \sum_{tu} V_{pqtrsu}\rho_{tu}$$



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NO wrt reference

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

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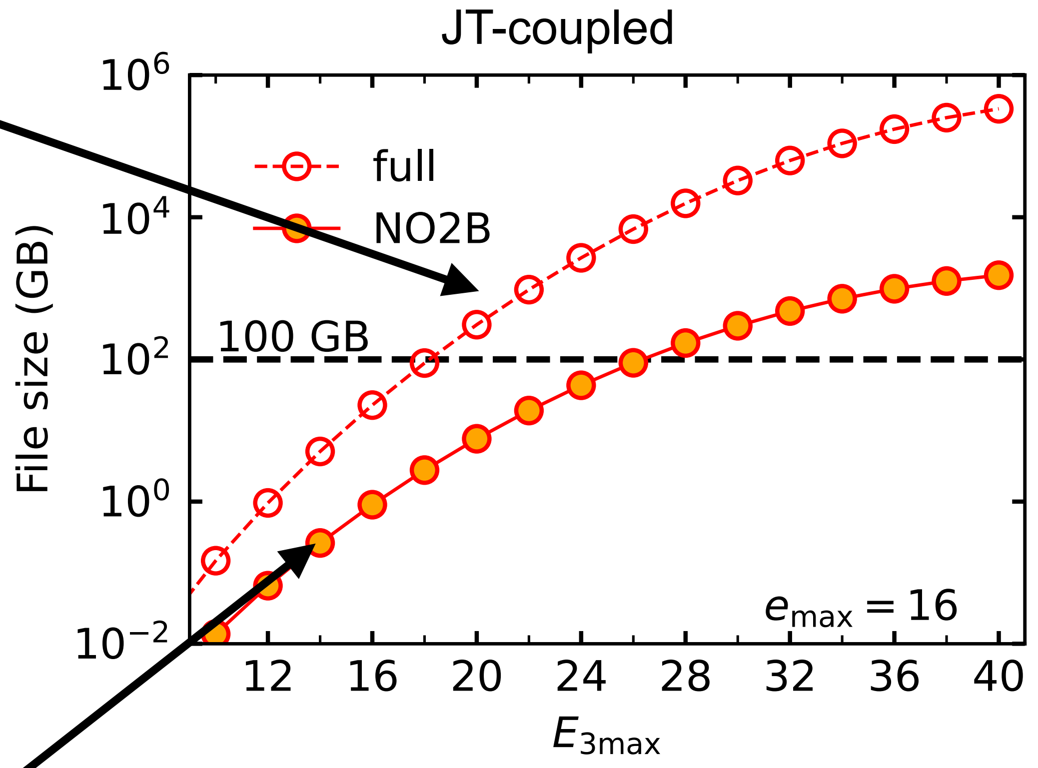
$$\Gamma_{pqrs} = V_{pqrs} + \sum_{tu} V_{pqtrsu} \rho_{tu}$$

If the reference state is spherically symmetric, $l_t = l_u$ and $j_t = j_u$.
The JT-coupled representation enters NO2B approximation:

$$\langle pqr : J_{pq} T_{pq} T | V^{3N,\mathrm{NO2B}} | stu : J_{st} T_{st} T \rangle = \delta_{l_r l_u} \delta_{j_r j_u} \delta_{J_{pq} J_{st}} \sum_J (2J+1) \langle pqr : J_{pq} T_{pq} J T | V^{3N} | stu : J_{st} T_{st} J T \rangle$$



* A new normal-ordering technique in the Jacobi coordinate is also available: K. Hebeler et al., arXiv: 2211.16262

Implementation of 3N TM transformation for NO2B approx.

- Matrix multiplication form

$$\langle p'q'r' : J_{p'q'}T_{p'q'}T | V^{3\mathrm{N,NO2B}} | pqr : J_{pq}T_{pq}T\rangle$$
$$= 6\delta_{l_{r'}l_r}\delta_{j_{r'}j_r}\delta_{J_{p'q'}J_{pq}} \sum_{JN_{\mathrm{cm}}L_{\mathrm{cm}}J_{\mathrm{rel}}} (2J+1) \sum_{E'i'} \sum_{Ei}$$
$$\times \langle p'q'r' : J_{p'q'}T_{p'q'}JT | N_{\mathrm{cm}}L_{\mathrm{cm}}E'i'J_{\mathrm{rel}} : JT\rangle$$
$$\times \langle E'i' : J_{\mathrm{rel}}T | V_{3\mathrm{N}} | Ei : J_{\mathrm{rel}}T\rangle$$
$$\times \langle N_{\mathrm{cm}}L_{\mathrm{cm}}EiJ_{\mathrm{rel}} : JT | pqr : J_{pq}T_{pq}JT\rangle$$

$$\langle N_{\mathrm{cm}}L_{\mathrm{cm}}EiJ_{\mathrm{rel}} : JT | pqr : J_{pq}T_{pq}JT\rangle$$
$$= \sum_{\alpha} \langle EiJ_{\mathrm{rel}}T | E\alpha J_{\mathrm{rel}}T\rangle$$
$$\times \langle N_{\mathrm{cm}}L_{\mathrm{cm}}E\alpha J_{\mathrm{rel}} : JT | pqr : J_{pq}T_{pq}JT\rangle$$
$$\alpha = \{n_{12}, l_{12}, s_{12}, j_{12}, n_3, l_3, j_3\}, \ (t_{12} = T_{pq})$$

Memory requirements for a channel:

- : CFP ~ O(1) GB
- : T coef. ~ O(100) GB
- : T coef. (Asym) ~ O(10) GB
- : 3NME (Jacobi) ~ O(1) GB
- : 3NME (Lab.) ~ O(0.1) GB

- Channel-by-channel MPI parallelization.
  - # of channels ~ 30000 (e_{max}=18, E_{3max}=28)

E_{3max}=28 takes 2-3 hours using 100 (nodes) x 48 (cores)

NuHamil code

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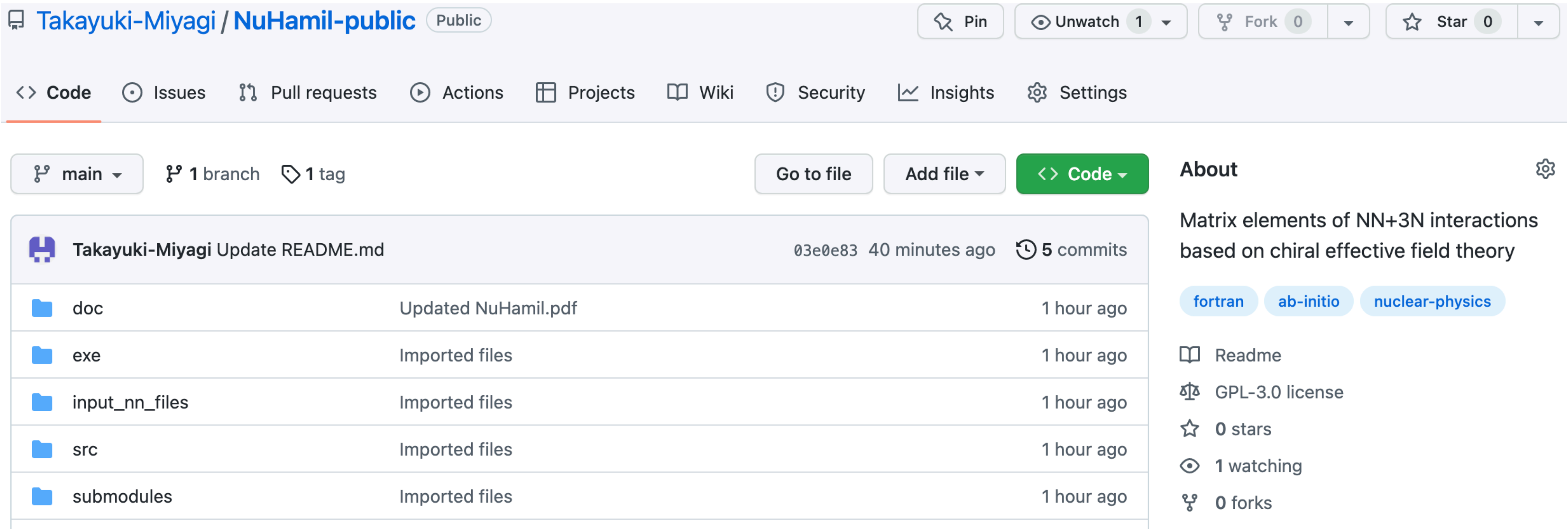
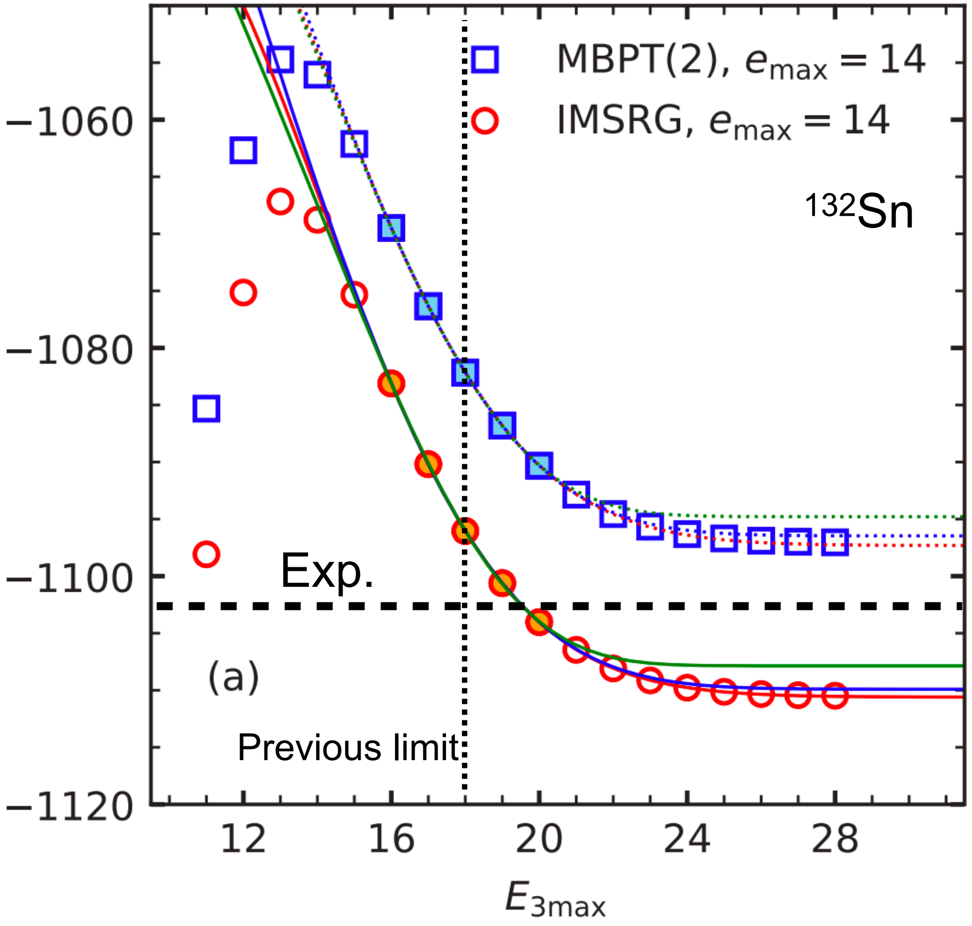
- A numerical code for the NN and 3N matrix elements is available.
  - ✦ https://github.com/Takayuki-Miyagi/NuHamil-public

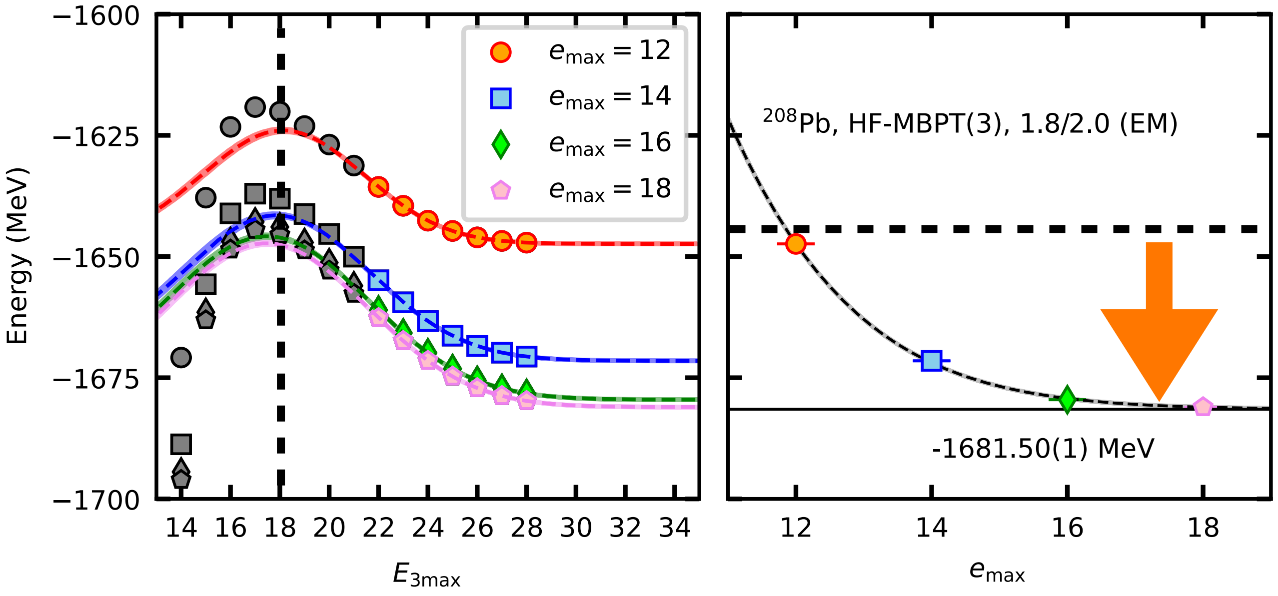


E_{3max} convergence in heavy nuclei

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

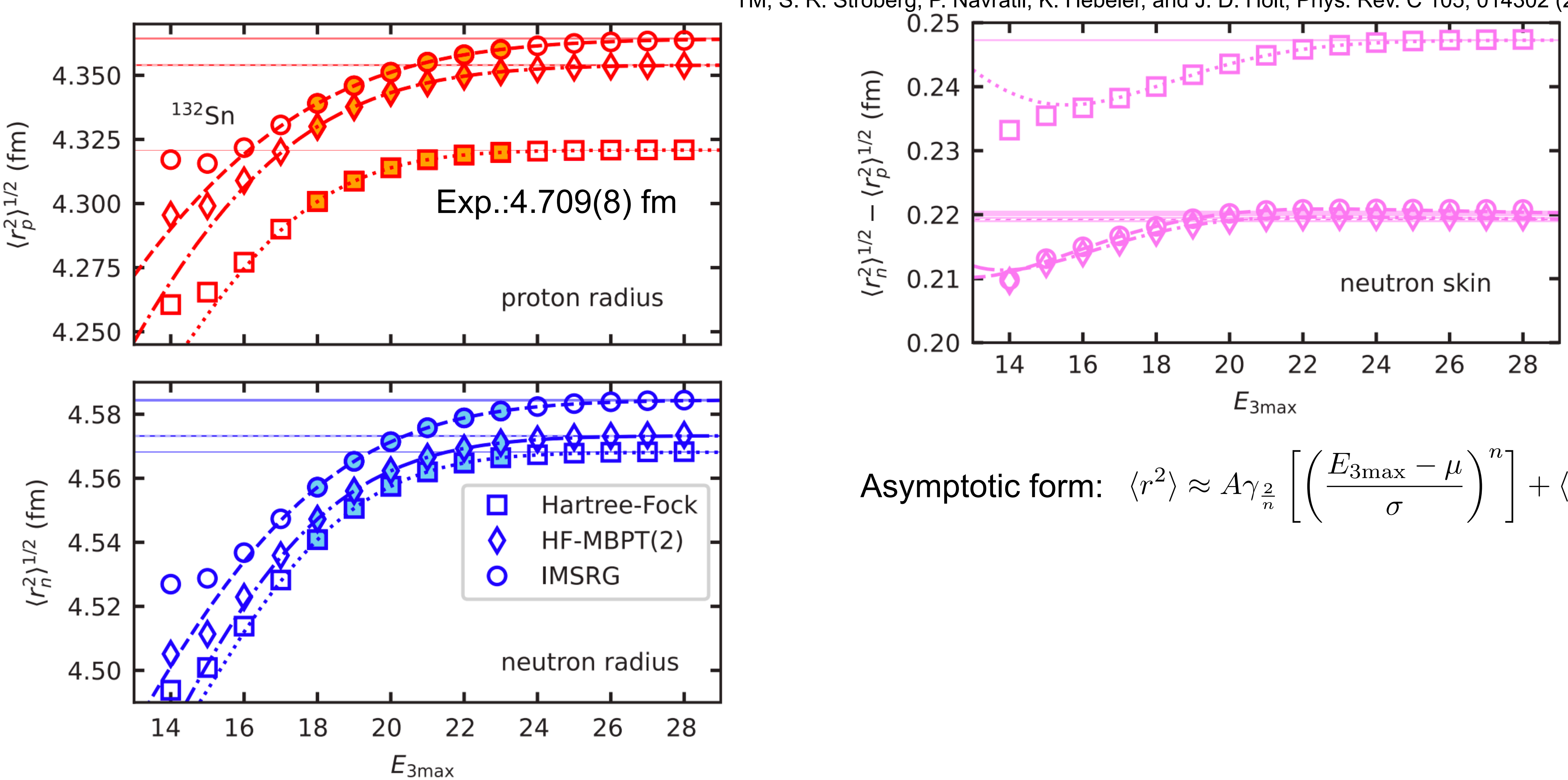


Asymptotic form: $E \approx A\gamma_{\frac{2}{n}}\left[\left(\frac{E_{3max}-\mu}{\sigma}\right)^n\right] + E_\infty$



Radii

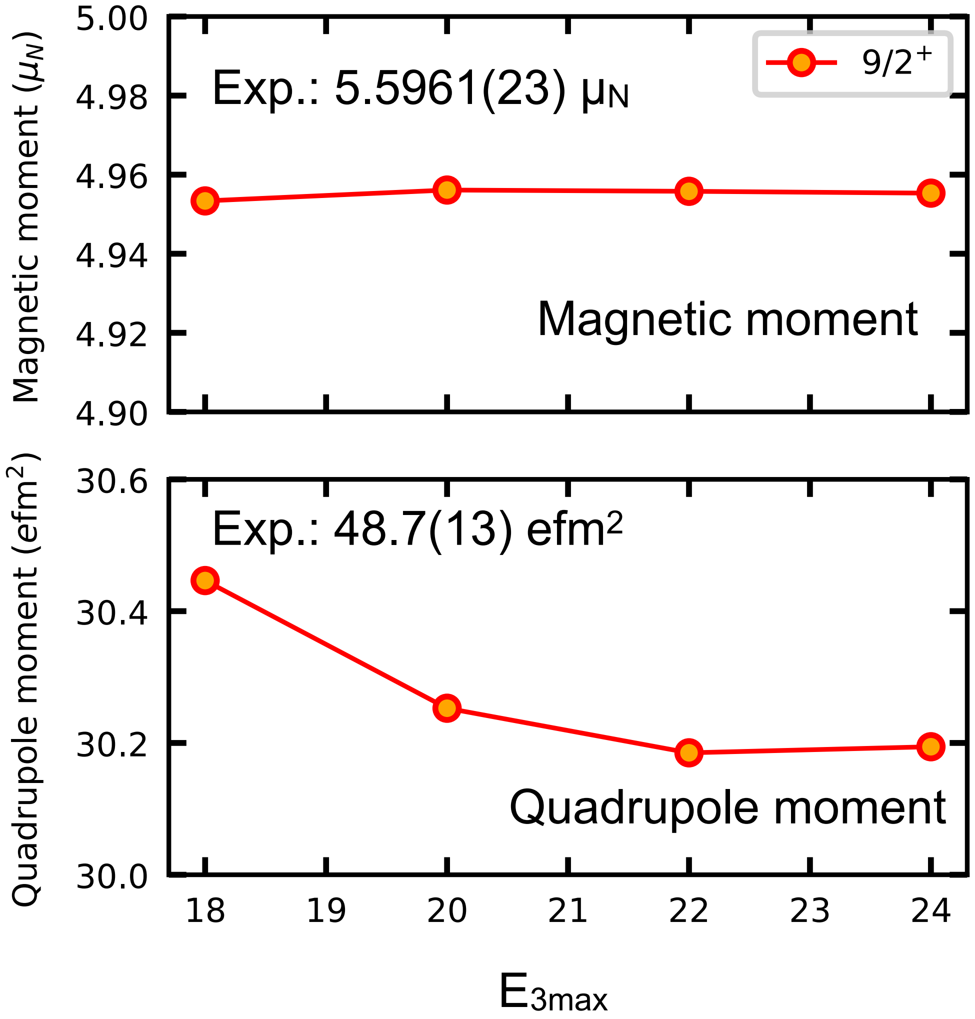
TM, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, Phys. Rev. C 105, 014302 (2022).

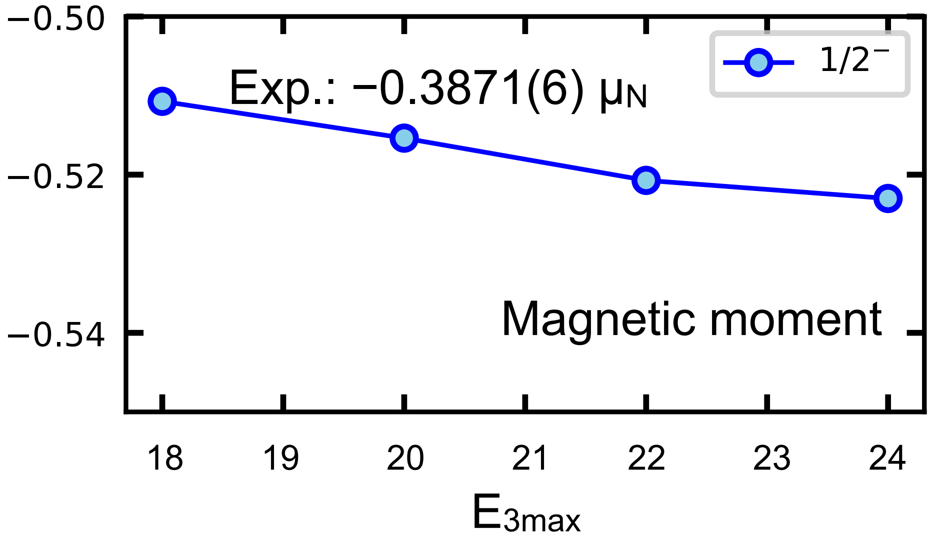


Asymptotic form: $\langle r^2\rangle \approx A\gamma_{\frac{2}{n}}\left[\left(\frac{E_{3\mathrm{max}}-\mu}{\sigma}\right)^n\right] + \langle r^2\rangle_\infty$

EM observables

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





Convergence is OK.

Disagreement with the experiment

- Nuclear Hamiltonian
- Many-body approximation
- Higher order EM current

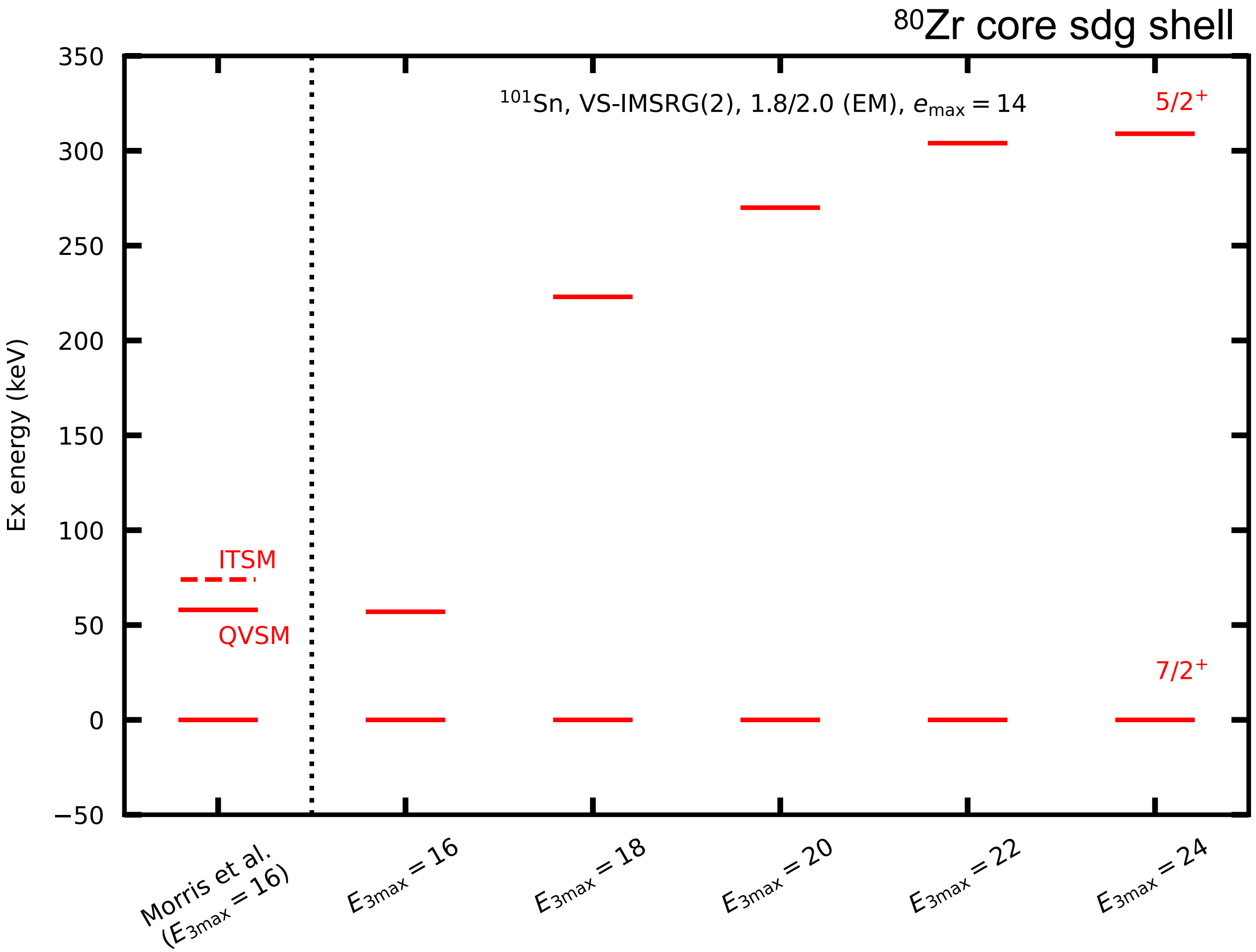
Experimental data: A. R. Vernon et al, Nature 607, 260 (2022).

^{101}Sn

- Near degenerate single-particle structure
- Valence-space IMSRG approach
- The valence-space dimension > ~ 10^{13}
  - Exact diagonalization is impossible
- Quasi-particle vacuum shell model (QVSM)
- Error of QVSM is the order of 10 keV

  N. Shimizu et al., Phys. Rev. C 103, 014312 (2021).

- A larger E_{3max} is needed in the light tin isotopes.



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

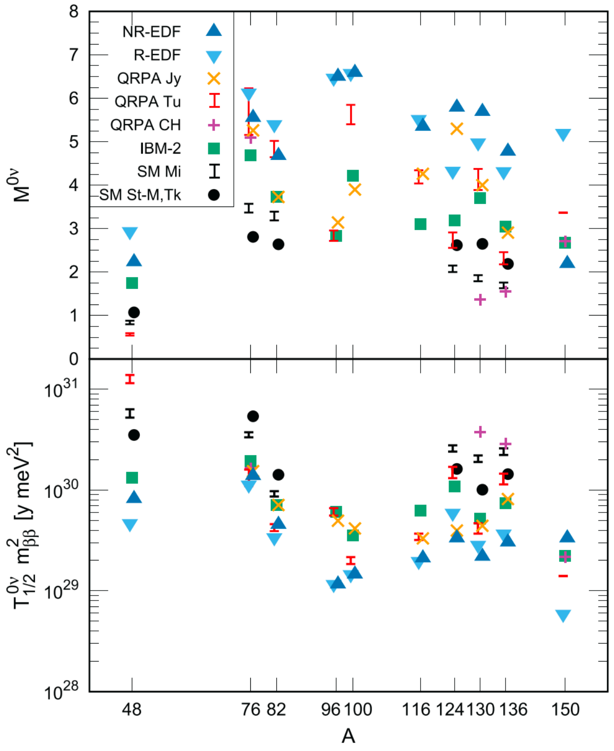
Neutrinoless double-beta decay

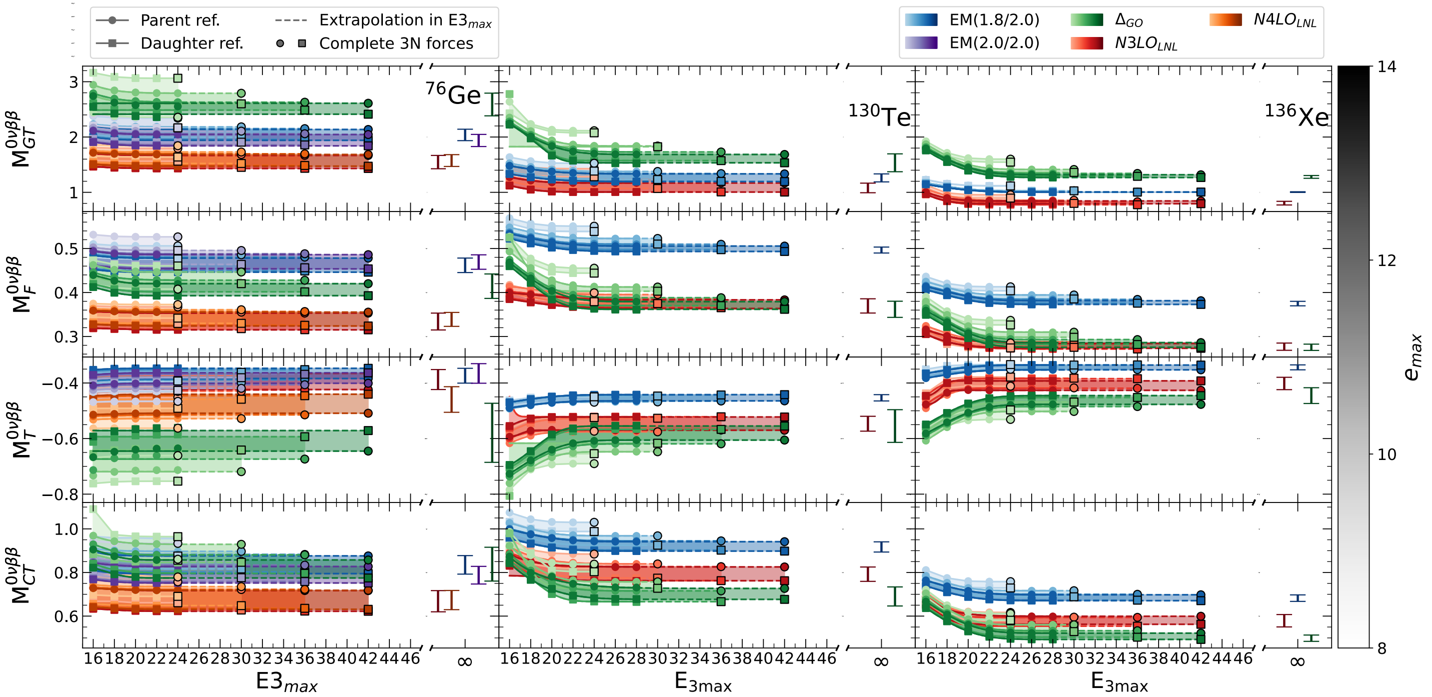
- Lifetime: $\frac{1}{T_{1/2}^{0\nu}} = G^{0\nu} |M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta} \rangle}{m_e} \right)^2$

Phase space factor
Nuclear matrix element
Neutrino mass

- NMEs depend on many-body methods (~ 10 times different in lifetime)

J. Engel and J. Menéndez, Reports Prog. Phys. 80, 046301 (2017).





VS-IMSRG result

$$M_{\mathrm{Ge}}^{0\nu\beta\beta} \in [2.10, 3.19]$$
$$M_{\mathrm{Te}}^{0\nu\beta\beta} \in [1.52, 2.40]$$
$$M_{\mathrm{Xe}}^{0\nu\beta\beta} \in [1.08, 1.90]$$

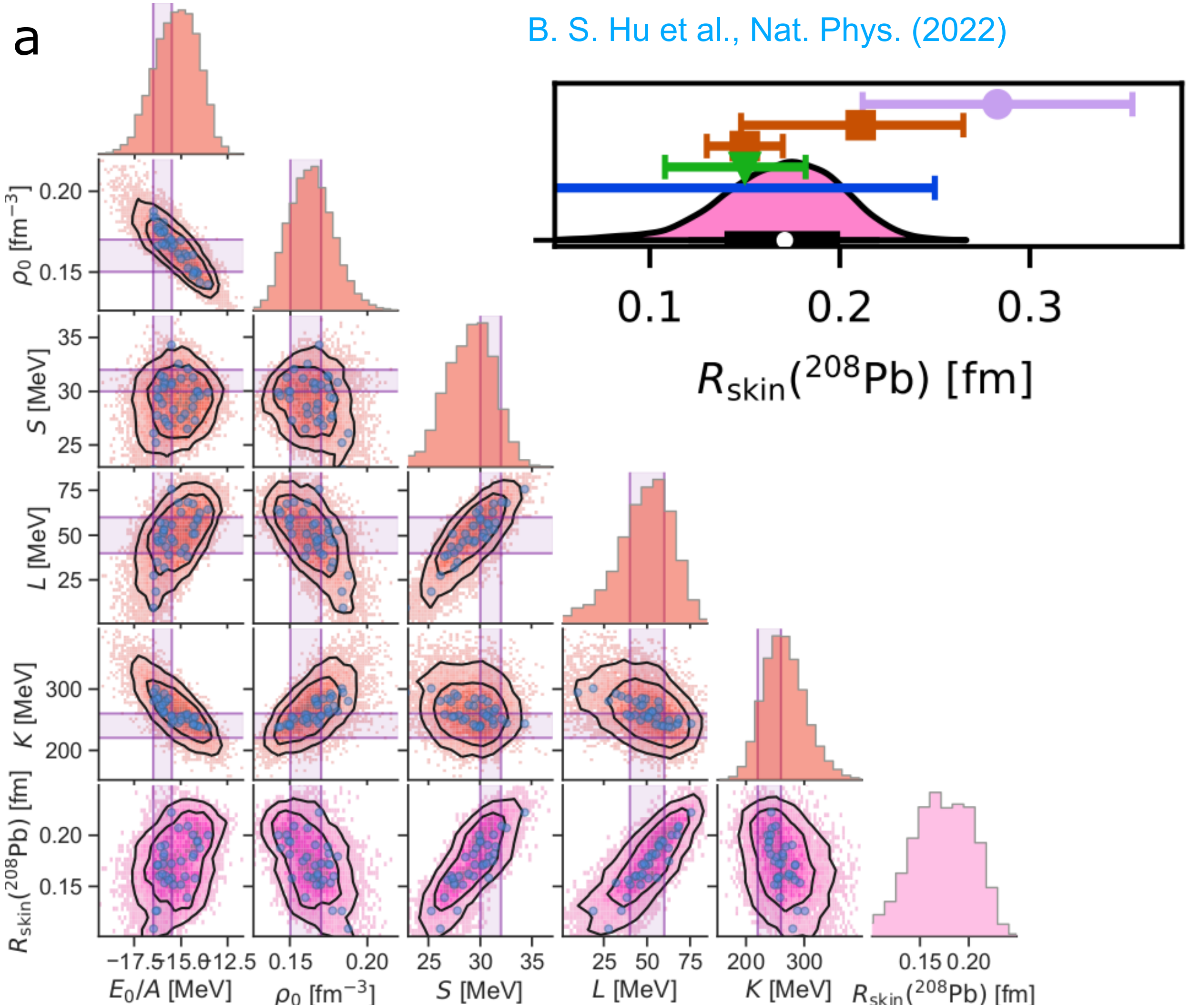
A. Belley et al., in prep.

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 N^{2}LO
- 34 NI interactions consistent with few-body and ^{16}O data
- Posterior predictive distribution
  - ✦ Calibrated by ^{48}Ca data
  - ✦ 0.14 < Rskin(^{208}Pb) < 0.20

See Christian Forssen's talk

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



Magnetic moment

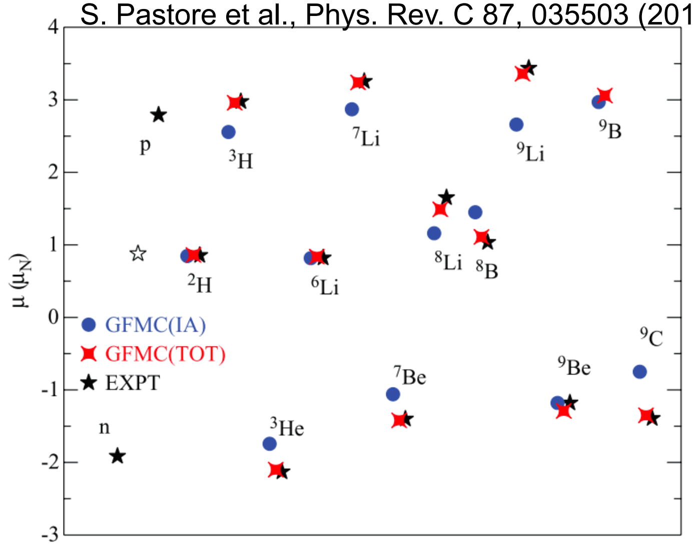
- The magnetic moment is also an indication of the magic number.
- Importance of 2BC is already shown in light nuclei and would be true for heavier systems.

- The analogy to the Gamow-Teller transition also suggests an effect of 2BC on the magnetic dipole operator is non-negligible.

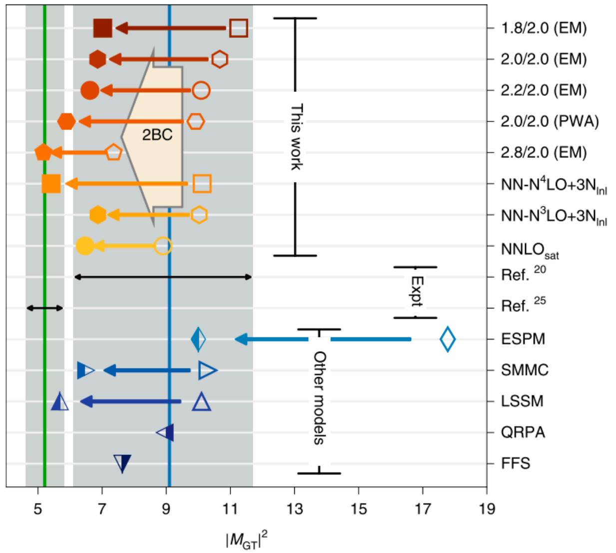
$$\boldsymbol{\mu} = \mu_N \sum_i \left[\frac{1}{2}(1+\tau_{z,i})\boldsymbol{l}_i + \frac{1}{2}(g^s_{\mathrm{IS}} + \tau_{i,z} g^s_{\mathrm{IV}})\boldsymbol{s}_i \right] \qquad g^s_{\mathrm{IS}} = 0.880,\ g^s_{\mathrm{IV}} = 4.706$$

$$GT = \sum_i \boldsymbol{s}_i \tau_{+,i}$$

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



P. Gysbers et al., Nat. Phys. 15, 428 (2019).



Magnetic moment

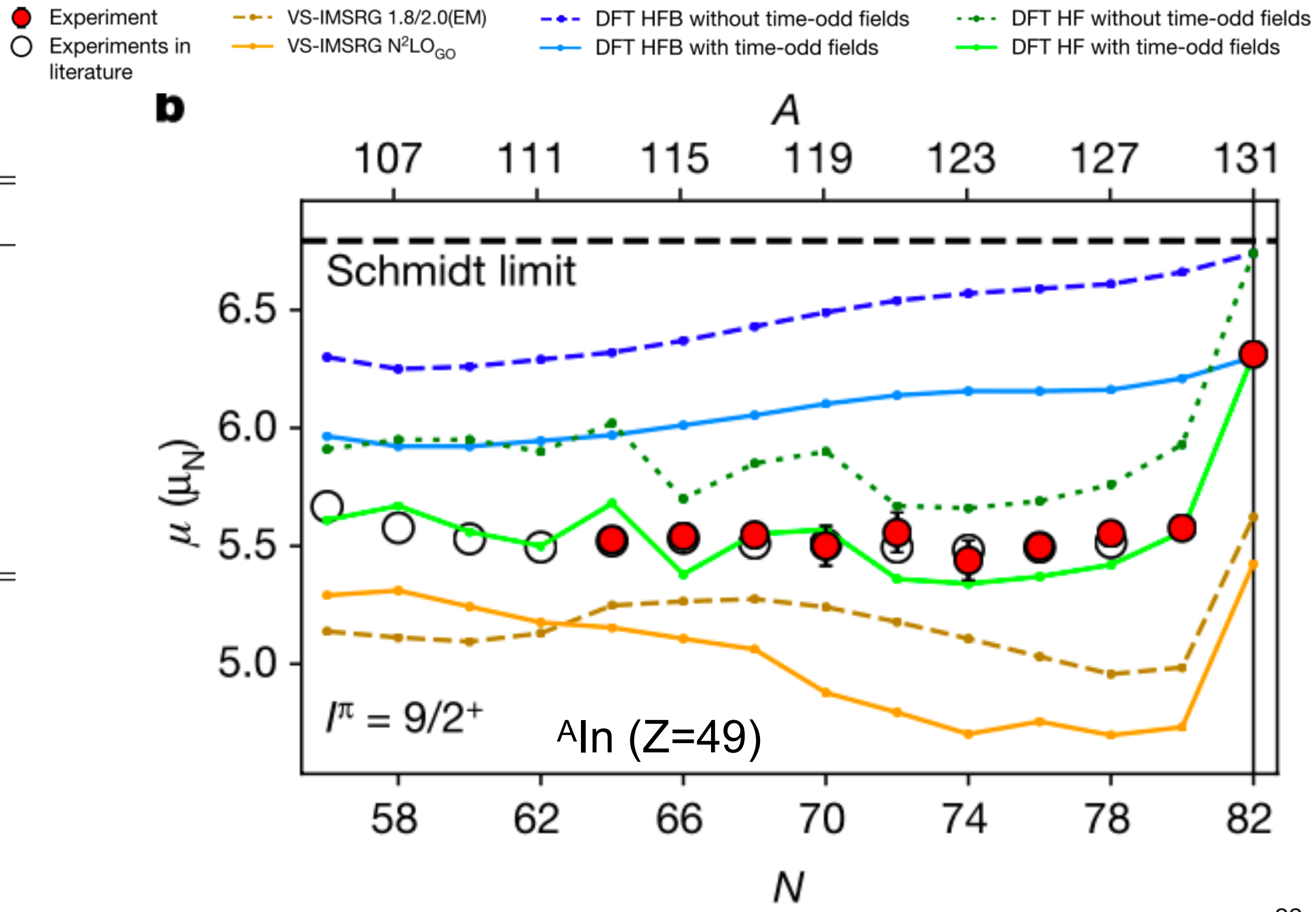
A. Klose et al., Phys. Rev. C 99, 061301 (2019).

VS-IMSRG, 1.8/2.0 (EM)

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).



LO 2B magnetic dipole operator

TECHNISCHE UNIVERSITÄT DARMSTADT

phD thesis by R. Seutin

- LO 2B contributions
  - ✦ Independent of LECs

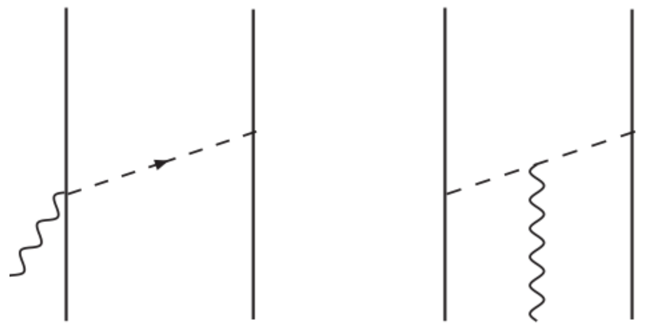
$$\boldsymbol{\mu}_{2\mathrm{B}} = \sum_{i<j} \boldsymbol{\mu}_{ij}^{\mathrm{intr}} + \boldsymbol{\mu}_{ij}^{\mathrm{Sachs}}$$

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

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

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

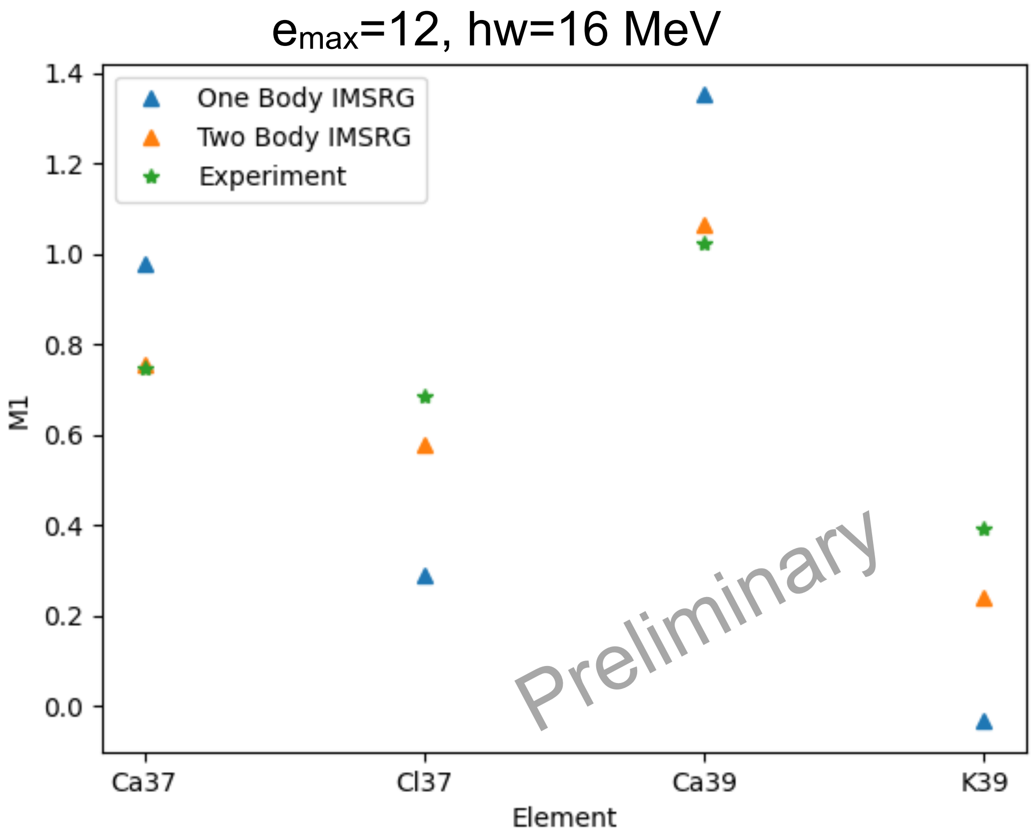
$$\boldsymbol{x}_{ij} = m_\pi \boldsymbol{r}_{ij}$$

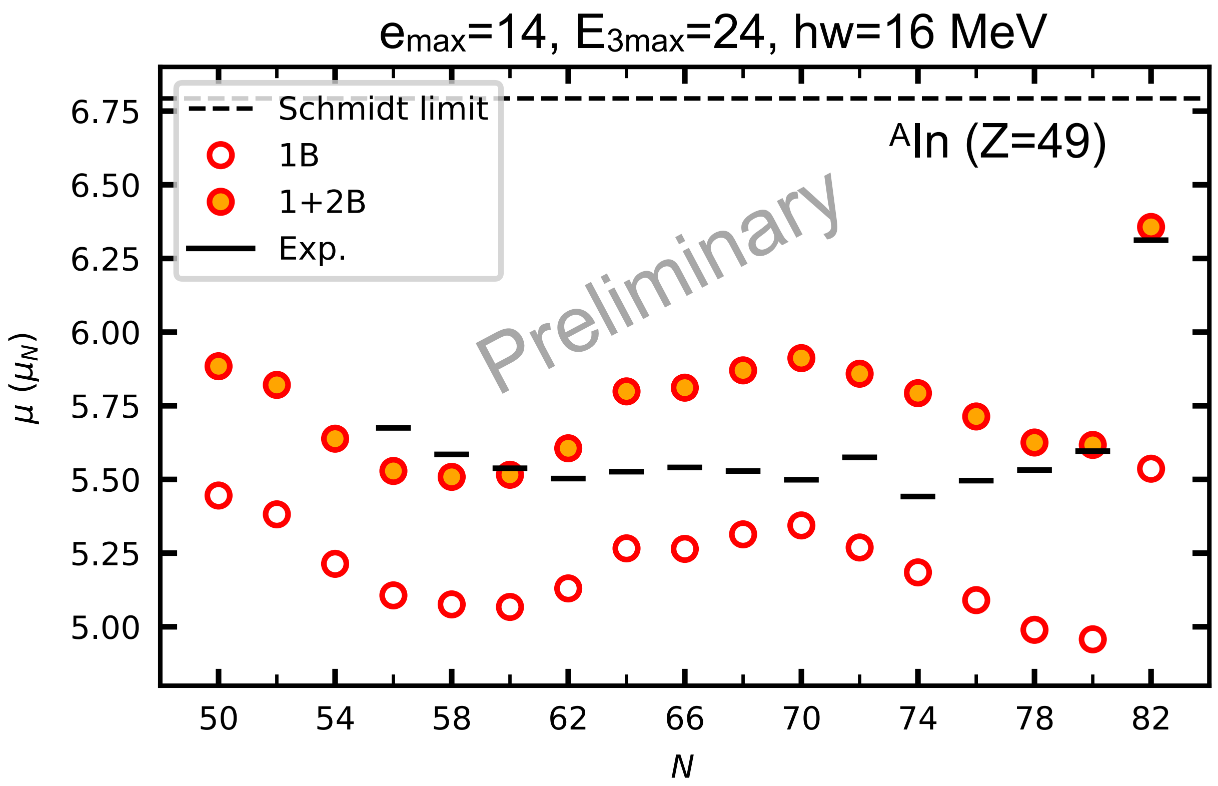


- Sachs term depends on the CM coordinate. The TM transformation becomes a little expensive.

Magnetic moments with 1+2BC

VS-IMSRG with 1.8/2.0 (EM) interaction





Sachs term is dominant in heavier systems: $\mu_{\text{Sachs}} > \mu_{\text{intr}}$

X. Cao et al., in prep.

Summary & outlook

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- Newly introduced 3N storage scheme [TM et al., Phys. Rev. C 105, 014302 (2022).]
  - Many applications:
    - Electromagnetic properties around ^{132}Sn
    - Neutrinoless double beta decay of ^{136}Xe [A. Belley et al., in prep.]
    - Neutron skin prediction for ^{208}Pb [B. S. Hu et al., Nat. Phys. 18, 1196 (2022).]
- 2B M1 operator improves the magnetic moments. [X. Cao et al., in prep.]

- Future perspective
  - Improvements in IMSRG frameworks for E2 observables.
  - M1 transitions with 1+2BC.

Faster T-coefficient calculation

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- Computation of T-coefficients can be a bottle neck.

Usual LS-like recoupling

$$\langle N_{\rm cm} L_{\rm cm} E \alpha J_{\rm rel} : JT | pqr : J_{pq} T_{pq} JT \rangle$$

$$= \delta_{t_{12} T_{pq}} \sum_{l_{pq}} \sqrt{[j_p][j_q][l_{pq}][s_{12}]} \left\{ \begin{matrix} l_p & s_p & j_p \\ l_q & s_q & j_q \\ l_{pq} & s_{12} & J_{pq} \end{matrix} \right\}$$

$$\times \sum_{N_{12} L_{12}} \langle N_{12} L_{12}, n_{12} l_{12} : l_{pq} | n_p l_p, n_q l_q : l_{pq} \rangle_1$$

$$\times \sum_{LS} \sqrt{[J_{pq}][j_r][L][S]} \left\{ \begin{matrix} l_{pq} & s_{12} & J_{pq} \\ l_r & s_r & j_r \\ L & S & J \end{matrix} \right\}$$

$$\times \sum_{\lambda} (-1)^{l_{12}+l_r+l_{pq}+\lambda} \sqrt{[l_{pq}][\lambda]} \left\{ \begin{matrix} l_{12} & L_{12} & l_{pq} \\ l_r & L & \lambda \end{matrix} \right\}$$

$$\times \langle N_{\rm cm} L_{\rm cm}, n_3 l_3 : \lambda | N_{12} L_{12}, n_c l_c : \lambda \rangle_2$$

$$\times \sum_{\Lambda} (-1)^{L_{\rm cm}+l_3+l_{12}+L} \sqrt{[\lambda][\Lambda]} \left\{ \begin{matrix} L_{\rm cm} & l_3 & \lambda \\ l_{12} & L & \Lambda \end{matrix} \right\}$$

$$\times (-1)^{L_{\rm cm}+\Lambda+S+J} \sqrt{[L][J_{\rm rel}]} \left\{ \begin{matrix} L_{\rm cm} & \Lambda & L \\ S & J & J_{\rm rel} \end{matrix} \right\}$$

$$\times (-1)^{l_3+l_{12}-Lambda} \sqrt{[j_{12}][j_3][\Lambda][S]} \left\{ \begin{matrix} l_{12} & s_{12} & j_{12} \\ l_3 & s_r & j_3 \\ \Lambda & S & J_{\rm rel} \end{matrix} \right\}$$

6 summations

New jj-like recoupling

$$\langle N_{\rm cm} L_{\rm cm} E \alpha J_{\rm rel} : JT | pqr : J_{pq} T_{pq} JT \rangle$$

$$= \delta_{t_{12} T_{pq}} \sum_{l_{pq}} \sqrt{[j_p][j_q][l_{pq}][s_{12}]} \left\{ \begin{matrix} l_p & s_p & j_p \\ l_q & s_q & j_q \\ l_{pq} & s_{12} & J_{pq} \end{matrix} \right\}$$

$$\times \sum_{N_{12} L_{12}} \langle N_{12} L_{12}, n_{12} l_{12} : l_{pq} | n_p l_p, n_q l_q : l_{pq} \rangle_1$$

$$\times (-1)^{L_{12}+s_{12}+l_{12}+J_{pq}} \sqrt{[l_{pq}][j_{12}]} \left\{ \begin{matrix} L_{12} & l_{12} & l_{pq} \\ s_{12} & J_{pq} & j_{12} \end{matrix} \right\}$$

$$\times \sum_{\Lambda} (-1)^{j_{12}+j_r+J_{pq}+\Lambda} \sqrt{[J_{pq}][\Lambda]} \left\{ \begin{matrix} j_{12} & L_{12} & J_{pq} \\ j_r & J & \Lambda \end{matrix} \right\}$$

$$\times \sum_{\lambda} (-1)^{L_{12}+l_r+s_r+\Lambda} \sqrt{[\lambda][j_r]} \left\{ \begin{matrix} L_{12} & l_r & \lambda \\ s_r & \Lambda & j_r \end{matrix} \right\}$$

$$\times \langle N_{\rm cm} L_{\rm cm}, n_3 l_3 : \lambda | N_{12} L_{12}, n_c l_c : \lambda \rangle_2$$

Equivalent to 12j

$$\times (-1)^{L_{\rm cm}+l_3+s_r+\Lambda} \sqrt{[\lambda][j_3]} \left\{ \begin{matrix} L_{\rm cm} & l_3 & \lambda \\ s_r & \Lambda & j_3 \end{matrix} \right\}$$

$$\times (-1)^{L_{\rm cm}+j_3+j_{12}+J} \sqrt{[\Lambda][J_{\rm rel}]} \left\{ \begin{matrix} L_{\rm cm} & j_3 & \Lambda \\ j_{12} & J & J_{\rm rel} \end{matrix} \right\} (-1)^{j_{12}+j_3-J_{\rm rel}}$$

4 summations

Benchmarks

- Jacobi NCSM
  - N^{3}LO (EM500)
  - SRG softened (1.8 fm^{-1}, NN-only)
  - Nmax = 2-20
- Consistent with Faddeev calculations
- Intrinsic term is dominant: $\mu_{\mathrm{intr}} > \mu_{\mathrm{Sachs}}$